85. *Explicit Formulae for Solutions of Schrödinger Equations with Quadratic Hamiltonians*

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This note is concerned with a global, explicit construction of the fundamental solution for the Cauchy problem

$$(1)\qquad \begin{aligned} &\frac{\partial}{i\partial t}\psi(t,x)=H\Big(t,x,\frac{\partial}{i\partial x}\Big)\psi(t,x), \qquad (t,x)\in \boldsymbol{R}^{n+1},\\ &\psi(0,x)=\psi(x),\end{aligned}$$

with a quadratic Hamiltonian H:

$$\begin{aligned} H(t,x,\xi)=&\frac{1}{2}\langle\alpha(t)\xi,\xi\rangle+\langle\beta(t)x,\xi\rangle+\frac{1}{2}\langle\gamma(t)x,x\rangle\\ &+\langle a_1(t),\xi\rangle-\langle a_2(t),x\rangle+c(t),\end{aligned}$$

where α, β, γ are real $n\times n$ matrices with α, γ symmetric and $a_1, a_2\in \boldsymbol{R}^n$, $c\in \boldsymbol{R}$. All the coefficients are assumed to be continuously dependent on t.

We shall construct a unitary map $\mathcal{U}_t: \psi(x)\to\psi(t,x)$ in $L^2(\boldsymbol{R}^n)$ which is strongly continuous in t and has an explicit form written by means of one or two integral transformations. One can obtain solutions for a more general class of Hamiltonians at the expense of such explicitness (Fujiwara [1], Kitada and Kumano-go [3]). As our tools we shall make use of Maslov indices and representations of the Heisenberg group and the metapletic group. Although they are well established facts, it would bear some meaning to review them in this connection.

To make $H(t,x,D)$ a symmetric operator, we shall assign to $\langle\beta x,\xi\rangle$ the operator

$$\frac{1}{2}(\langle\beta x, D\rangle+\langle D,\beta x\rangle),$$

while to the rest of the symbol an operator in the usual way. One can write $H=H_1+H_2$ with

$$H_1(t,x,\xi)=-\sigma(a,(x,\xi))+c(t)$$

where $a=(a_1,a_2)$ and σ denotes the symplectic form $\sigma((x,\xi),(x',\xi'))=\langle x',\xi\rangle-\langle x,\xi'\rangle$.

1. Heisenberg group. When a is independent of t, the fundamental solution of

$$(2)\qquad D_t\psi=H_1(t,x,D)\psi, \qquad \psi(0,x)=\psi(x)\in\mathcal{S}(\boldsymbol{R}^n)$$

is given by $V_t(a,c)=e^{i\tilde{c}(t)}V(ta)$, where

$$\tilde{c}(t)=\int_0^t c(\tau)d\tau, \qquad V(a)(\psi)=\exp\left\{i\left(-\langle a_2, x\rangle+\frac{\langle a_1, a_2\rangle}{2}\right)\right\}\psi(x+a_1).$$

The relation

$$V(a)V(a')=V(a+a')e^{-(i/2)\sigma(a,a')} \tag{3}$$

implies the group action

$$X \ni (a, z) \mapsto zV(a)(\psi)$$

of the Heisenberg group X on $L^2(\boldsymbol{R}^n)$ as unitary operators. X is defined by

$$X=\boldsymbol{R}^{2n}\times \boldsymbol{T}, \qquad \boldsymbol{T}=\{z\in \boldsymbol{C}\,;\,|z|=1\}$$

with the multiplication law

$$(a, z)(a', z')=(a+a', zz'e^{-(i/2)\sigma(a,a')}).$$

In the general case when $a(t)$ may depend on t, the fundamental solution can be realized as a curve in X in the following way. Let R_u, $u\in X$, be the right translation of X, $R_u(a, z)=(a, z)u$, and $u(t)$ be the solution of

$$\frac{d}{dt}u(t)=dR_u(a(t), 0), \qquad u(0)=(0, 1), \tag{4}$$

where $(a(t), 0)$ is regarded as a tangent vector to X at (0.1). Writing $u=(v, w)$ with $v\in \boldsymbol{R}^{2n}$, $w\in \boldsymbol{T}$, we have

$$v(t)=\int_0^t a(\tau)d\tau, \qquad w(t)=\exp\left(-\frac{i}{2}\int_0^t \sigma(a(\tau), v(\tau))d\tau\right).$$

Now defining

$$V_t(a, c)(\psi)=e^{i\tilde{c}(t)}u(t)(\psi)=e^{i\tilde{c}(t)}w(t)V(v)(\psi)$$

we get the fundamental solution of (2) in this general case.

Since the transformation $(x, \xi)\mapsto(x, \xi)+v(t)$ is generated by the Hamiltonian system

$$\dot{x}=H_{1\xi}=a_1, \qquad \dot{\xi}=-H_{1x}=a_2,$$

it is natural to ask what form V_T takes when $v(T)=0$ for some $T>0$. Let $\gamma=\{v(t)\,;\,0\leqq t\leqq T\}$ be the closed curve, then

$$-\frac{i}{2}\int_0^t \sigma(a(\tau), v(\tau))d\tau=-\frac{i}{2}\int_\gamma \langle v_1, dv_2\rangle-\langle v_2, dv_1\rangle=i\int_S \sigma,$$

where S is a two dimensional surface with γ as its boundary. So we have

$$V_T=\exp\left(i\tilde{c}(T)+i\int_S \sigma\right).$$

2. Metaplectic group. Let us proceed to the equation

$$D_t\psi=H_2(t, x, D)\psi, \qquad \psi(0, x)=\psi(x)\in \mathcal{S}(\boldsymbol{R}^n). \tag{5}$$

We shall associate H_2 with a curve $F(t)$ in the Lie algebra $sp(n)$ of the real symplectic group $Sp(n)$:

$$F(t)=\begin{bmatrix}\beta & \alpha\\ -\gamma & -{}^t\beta\end{bmatrix}, \quad {}^tFJ+JF=0, \quad J=\begin{bmatrix} & -I\\ I & \end{bmatrix}.$$

The $2n\times 2n$ matrix solution of the linear ordinary differential equation

(6) $$\frac{d}{dt}s(t) = -F(t)s(t), \qquad s(0) = I$$

satisfies the identity ${}^t sJs = J$, thus belonging to $Sp(n)$.

$Sp(n)$ is nothing but the group of linear canonical transformations, so it is well known that under a suitable condition s is described by a generating function.

Lemma. *Let* $s = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ *be an element of* $Sp(n)$. *Then the following conditions on* s *are equivalent.*

(a) $\det b \neq 0$.

(b) *One can find a real quadratic form*

$$S(x, x') = \frac{1}{2}\langle Px, x\rangle - \langle Lx, x'\rangle + \frac{1}{2}\langle Qx', x'\rangle$$

with some symmetric P, Q *and invertible* L *such that the graph of the map* $s : (x', \xi') \mapsto (x, \xi)$ *is equivalently described by* $\xi = \partial S/\partial x$, $\xi' = -\partial S/\partial x'$.

The proof of this lemma shows that, if $\det b \neq 0$, we have

(7) $$P = db^{-1}, \quad Q = b^{-1}a \quad \text{and} \quad L = b^{-1}.$$

Now let $\Sigma = \{s \in Sp(n) ; \det b = 0\}$ and $\Sigma_0 = \{t \in \boldsymbol{R} ; s(t) \in \Sigma\}$. The above lemma allows us to define a unitary operator

(8) $$U(s)(\psi) = (2\pi)^{-n/2} |\det L|^{1/2} \int e^{iS(x,x')} \psi(x') dx'$$

for every $s \in Sp(n) \backslash \Sigma$. $U(s)$ induces the automorphisms of $\mathcal{S}(\boldsymbol{R}^n)$ and of $\mathcal{S}'(\boldsymbol{R}^n)$ in an obvious way, and has an important property:

(9) $$U(s)L(x, D)U(s)^{-1} = L \circ s^{-1}(x, D)$$

for every *linear* function $L(x, \xi)$ of x, ξ.

Moreover, putting $U_t = U(s(t))$, we claim that

(10) $$D_t U_t(\psi) = H_2(t, x, D) U_t(\psi), \quad \psi \in \mathcal{S}, \quad t \notin \Sigma_0.$$

Sketch of the proof of (10). From (9) we have

$$D_t \int e^{iS} \psi dx' = \int e^{iS} S'(t, x, x') \psi dx' = S'(t, x, {}^t dx - {}^t bD) \int e^{iS} \psi dx'.$$

A careful calculation in the light of the definition (6) of $s(t)$ now gives

$$S'(t, x, {}^t dx - {}^t bD) = H_2(t, x, D) - \frac{1}{2i} \operatorname{Tr}(L^{-1}L').$$

Furthermore, the fact that $D_t |\det L|^{1/2} = (1/2i) |\det L|^{1/2} \operatorname{Tr}(L^{-1}L')$ enables us to come to the conclusion (10).

We have yet to define U_t for $t \in \Sigma_0$. In doing so, we shall recall some results of Leray [4] concerning the unitary representation of the metaplectic group. First, $U(s)$ fails to have the group theoretical property: If $s_1 s_2 s_3 = I$, $s_j \notin \Sigma$, then

(11) $$U(s_1)U(s_2)U(s_3) = \exp\{(\pi i/4) \operatorname{sgn}(s_1, s_2, s_3)\},$$
$$\operatorname{sgn}(s_1, s_2, s_3) = \operatorname{sgn}(P_2 + Q_1) = \operatorname{sgn}(P_3 + Q_2) = \operatorname{sgn}(P_1 + Q_3),$$

with P_j, Q_j defined from s_j through (7). Let $Mp(n)$ be the connected double covering group of $Sp(n)$ with the projection $p : Mp(n) \to Sp(n)$.

We shall write $\tilde{\Sigma}=p^{-1}(\Sigma)$ and $\tilde{I}$ for the unit element of $Mp(n)$. The following is due to Leray [4]. (See also [5], [2].)

Theorem. *There exists a unique function $m(\tilde{s})$ of $Mp(n)\backslash\tilde{\Sigma}$ with values in Z_4 for even n, in $(Z+1/2)_4$ for odd n such that m is locally constant and satisfies*

(12) $$m(\tilde{s}^{-1})=-m(\tilde{s}),$$

(13) $$\frac{1}{2}\operatorname{sgn}(s_1, s_2, s_3)=m(\tilde{s}_1)+m(\tilde{s}_2)+m(\tilde{s}_3) \quad \text{mod. } 4,$$

$$\text{if } \tilde{s}_1\tilde{s}_2\tilde{s}_3=\tilde{I}, \quad \tilde{s}_j \notin \tilde{\Sigma}, \quad s_j=p(\tilde{s}_j).$$

Let us define for $\tilde{s}\in Mp(n)\backslash\tilde{\Sigma}$

$$U(\tilde{s})=e^{-(\pi i/2)m(\tilde{s})}U(s)$$

and for general $\tilde{s}\in Mp(n)$

(14) $$U(\tilde{s})=U(\tilde{s}_1)U(\tilde{s}_2) \quad \text{with} \quad \tilde{s}=\tilde{s}_1\tilde{s}_2, \quad \tilde{s}_j\notin\tilde{\Sigma}.$$

From (11), (13) we get the unitary representation of $Mp(n)$ (faithful but not irreducible). This in turn leads to the definition of the fundamental solution:

$$\tilde{U}_t=U(\tilde{s}(t)),$$

where $\tilde{s}(t)$ is the unique continuous lift-up of $s(t)$ to $Mp(n)$ with $\tilde{s}(0)=\tilde{I}$.

To prove that $\tilde{U}_t\psi$ is the solution of (5), it suffices to notice the following: In a local decomposition $s(t)=s_1(t)s_2$, $s_1, s_2\notin\Sigma$, with constant s_2, $s_1(t)$ also fulfills the first equation of (6). And in proving (10) we have used only that condition of s, aside from that $s\in Sp(n)\backslash\Sigma$. Strong continuity of $\tilde{U}(t)$ follows easily from (8) and (14).

As in §2, it is of our concern to study $\tilde{U}_T$ for a $T>0$ with $s(T)=I$, because $s(t)$ is the Hamiltonian flow of $-H_2$. With any $\tilde{s}_1\notin\tilde{\Sigma}$, we have

$$U(\tilde{s}(T))=\exp\left(-\frac{\pi i}{2}(m(\tilde{s}(T)\tilde{s}_1)-m(\tilde{s}_1))\right)I.$$

This index depends only on the homotopy class of the closed curve $\Gamma=\{s(t)\,;\,0\leqq t\leqq T\}$ in $Sp(n)$. So we can write

$$U(\tilde{s}(T))=i^{-m(\Gamma)}I$$

with the integer

$$m(\Gamma)=m(\tilde{s}(T)\tilde{s}_1)-m(\tilde{s}_1).$$

3. Conclusion and a remark. We are now in a position to conclude that the unitary operator

$$\mathcal{U}_t=\tilde{U}_t\cdot V(s(t)^{-1}a, c)$$

becomes the fundamental solution of (1). $\mathcal{U}_t$ is strongly continuous in t and further satisfies

$$\mathcal{U}_T=i^{-m(\Gamma)}\exp\left\{i(\tilde{c}(T)+\int_S\sigma)\right\}$$

when $\int_0^T s(\tau)^{-1}a(\tau)d\tau=0$ and $s(T)=I$.

While $V(a, c)$ and U_t are in principle explicitly calculated from H_1 and H_2, the Maslov index $m(\tilde{s})$ has been rather abstractly introduced.

But a method of Souriau [5] provides us with a practical way to calculate it. To sketch this, we identify $\boldsymbol{R}^{2n}$ with $\boldsymbol{C}^n$ by the map $(x,\xi)\to x+i\xi$. Let A be an element of $GL(n,\boldsymbol{C})$ with no eigenvalues on the negative real axis. For such A the logarithm of A can be defined by

$$\operatorname{Log}(A)=\int_{-\infty}^{0}\{(\tau I-A)^{-1}-(\tau-1)^{-1}I\}d\tau.$$

$s(t)$ may be only an $\boldsymbol{R}$-linear map in $\boldsymbol{C}^n$ by the above identification. But a fact concerning Lagrangian planes makes it possible to find a unitary map $u(t)$ satisfying $s(t)(i\boldsymbol{R}^n)=u(t)(i\boldsymbol{R}^n)$, along with a continuous function $\theta(t)$ such that $\det(u\bar{u}^{-1})=\exp(i\theta(t))$ with $\theta(0)=0$. The following formula is then valid.

$$m(\tilde{s}(t))=\frac{1}{2\pi}\{-\theta(t)+i\operatorname{Tr}\operatorname{Log}(-\bar{u}(t)u(t)^{-1})\}.$$

The condition that $-\bar{u}(t)u(t)^{-1}$ has no eigenvalue equal to -1 is equivalent to saying that $t\notin\Sigma_0$.

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