数理解析研究所講究録
1047 巻 1998 年 12-25

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

ATSUSHI INOUE (井上 淳)

Department of Mathematics, Tokyo Institute of Technology

§1. PROBLEM AND RESULT

Problem: Construct a parametrix which exhibits clearly how quantities from Hamiltonian mechanics are related to quantum mechanics: ("**Hamiltonian path-integral quantization**" in $L^2(\mathbb{R}^m)$)

$$\begin{cases} \dfrac{\hbar}{i}\dfrac{\partial u(t,x)}{\partial t} + \mathbb{H}\left(t, x, \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}\right) u(t,x) = 0, \\ u(0,x) = \underline{u}(x) \end{cases} \tag{1}$$

with

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

Assumptions:

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

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

where

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

(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

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

Outline of the strategy of quantization:

(I) Let $H(t, x, \xi)$ be given (e.g. the complete symbol of $\mathbb{H}(t, x, -i\hbar\partial_x)$). Solve

$$\begin{cases} \dot{x}(t) = \partial_\xi H(t, x(t), \xi(t)), \\ \dot{\xi}(t) = -\partial_x H(t, x(t), \xi(t)). \end{cases} \tag{2}$$

(II) Under Assumptions (A) and (V), construct a phase function $S(t, s, x, \xi)$ (Hamilton-Jacobi equation):

$$\begin{cases} \partial_t S(t, s, x, \xi) + H(t, x, \partial_x S(t, s, x, \xi)) = 0, \\ S(s, s, x, \xi) = x \cdot \xi. \end{cases} \tag{3}$$

Then, $D(t, s, x, \xi) = \det(\partial^2_{x_j \xi_k} S(t, s, x, \xi))$ satisfies the continuity equation:

$$\begin{cases} \partial_t D(\cdot) + \partial_x \big[D(\cdot) \partial_\xi H(t, x, \partial_x S(t, s, x, \xi)) \big] = 0, \\ D(s, s, x, \xi) = 1. \end{cases} \tag{4}$$

(III) Define a Fourier Integral Operator on $\mathbb{R}^m$ as

$$E(t, s)u(x) = c_m \int_{\mathbb{R}^m} d\xi \, D^{1/2}(t, s, x, \xi) \, e^{i\hbar^{-1} S(t,s,x,\xi)} \hat{u}(\xi) \tag{5}$$

where $c_m = (2\pi\hbar)^{-m/2}$ and

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

(IV) This operator gives a **good parametrix** for (1) on $L^2(\mathbb{R}^m)$, by virtue of (3) and (4).

For a subdivision Δ of (s, t), put

$$\Delta : t_0 = s < t_1 < \cdots < t_{\ell-1} < t_\ell = t, \quad \delta(\Delta) = \max_{j=1,\cdots,\ell} |t_j - t_{j-1}|,$$
$$E(\Delta | t, s)u = E(t, t_{\ell-1}) E(t_{\ell-1}, t_{\ell-2}) \cdots E(t_1, s).$$

Main Theorem. *Fix $T > 0$ arbitrarily. Assume (A) and (V). $(t, s) \in [-T, T]^2$.*

(0) $\{E(\Delta | t, s)\}$ converges to $\mathbb{U}(t, s)$ when $\delta(\Delta) \to 0$ in $L^2(\mathbb{R}^m)$ s.t.

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

(1) $\mathbb{U}(t, s) \in \mathbb{B}(L^2(\mathbb{R}^m) : L^2(\mathbb{R}^m))$.

(2) $\mathbb{U}(t,s)$ *is* $L^2(\mathbb{R}^m)$*-valued continuous and*

$$\begin{cases} \mathbb{U}(s,s) = I, \\ \mathbb{U}(t,s)\mathbb{U}(s,r) = \mathbb{U}(t,r). \end{cases}$$

(3) If $u \in C_0^\infty(\mathbb{R}^m)$, $\mathbb{U}(t,s)u$ *satisfies*

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

§2. Feynman's heuristic argument

Consider the following initial value problem:

$$(*) \qquad \begin{cases} i\hbar\frac{\partial}{\partial t}u(x,t) = -\frac{\hbar^2}{2}\Delta u(x,t) + V(x)u(x,t), \\ u(x,0) = \underline{u}(x). \end{cases}$$

Here, the Hamiltonian is given formally as

$$H = -\frac{\hbar^2}{2}\Delta + V(\cdot) = H_0 + V, \quad \Delta = \sum_{j=1}^m \frac{\partial^2}{\partial x_j^2}.$$

Assuming H is essentially selfadjoint in $L^2(\mathbb{R}^m)$, by Stone's theorem, we have the solution of (*) as

$$u(x,t) = (e^{-\frac{i}{\hbar}tH}\underline{u})(x).$$

On the other hand, by the Lie-Trotter-Kato product formula, we have

$$e^{-\frac{i}{\hbar}tH} = \operatorname*{s-lim}_{k\to\infty}\Big(e^{-\frac{i}{\hbar}\frac{t}{k}V}e^{-\frac{i}{\hbar}\frac{t}{k}H_0}\Big)^k.$$

If the initial data $\underline{u}$ belongs to $\mathcal{S}(\mathbb{R}^m)$, we get

$$(e^{-\frac{i}{\hbar}tH_0}\underline{u})(x) = (2\pi i\hbar t)^{-m/2}\int_{\mathbb{R}^m} dy\, e^{i(x-y)^2/(2\hbar t)}\underline{u}(y).$$

Therefore,

$$(e^{-\frac{i}{\hbar}tH}\underline{u})(x) = \int dy\, F(t,x,y)\underline{u}(y),$$

with

$$F(t,x,y) = \operatorname*{s-lim}_{k\to\infty}(2\pi i\hbar t)^{-km/2}\int\cdots\int dx^{(1)}\cdots dx^{(k-1)} e^{\frac{i}{\hbar}S_t(x,x^{(k-1)},\cdots,x^{(1)},y)}.$$

Here, we put $x^{(k)} = x,\ x^{(0)} = y$,

$$S_t(x^{(k)},\ldots,x^{(0)}) = \sum_{j=1}^{k}\left[\frac{1}{2}\frac{(x^{(j)}-x^{(j-1)})^2}{(t/k)^2} - V(x^{(j)})\right]\frac{t}{k}.$$

Feynman's interpretation: Let

$$C_{t,x,y} = \{\gamma(\cdot)\in AC([0,t]:\mathbb{R}^m)\,|\,\gamma(0)=y,\gamma(t)=x\}.$$

For any path $\gamma\in C_{t,x,y}$, $S_t(x^{(k)},\ldots,x^{(0)})$ is regarded as the Riemann sum for the classical action $S_t(\gamma)$, i.e.

$$S_t(\gamma) = \int_0^t L(\gamma(\tau),\dot\gamma(\tau))d\tau = \lim_{k\to\infty} S_t(x^{(k)},\ldots,x^{(0)}),$$

where

$$L(\gamma,\dot\gamma) = \frac{1}{2}\dot\gamma^2 - V(\gamma)\in C^\infty(T\mathbb{R}^m)$$

When $k\to\infty$, the 'limit' of the measure $dx^{(1)}\cdots dx^{(k-1)}$ is denoted by

$$d_F\gamma = \prod_{0<\tau<t} d\gamma(\tau)$$

and considered as the 'measure' on the path space $C_{t,x,y}$ (See S.A. Albeverio & R.J. Hoegh-Krohn [1]).

Feynman's conclusion:

$$F(t,x,y) = \int_{C_{t,x,y}} d_F\gamma\, e^{\frac{i}{\hbar}\int_0^t L(\gamma(\tau),\dot\gamma(\tau))d\tau}.$$

On the other hand, it is proved unfortunately that there exists no non-trivial 'Feynman measure' on ∞-dimensional spaces.

Problem 1. Give a meaning to

$$\int d_F\gamma\, e^{i\hbar^{-1}\int_0^t L(\gamma(\tau),\dot\gamma(\tau))d\tau}.$$

A partial solution of this problem is presented by Fujiwara [12], when $|\partial_x^\alpha V(x)| \le C_\alpha$ for $|\alpha| \ge 2$.

Problem 2. As a Hamiltonian counter part of above, how do we define

$$\iint d_F x d_F \xi \, e^{i\hbar^{-1}\int_0^t H(x(\tau),\xi(\tau))d\tau} ?$$

See, Inoue [17].

Method of characteristics as quantization

On the region Ω in $\mathbb{R}^{m+1}$, we consider the following initial value problem:

$$\begin{cases} \dfrac{\partial}{\partial t}u(t,q) + \displaystyle\sum_{j=1}^m a_j(t,q)\frac{\partial}{\partial q_j}u(t,q) = b(t,q)u(t,q) + f(t,q), \\ u(\underline{t},q) = \underline{u}(q). \end{cases}$$

Corresponding characteristics are given by

$$\begin{cases} \dfrac{d}{dt}q_j(t) = a_j(t,q(t)), \\ q_j(\underline{t}) = \underline{q}_j \quad (j=1,\cdots,m). \end{cases}$$

When this is solved nicely, we denote them as

$$q(t) = q(t,\underline{t};\underline{q}) = (q_1(t),\cdots,q_m(t)) \in \mathbb{R}^m.$$

Following theorem is well-known.

Theorem. *Let $a_j \in C^1(\Omega:\mathbb{R})$ and $b,f \in C(\Omega:\mathbb{R})$. For any point $(\underline{t},\underline{q}) \in \Omega$, we asume that $\underline{u}$ is C^1 in a neighbourhood of $\underline{q}$.*

Then, in a neighbourgood of $(\underline{t},\underline{q})$, there exists uniquely a solution $u(t,q)$. More precisely, putting

$$U(t,\underline{q}) = e^{\int_{\underline{t}}^t d\tau\, B(\tau,\underline{q})}\left\{\int_{\underline{t}}^t ds\, e^{-\int_{\underline{t}}^s d\tau\, B(\tau,\underline{q})}F(s,\underline{q}) + \underline{u}(\underline{q})\right\},$$

solution is represented by

$$u(t,\bar{q}) = U(t,y(t,\underline{t};\bar{q}))$$

where $B(t,\underline{q}) = b(t,q(t,\underline{t};\underline{q}))$, $F(t,\underline{q}) = f(t,q(t,\underline{t};\underline{q}))$ and $\underline{q} = y(t,\underline{t};\bar{q})$ is a inverse function defined from $\bar{q} = q(t,\underline{t};\underline{q})$.

We apply above theorem to the simplest case:

$$\begin{cases} i\hbar\dfrac{\partial}{\partial t}u(t,q) = a\dfrac{\hbar}{i}\dfrac{\partial}{\partial q}u(t,q) + bqu(t,q), \\ u(0,q) = \underline{u}(q). \end{cases}$$

From the right-hand side of above, we define a Hamiltonian as follows (more precisely, Weyl symbol should be considered):

$$H(q,p) = e^{-i\hbar^{-1}qp}\Big(a\frac{\hbar}{i}\frac{\partial}{\partial q} + bq\Big)e^{i\hbar^{-1}qp} = ap + bq.$$

The classical mechanics associated to that Hamiltonian is given by

$$\begin{cases} \dot{q}(t) = H_p = a, \\ \dot{p}(t) = -H_q = -b \end{cases} \text{with } \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} = \begin{pmatrix} \underline{q} \\ \underline{p} \end{pmatrix}$$

which is readily solved as

$$q(s) = \underline{q} + as, \quad p(s) = \underline{p} - bs.$$

From above theorem, putting $\underline{t} = 0$, we get readily that

$$U(t,\underline{q}) = \underline{u}(\underline{q})e^{-i\hbar^{-1}(b\underline{q}t + 2^{-1}abt^2)}.$$

As the inverse function of $\bar{q} = q(t,\underline{q})$ is given by$\underline{q} = y(t,\bar{q}) = \bar{q} - at$, we get

$$u(t,\bar{q}) = U(t,\underline{q})|_{\underline{q}=y(t,\bar{q})} = \underline{u}(\bar{q} - at)e^{-i\hbar^{-1}(b\bar{q}t - 2^{-1}abt^2)}.$$

Another point of view: Put

$$S_0(t,\underline{q},\underline{p}) = \int_0^t ds\,[\dot{q}(s)p(s) - H(q(s),p(s))] = -b\underline{q}t - 2^{-1}abt^2,$$

$$S(t,\bar{q},\underline{p}) = \underline{q}\,\underline{p} + S_0(t,\underline{q},\underline{p})|_{\underline{q}=y(t,\bar{q})} = \bar{q}\underline{p} - a\underline{p}t - b\bar{q}t + 2^{-1}abt^2.$$

$S(t,\bar{q},\underline{p})$ satisfies the Hamilton-Jacobi equation.

$$\begin{cases} \frac{\partial}{\partial t}S + H(\bar{q}, \partial_{\bar{q}}S) = 0, \\ S(0,\bar{q},\underline{p}) = \bar{q}\,\underline{p}. \end{cases}$$

On the other hand, the van Vleck determinant is

$$D(t,\bar{q},\underline{p}) = \frac{\partial^2 S(t,\bar{q},\underline{p})}{\partial\bar{q}\partial\underline{p}} = 1.$$

This quantity satisfies the continuity equation:

$$\begin{cases} \frac{\partial}{\partial t}D + \frac{1}{2}\partial_{\bar{q}}(DH_p) = 0 \quad \text{where } H_p = \frac{\partial H}{\partial p}(\bar{q}, \frac{\partial S}{\partial \bar{q}}), \\ D(0,\bar{q},\underline{p}) = 1. \end{cases}$$

As an interpretation of Feynman's idea, we regard that the transition from classical to quantum is to study the following quantity or the one represented by this (the term "quantization" is not so well-defined mathematically):

$$u(t,\overline{q}) = (2\pi\hbar)^{-1/2}\int_{\mathbb{R}} d\underline{p}\, D^{1/2}(t,\overline{q},\underline{p})e^{i\hbar^{-1}S(t,\overline{q},\underline{p})}\hat{\underline{u}}(\underline{p}).$$

That is, in our case at hand, we should study the quantity defined by

$$\begin{aligned} u(t,\overline{q}) &= (2\pi\hbar)^{-1/2}\int_{\mathbb{R}} d\underline{p}\, e^{i\hbar^{-1}S(t,\overline{q},\underline{p})}\hat{\underline{u}}(\underline{p}) \\ &= (2\pi\hbar)^{-1}\iint_{\mathbb{R}^2} d\underline{p}d\underline{q}\, e^{i\hbar^{-1}(S(t,\overline{q},\underline{p})-\underline{q}\,\underline{p})}\underline{u}(\underline{q}) = \underline{u}(\overline{q}-at)e^{i\hbar^{-1}(-b\overline{q}t+2^{-1}abt^2)}. \end{aligned}$$

[Problem] Can we extend the above argument to a system of PDE? For example, Dirac, Weyl or Pauli equations, quantum mechanical equations with spin. See, Inoue [17-19] and Inoue & Maeda [21].

§3. Composition formulas.

Now, we put

$$\begin{aligned} \hat{H}^W(x,D_x^\hbar) &= c_m^2\int_{\mathbb{R}^{2m}} d\xi\, dx' e^{i\hbar^{-1}(x-x')\cdot\xi}H\Big(\frac{x+x'}{2},\xi\Big)u(x'), \\ F(a,\phi)u(x) &= c_m\int_{\mathbb{R}^m} d\xi\, a(x,\xi)e^{i\hbar^{-1}\phi(x,\xi)}\hat{u}(\xi). \end{aligned}$$

Theorem. *For suitablly given $a(x,\xi)$, $\phi(x,\xi)$, $H(x,\xi)$, we have the following:*

(1) There exists $c_L{=}c_L(x,\eta)\in C^\infty(\mathbb{R}^{2m})$ s.t.
$\hat{H}^W(x,D_x^\hbar)F(a,\phi) = F(c_L,\phi)$ with

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

Here, $H = H(x,\partial_x\phi)$, $\phi=\phi(x,\eta)$ and $r_L = r_L(x,\eta)$,

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

(2) There exists $c_R = c_R(x,\xi)\in C^\infty(\mathbb{R}^{2m})$ s.t.
$F(a,\phi)\hat{H}^W(x,D_x^\hbar) = F(c_R,\phi)$ with

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

Here, $H = H(\partial_\xi\phi(x,\xi),\xi)$, $c_R = c_R(x,\xi)$, $a=a(x,\xi)$ and $\phi=\phi(x,\xi)$,

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

§4. Properties of parametrix

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

$$\|E(t,s)u\| \leq C\|u\|.$$

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

$$\underset{|t-s|\to 0}{\text{s-lim}}\ E(t,s)u = u \qquad in \quad L^2(\mathbb{R}^m).$$

(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 $L^2(\mathbb{R}^m)$.

Proposition. *Let $u \in C_0^\infty(\mathbb{R}^m)$.*

$$\frac{\hbar}{i}\frac{\partial}{\partial t}E(t,s)u(x) = -\hat{H}^W(t,x,D_x)E(t,s)u(x) + G(t,s)u(x),$$
$$\|G(t,s)u\| \leq C\hbar^2|t-s|\|u\|.$$

Proof. Using the Hamilton-Jacobi and the continuity equations with the product formula, we get

$$\frac{\hbar}{i}(\mu_t + i\hbar^{-1}S_t\,\mu) = \frac{\hbar}{i}(\cdots) - \mu\,H$$
$$= -[\text{amplitude part of the “symbol” of } (\hat{H}^W(t,x,D_x)E(t,s))] - r_L.$$

$r_L = -\frac{\hbar^2}{2}\Delta_x\mu(t,s,x,\xi)$, $\mu = \mu(\cdots)$ and $S = S(\cdots)$, $H = H(x, \partial_x S(t,s,x,\xi))$.

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

Use Calderon-Vaillancourt's theorem. □

Proposition. *Let $|||u|||_1 = \|\langle x\rangle u\| + \|\partial_x u\|$.*

$$\frac{\hbar}{i}\frac{\partial}{\partial s}E(t,s)u(x) = E(t,s)\hat{H}^W(s,x,D_x)u(x) + \tilde{G}(t,s)u(x),$$
$$\|\tilde{G}(t,s)u\| \leq C\hbar^2|t-s|\,|||u|||_1$$

Remark. The above estimate is crucial why we can't proceed as in the Lagarngian formalism. But in case $A_i(t,x) = a_{ij}(t)x_j$, we have

$$\|\tilde{G}(t,s)u\| \leq C\hbar^2|t-s|\|u\|.$$

Proceeding as in Fujiwara, we have

Propositon.

$$(**)\qquad \|(E(t,s)E(s,r)-E(t,r))u\| \le C\hbar(|t-s|^2+|s-r|^2)|||u|||_1,$$

$$(***)\qquad \|(E(s,t)^*E(s,r)-E(t,r))u\| \le C\hbar(|t-s|^2+|s-r|^2)\|u\|.$$

Corollary. *From (***), we have*

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

§5. Composition of FIOs

Let $|t-s|+|s-r|$ be sufficiently small. We want to calculate the quantity $\|E(t,s)E(s,r)u-E(t,r)u\|$ directly without using the adjoint operation.

Lemma. *For any x,ξ, there exists a unique solution (X,Ξ) of*

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

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

Put $X = X(t,s,r,x,\xi)$, $\Xi = \Xi(t,s,r,x,\xi)$ and

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

Lemma. *As we calculate easily*

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

we get

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

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 $S(t,s,x,\cdot)\#S(s,r,\cdot,\xi)$.

Now, we have, as an oscillatory integral,

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

Using the change of variables

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

we have

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

with

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

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

Propositon. *[Taniguchi [29]]*

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

In spite of the estimate (**), we have

Corollary.

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

§6. The comparison with two formalisms

Theorem. *[Lagrangian formulation] A parametrix of the initial value problem (1) is given by*

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

$\tilde{c}_m = (2\pi i\hbar)^{-m/2} = c_m e^{-m\pi i/4}$, $\tilde{S}(t,s) = \tilde{S}(t,s,x,y)$ satisfies

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

and $\tilde{\mu}(t,s) = \tilde{\mu}(t,s,x,y)$ satisfies

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

Corollary.

$$\begin{aligned} &\partial_s \tilde{S}(t,s) - H(s,y,-\partial_y \tilde{S}(t,s)) = 0, \\ &\partial_s \tilde{\mu}(t,s) - \partial_{y_k}\tilde{\mu}(t,s) H_{\xi_k}(s,y,-\partial_y \tilde{S}(t,s)) \\ &\qquad\qquad - \frac{1}{2}\tilde{\mu}(t,s)\frac{\partial}{\partial y_k} H_{\xi_k}(s,y,-\partial_y \tilde{S}(t,s)) = 0. \end{aligned}$$

Here, we put

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

Proposition.

$$\begin{aligned} &\frac{\partial}{\partial t}\tilde{E}(t,s)u + \mathbb{H}(t,x,D_x^\hbar)\tilde{E}(t,s)u = \tilde{G}_L(t,s)u, \\ &\qquad \|\tilde{G}_L(t,s)u\| \le C\hbar^2|t-s|\|u\|. \end{aligned}$$

Proposition.

$$\begin{aligned} &\frac{\partial}{\partial s}\tilde{E}(t,s)u - \tilde{E}(t,s)\mathbb{H}(s,y,D_y^\hbar)u = \tilde{G}_R(t,s)u, \\ &\qquad \|\tilde{G}_R(t,s)u\| \le C\hbar^2|t-s|\|u\|. \end{aligned}$$

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

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

From these propositions, we have

Proposition.

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

The difference.

(1) $\hat{H}^W(t,x,D_x^\hbar)$ is derived from $H(t,x,\xi)$ using the Fourier transformation, while $\mathbb{H}(t,x,D_x^\hbar)$ is used 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. *Under Assumptions (A) and (V), we have*

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

Therefore, we have

Corollary.

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

Now, we have

Proposition. *Under these circumstance, we have*

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

Though in the Hamiltonian formulation, this relation does not seem to hold in general, we have

Proposition.

$$\|E(t,s)^* - E(s,t)\| \le C|t-s|^2.$$

REFERENCES

1. S.A. Albeverio and R.J. Hoegh-Krohn, *Mathematical Theory of Feynman Integrals*, vol. 523, Lecture Notes in Mathematics, Springer-Verlag, Heidelberg, New York, 1976.
2. L. Alvarez-Gaumé, *Supersymmetry and the Atiyah-Singer Index Theorem*, Commun.Math.Phys. **90** (1983), 161-173.
3. V.S. Buslaev, *Continuum integrals and the asymptoticbehavior of the solutions of parabolic equations as $t \to 0$, Applications to diffraction*, Topics in Math.Physics (M.Sh. Birman, eds.), vol. 2, 1968.
4. P. Cartier and C. deWitt-Morette, *A new perspective on funational integration*, preprint, IHES/M/96/25.
5. B. DeWitt, *Dynamical theory in curved spaces. I. A review of the classical and quantum action principles*, Reviews of modern physics **29** (1984), 377-397.
6. C. DeWitt -Morette and T.R. Zhang, *Path integrals and conservation laws*, Physical Review D **28** (1983), 2503-2516.
7. ______, *Feynman-Kac formula in phase space with application to coherent-state transition*, Physical Review D **28** (1983), 2517-2525.
8. C. DeWitt -Morette, B. Nelson and T.R. Zhang, *Causitics problems in quantum mechanics with applications to scattering theory*, Physical Review D **28** (1983), 25262546.
9. I.H. Duru and H. Kleinert, *Quantum mechanics of H-atom from path integrals*, Fortschritte der Physik **30** (1982), 401-435.
10. M.V. Fedoryuk, *The stationary phase method and pseudodifferential operators*, Russian Math Survey (1970), 65-115.
11. R. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill Book Co., New York, 1965.
12. D. Fujiwara, *A construction of the fundamental solution for the Schrödinger equation*, J. D'Analyse Math. **35** (1979), 41-96.
13. ______, *Remarks on the convergence of the Feynman path integrals*, Duke Math.J. **47** (1980), 41-96.
14. C. Garrod, *Hamiltonian path-integral methods*, Reviews of Modern Physics **38** (1966), 483-494.
15. E. Getzler, *Pseudo-differential operators on supermanifolds and the Atiyah–Singer index theorem*, Commun. Math. Phys. **92** (1983), 163-178.
16. M.C. Gutzwiller, *Path integrals and the relation between classical and quantum mechanics*, Path Integrals (G.J. Papadopoulos and J.T. Devreese, eds.), Plenum Pub.Corp., New York, 1978, pp. 163-200.
17. A. Inoue, *On a "Hamiltonian path-integral" derivation of the Schrödinger equation*, Preprint series of Math.TITECH #61(07-96), submitted to Osaka J.Math.
18. ______, *On a construction of the fundamental solution for the free Weyl equation by Hamiltonian path-integral method —an exactly solvable case with "odd variable coefficients"*, Tohoku J.Math. "" (1998), ??.
19. ______, *On a construction of the fundamental solution for the free Dirac equation by Hamiltonian path-integral method —the classical counterpart of Zitterbewegung* (to appearJapanese J.Math.).

20. A. Inoue and Y. Maeda, *On integral transformations associated with a certain Lagrangian – as a pototype of quantization*, J.Math.Soc.Japan **37** (1985), 219-244.

21. ———, *Super oscillatory integrals and a path integral for a non-relativistic spinning particle*, Proc. Japan Acad. Ser. A **63** (1987), 1-3.

22. ———J.B. Keller and D.W. McLaughlin, *The Feynman Integral*, Amer.Math.Sci.Monthly **82** (1975), 451-465.

23. J. Klauder, *Is quantization Geometry?*, I.H.E.S. preprint (1996).

24. M.L. Lapidus, *The Feynman integral and Feynman's operational calculus: A heuristic and mathematical introduction*, I.H.E.S. preprint (1996).

25. R.G. Littlejohn and W.O. Flynn, *Geometric phases in the asymptotic theory of coupled wave equations*, Physical Review A **44** (1991), 5239-5256.

26. O.N. Naida and A.G. Prudkovskii, *The WKB method for the system* $(-i\hbar\partial_t - \mathcal{A}(x,t,-i\hbar\partial_x))U = 0$ *when the characteristics have variable multiplicity*, Differential Equations **13** (1978), 1169-1179.

27. L. Schulman, *A path integral for spin*, Physical Review **176** (1968), 1558-1142.

28. ———, *Techniques and Applications of Path Integration*, Wiley, New York, 1981.

29. K. Taniguchi, *A remark on composition formula od ceratin Fourier integral operators*, preprint, June 1997.

30. B. Thaller, *The Dirac Equation*, Springer-Verlag, Texts and Monographs in Physics, Heidelberg, New York, 1992.

31. K. Yajima, *Schrödinger evolution equations with magnetic fields*, J.d'Analyse Math. **56** (1991), 29-76.

32. ———, *Smoothness and non-smoothness of the fundamental solution of time-dependent Schrödinger equations*, Commun.Math.Phys. **181** (1996), 605-629.

Oh-okayama, Meguro-ku, Tokyo, 152, Japan