3. A Construction of the Fundamental Solution for the Schrödinger Equations

By Daisuke FUJIWARA
Department of Mathematics, University of Tokyo

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§ 1. **Introduction.** The aim of this note is to improve the results of [6], that is, to show that the main results of [6] hold even if we substitute the amplitude function $a(\lambda, t, s, x, y)$ of (10) in [6] by the constant function 1. We shall consider the Schrödinger equation

$$(1)\qquad \frac{\partial}{\lambda\partial t}u(t,x)+\frac{1}{2}\sum_{j=1}^{n}\left(\frac{\partial}{\lambda\partial x_j}\right)^2 u(t,x)+V(t,x)u(t,x)=0,\qquad (t,x)\in \mathrm{R}\times\mathrm{R}^n$$

and the initial condition

$$(2)\qquad u(s,x)=\varphi(x).$$

Here $\lambda=ih^{-1}$ is a pure imaginary parameter and h is a small parameter $0<h\leq 1$. The potential $V(t,x)$ is assumed to satisfy the following two conditions;

(V-I) $V(t,x)$ is real valued. For any fixed $t\in\mathrm{R}$, $V(t,x)$ is a C^∞ function of $x\in\mathrm{R}^n$. $V(t,x)$ is measurable in $(t,x)\in\mathrm{R}\times\mathrm{R}^n$.

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

$$(3)\qquad M_\alpha(t)=\sup_{x\in\mathrm{R}^n}\left|\left(\frac{\partial}{\partial x}\right)^\alpha V(t,x)\right|+\sup_{|x|\leq 1}|V(t,x)|$$

is essentially bounded on every compact interval of R^1.

We fix $L\geq 10(m+n+10)$. We put $T=\infty$ if $\operatorname{ess.sup.}_{|\alpha|=L,t\in\mathrm{R}} M_\alpha(t)<\infty$. Otherwise we let T denote an arbitrarily fixed positive number. Every discussion will be made in the interval $(-T,T)$ throughout this paper.

We shall consider the integral transformation

$$(4)\qquad E(\lambda,t,s)\varphi(x)=\left(\frac{-\lambda}{2\pi(t-s)}\right)^{(1/2)n}\int_{\mathrm{R}^n} e^{\lambda S(t,s,x,y)}\varphi(y)dy,$$

where $S(t,s,x,y)$ is the classical action along the classical orbit starting the point y at the time s and reaching the point x at the time t. (If $|t-s|$ is small enough, such an orbit is uniquely determined. See Proposition 1 below.) The integral transformation (4) is exactly the same transformation as Feynman used in [3] and [4].

Let $[s,t]\subset(-T,T)$ be an arbitrary interval. Let

$$\Delta\,;\ s=t_0<t_1<t_2<\cdots<t_{L-1}<t_L=t$$

be an arbitrary subdivision of the interval $[s,t]$. We put

$$\delta(\Delta)=\max|t_j-t_{j-1}|.$$

Define $E_\Delta(\lambda, t, s)=E(\lambda, t, t_{L-1})E(\lambda, t_{L-1}, t_{L-2})\cdots E(\lambda, t_1, s)$ and

$$E_\Delta(\lambda, s, t)=E(\lambda, s, t_1)E(\lambda, t_1, t_2)\cdots E(\lambda, t_{L-1}, t).$$

We shall prove that $E_\Delta(\lambda, t, s)$ and $E_\Delta(\lambda, s, t)$ converge to the fundamental solution when $\delta(\Delta)$ tends to 0.

§ 2. **Main results.** Our main results are the following theorems.

Theorem 1. *Assume that $V(t, x)$ satisfies the assumptions* (V-I)–(V-II). *Let $[s, t]$ be an arbitrary subinterval of $(-T, T)$. Then there exist unitary operators $U(\lambda, t, s)$ and $U(\lambda, s, t)$ of the Hilbert space $L^2(\mathrm{R}^n)$ such that*

$$\text{(5)}\qquad \lim_{\delta(\Delta)\to 0}\|U(\lambda, t, s)-E_\Delta(\lambda, t, s)\|=0,$$

$$\text{(6)}\qquad \lim_{\delta(\Delta)\to 0}\|U(\lambda, s, t)-E_\Delta(\lambda, s, t)\|=0.$$

More precisely, there exists a positive constant γ_0 such that

$$\text{(7)}\qquad \|U(\lambda, t, s)-E_\Delta(\lambda, t, s)\|\le\gamma_0|t-s|\,\delta(\Delta)\exp\gamma_0|t-s|,$$

$$\text{(8)}\qquad \|U(\lambda, s, t)-E_\Delta(\lambda, s, t)\|\le\gamma_0|t-s|\,\delta(\Delta)\exp\gamma_0|t-s|.$$

Where γ_0 depends on T but not on particular choice of t, s, λ and subdivision Δ if $|\lambda|\ge 1$.

This theorem means that Feynman path integral converges in the uniform operator topology if the potential satisfies (V-I)–(V-II).

Theorem 2. *Put $U(\lambda, t, t)=I$ for any $t\in\mathrm{R}$. Then $\{U(\lambda, t, s)\}_{(t,s)\in\mathrm{R}^2}$ is a family of unitary operators satisfying the following properties;*

(i) $U(\lambda, t, t)=I$.

(ii) $U(\lambda, t, s)=U(\lambda, t, s_1)U(\lambda, s_1, s)$ *for any* t, s_1, s *in* R.

(iii) $U(\lambda, t, s)$ *is strongly continuous in* $(t, s)\in\mathrm{R}^2$.

(iv) $U(\lambda, t, s)$ *is a topological linear isomorphism of* $\mathcal{S}(\mathrm{R}^n)$.

For any $\varphi\in\mathcal{S}(R^n)$, let $u(t, x)=U(\lambda, t, s)\varphi(x)$. Then, $u(t, x)$ satisfies the initial condition $u(s, x)=\varphi(x)$ and the equation

$$\text{(9)}\qquad \frac{\partial}{\lambda\partial t}u(t, x)+H(\lambda, t)u(t, x)=0 \qquad \text{at almost every } t,$$

where $H(\lambda, t)$ is the Hamiltonian operator $(1/2)\sum_{j=1}^n(\partial/\lambda\partial x_j)^2+V(t, x)$ restricted to $\mathcal{S}(\mathrm{R}^n)$.

Remark. If we assume, in addition to (V-I)–(V-II), that $V(t, x)$ is continuous in $(t, x)\in\mathrm{R}^{n+1}$, then, the equation (9) holds everywhere.

§ 3. **Sketch of the proofs.** The classical mechanics corresponding to (1) is described by the Hamiltonian canonical equations

$$\text{(10)}\qquad \frac{dx}{dt}=\xi, \qquad \frac{d\xi}{dt}=-\frac{\partial V(t, x)}{\partial x}.$$

We consider these under the initial condition

$$\text{(11)}\qquad x(s)=y, \qquad \xi(s)=\eta.$$

We denote the solution of these as $x(t)=x(t, s, y, \eta)$ and $\xi(t)=\xi(t, s, y, \eta)$. By studying this orbit in detail, we obtain the following propositions.

Proposition 1. *Assume the assumptions* (V-I)–(V-II). *Then,* *there exists a positive constant* $\delta_1(T)>0$ *such that* $S(t,s,x,y)$ *is well defined if* $|t-s|\leq\delta_1(T)$.

Proposition 2. *Assume that* $|t-s|\leq\delta_1(T)$. *Let s be fixed. Then, the function* $S(t,s,x,y)$ *of* (t,x,y) *is totally differentiable at almost everywhere in* $(s-\delta_1(T), s+\delta_1(T))\times\mathbf{R}^n\times\mathbf{R}^n$. *It satisfies the Hamilton-Jacobi partial differential equation*

$$\frac{\partial}{\partial t}S(t,s,x,y)+\frac{1}{2}\left|\frac{\partial}{\partial x}S(t,s,x,y)\right|^2+V(t,x)=0 \tag{12}$$

almost everywhere.

Proposition 3. *Assume that* $0<|t-s|\leq\delta_1(T)$. *Then the action* $S(t,s,x,y)$ *is of the form*

$$S(t,s,x,y)=\frac{1}{2}\frac{|x-y|^2}{t-s}+(t-s)\omega(t,s,x,y). \tag{13}$$

For any pair of multi-indices α *and* β *with length* $|\alpha|+|\beta|\geq 2$, *we have*

$$\left|\left(\frac{\partial}{\partial x}\right)^\alpha\left(\frac{\partial}{\partial y}\right)^\beta\omega(t,s,x,y)\right|\leq C_{\alpha\beta} \tag{14}$$

where $C_{\alpha\beta}$ *is a positive constant independent of* (t,s,x,y).

The next proposition follows from this and the result in [5].

Proposition 4. i) *There exists a positive constant* γ_1 *such that*

$$\|E(\lambda,t,s)\varphi\|\leq\gamma_1\|\varphi\| \quad \text{for any } \varphi \text{ in } C_0^\infty(\mathbf{R}^n) \tag{15}$$

if $|t-s|\leq\delta_1(T)$. γ_1 *depends on T but not on* t, s, λ *and* φ.

ii) $s\text{-}\lim_{t\to s}E(\lambda,t,s)\varphi=\varphi$ *for any* φ *in* $L^2(\mathbf{R}^n)$.

As a consequence of Proposition 3, direct computation yields

$$\left(\frac{\partial}{\lambda\partial t}+\frac{1}{2}\sum_j\left(\frac{\partial}{\lambda\partial x_j}\right)^2+V(t,x)\right)\left(\left(\frac{-\lambda}{2\pi(t-s)}\right)^{n/2}e^{\lambda S(t,s,x,y)}\right) \tag{16}$$
$$=\left(\frac{-\lambda}{2\pi(t-s)}\right)^{n/2}\frac{(t-s)}{2\lambda}\Delta_x\omega(t,s,x,y)e^{\lambda S(t,s,x,y)}$$

almost everywhere.

Definition 5. We introduce the integral operator

$$G(\lambda,t,s)\varphi(x) \tag{17}$$
$$=\left(\frac{-\lambda}{2\pi(t-s)}\right)^{n/2}\frac{(t-s)}{2\lambda}\int_{\mathbf{R}^n}\Delta_x\omega(t,s,x,y)e^{\lambda S(t,s,x,y)}\varphi(y)dy.$$

Just as in Proposition 4, we can prove

Proposition 6. *There exists a positive constant* γ_2 *such that*

$$\|G(\lambda,t,s)\varphi\|\leq\gamma_2|t-s||\lambda|^{-1}\|\varphi\|. \tag{18}$$

γ_2 *is independent of* t, s, λ, φ *but it depends on T.*

Let $H(\lambda,t)$ denote the minimal closed extension of the Hamiltonian operator restricted to $\mathcal{S}(\mathbf{R}^n)$. We introduce the following pseudo-differential operators.

Definition 7. We put, for $j=1,2,\cdots,n$,

$$X_j(\lambda,t,s)\varphi(x)=\left(\frac{\lambda}{2\pi}\right)^n\iint_{\mathbf{R}^n\times\mathbf{R}^n}e^{\lambda(x-y)\cdot\eta}x_j(t,s,y,\eta)\varphi(y)dyd\eta \tag{19}$$

and

(20) $$\Xi_j(\lambda, t, s)\varphi(x)=\left(\frac{\lambda}{2\pi}\right)^n \iint_{\mathbf{R}^n\times\mathbf{R}^n} e^{i\lambda(x-y)\cdot\eta}\xi_j(t, s, y, \eta)\varphi(y)dyd\eta.$$

Using the results of Asada-Fujiwara [1], we obtain

Proposition 8. *We have the formulae, for* $j, k=1, 2, \cdots, n$,

(21) $$\left(\frac{\partial}{\lambda\partial x_j}\frac{\partial}{\lambda\partial x_k}E(\lambda, t, s)-E(\lambda, t, s)\Xi_j(\lambda, t, s)\Xi_k(\lambda, t, s)\right)\varphi(x)$$
$$=\left(\frac{t-s}{\lambda}\right)(P_j(\lambda, t, s)\Xi_j(\lambda, t, s)+P_k(\lambda, t, s)\Xi_k(\lambda, t, s))\varphi(x)$$
$$+\left(\frac{t-s}{\lambda}\right)^2 P_{jk}(\lambda, t, s)\varphi(x)$$

and

(22) $$(x_jx_kE(\lambda, t, s)-E(\lambda, t, s)X_j(\lambda, t, s)X_k(\lambda, t, s))\varphi(x)$$
$$=\left(\frac{t-s}{\lambda}\right)(Q_j(\lambda, t, s)X_j(\lambda, t, s)+Q_k(\lambda, t, s)X_k(\lambda, t, s))\varphi(x)$$
$$+\left(\frac{t-s}{\lambda}\right)^2 Q_{jk}(\lambda, t, s)\varphi(x).$$

The norm of operators $P_j(\lambda, t, s)$, $P_{jk}(\lambda, t, s)$, $Q_j(\lambda, t, s)$ *and* $Q_{jk}(\lambda, t, s)$ *are bounded uniformly in* t, s *and* λ *if* $|\lambda|\geq 1$.

Since $\Xi_j(\lambda, t, s)$ and $X_j(\lambda, t, s)$ maps $\mathcal{S}(\mathbf{R}^n)$ into itself, we obtain

Proposition 9. *If* $\varphi\in\mathcal{S}(\mathbf{R}^n)$, *then* $E(\lambda, t, s)\varphi$ *belongs to the domain* $D(H(\lambda, t))$ *of the operator* $H(\lambda, t)$. *Moreover, we have*

(23) $$E(\lambda, t, s)\varphi-\varphi=-\lambda\int_s^t H(\lambda, \sigma)E(\lambda, \sigma, s)\varphi d\sigma+\lambda\int_s^t G(\lambda, \sigma, s)\varphi d\sigma.$$

The right hand side is the Bochner integral in $L^2(\mathbf{R}^n)$.

Using this, we can prove the following basic properties of $E(\lambda, t, s)$.

Proposition 10. *For any* t, s *and* s_1 *satisfying* $|t-s|\leq\delta_1(T)$, $|s-s_1|\leq\delta_1(T)$ *and* $|t-s_1|\leq\delta_1(T)$, *we have the following estimates;*

(i) $\|E(\lambda, t, s_1)^*E(\lambda, t, s)-E(\lambda, s_1, s)\|\leq\gamma_3(|t-s_1|^2+|s_1-s|^2)$,

(ii) $\|E(\lambda, t, s)\|\leq\exp\gamma_3|t-s|^2$,

(iii) $\|E(\lambda, t, s)-E(\lambda, t, s_1)E(\lambda, s_1, s)\|\leq\gamma_3(|t-s_1|^2+|s_1-s|^2)$,

(iv) $\|E(\lambda, t, s)^*-E(\lambda, t, s)^{-1}\|\leq\gamma_3|t-s|^2$,

(v) $\|E(\lambda, t, s)E(\lambda, s, t)-I\|\leq\gamma_3|t-s|^2$,

where γ_3 *is a positive constant independent of* t, s, s_1 *and* λ *provided* $|t-s|\leq\delta_1(T)$, $|s_1-s|\leq\delta_1(T)$, $|t-s_1|\leq\delta_1(T)$ *and* $|\lambda|\geq 1$.

Theorem 1 follows from Proposition 10.

To prove Theorem 2, we use the following fact.

Proposition 11. *For any* t, τ, s *in* $\mathbf{R}$, *we have*

(24) $$(\Xi_j(\lambda, t, \tau)U(\lambda, \tau, s)-U(\lambda, \tau, s)\Xi_j(\lambda, t, s))\varphi$$
$$=\lambda^{-1}\int_s^\tau U(\lambda, \tau, \sigma)\tilde{P}_j(\lambda, t, \sigma)U(\lambda, \sigma, s)\varphi d\sigma$$

and

$$(25)\qquad (X_j(\lambda,t,\tau)U(\lambda,\tau,s)-U(\lambda,\tau,s)X_j(\lambda,t,s))\varphi = \lambda^{-1}\int_s^\tau U(\lambda,\tau,\sigma)\tilde{Q}_j(\lambda,t,\sigma)U(\lambda,\sigma,s)\varphi d\sigma,$$

where

$$\tilde{P}_j(\lambda,t,s)=\frac{d}{ds}\Xi_j(\lambda,t,s)+\lambda[H(\lambda,s),\Xi_j(\lambda,t,s)]$$

and

$$\tilde{Q}_j(\lambda,t,s)=\frac{d}{ds}X_j(\lambda,t,s)+\lambda[H(\lambda,s),X_j(\lambda,t,s)]$$

are pseudo-differential operators of Calderón-Vaillancourt type in [2].

Since $\tilde{P}_j(\lambda,t,s)$ and $\tilde{Q}_j(\lambda,t,s)$ are pseudo-differential operators which are bounded in $L^2(\mathrm{R}^n)$, $(\partial/\lambda\partial x_j)U(\lambda,t,s)\varphi\in L^2(\mathrm{R}^n)$ if both $\Xi_j(\lambda,t,s)\varphi$ and φ belong to $L^2(\mathrm{R}^n)$. Repeating similar discussions, we can prove that for any pair of multi-indices α and β, $x^\alpha(\partial/\lambda\partial x)^\beta U(\lambda,t,s)\varphi\in L^2(\mathrm{R}^n)$ if $\varphi\in\mathcal{S}(\mathrm{R}^n)$, which proves that $U(\lambda,t,s)\varphi\in\mathcal{S}(\mathrm{R}^n)$. The closed graph theorem proves that $U(\lambda,t,s)$ is a topological linear isomorphism of $\mathcal{S}(\mathrm{R}^n)$. Theorem 2 is proved.

References

[1] Asada, K., and Fujiwara, D.: On some oscillatory integral transformations in $L^2(\mathrm{R}^n)$ (to appear in Jap. J. Math., **4**).
[2] Calderón, A. P., and Vaillancourt, R.: On the boundedness of pseudo-differential operators. J. Math. Soc. Japan., **23**, 374–378 (1970).
[3] Feynman, R. P.: Space time approach to non-relativistic quantum mechanics. Rev. Mod. Phys., **20**, 367–387 (1948).
[4] Feynman, R. P., and Hibbs, A. R.: Quantum mechanics and path integrals. Mcgraw-Hill, New York (1965).
[5] Fujiwara, D.: On the boundedness of integral transformations with highly oscillatory kernels. Proc. Japan Acad., **51**, 96–99 (1975).
[6] ——: Fundamental solution of partial differential operators of Schrödinger's type. III. Ibid., **54A**, 62–66 (1978).