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Remarks on Fundamental Solutions to Schrödinger Equation with Variable Coefficients[*]

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1 Introduction.

1.1 Problem:

We consider

H : Schrödinger operator with variable coefficients,

$H_0 = -\dfrac{1}{2}\triangle$: Free Schrödinger operator.

We are interested in the following problems:

Q1 : $W(t) = e^{itH_0}e^{-itH}$ is a Fourier integral operator (FIO)?
If so, we have a representation:

$$e^{-itH} = e^{-itH_0}W(t) \quad \text{with } W(t) \text{ an FIO}.$$

(Not obvious even if $H = H_0 + V(x)$).

Q2 : $W_{\pm} = \underset{t\to\pm\infty}{\text{s-lim}}\, e^{itH}e^{-itH_0}$ is an FIO?

Answer: Yes (under certain assumptions).

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[*]This note is an edited version of the slides used in the seminar talk given by Nakamura.

1.2 Model:

The equation is

$$i\frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x), \quad t \in \mathbb{R}, x \in \mathbb{R}^n$$

with $\psi(0,x) = \psi_0(x) \in L^2(\mathbb{R}^n)$. The Hamiltonian is

$$H = -\frac{1}{2}\sum_{j,k=1}^{n}\frac{\partial}{\partial x_j}a_{jk}(x)\frac{\partial}{\partial x_k} + V(x),$$

where $a_{jk}, V \in C^\infty(\mathbb{R}^n;\mathbb{R})$, $(a_{jk}(x))_{j,k} > 0 \ (\forall x)$.

Assumption (A):

$$|\partial_x^\alpha(a_{jk}(x) - \delta_{jk})| \le C_\alpha\langle x\rangle^{-\mu-|\alpha|}, \quad |\partial_x^\alpha V(x)| \le C_\alpha\langle x\rangle^{2-\mu-|\alpha|}$$

for any $\alpha \in \mathbb{Z}_+^n$ with some $\mu > 1$ (short range).

1.3 Classical flow:

The classical hamiltonians are:

$$k(x,\xi) = \frac{1}{2}\sum_{j,k=1}^{n}a_{jk}(x)\xi_j\xi_k, \quad p(x,\xi) = k(x,\xi) + V(x).$$

Hamilton vector fields on $T^*\mathbb{R}^n$ are

$$H_k = \sum_{j=1}^{n}\left[\frac{\partial k}{\partial \xi_j}\frac{\partial}{\partial x_j} - \frac{\partial k}{\partial x_j}\frac{\partial}{\partial \xi_j}\right], \quad H_p = \sum_{j=1}^{n}\left[\frac{\partial p}{\partial \xi_j}\frac{\partial}{\partial x_j} - \frac{\partial p}{\partial x_j}\frac{\partial}{\partial \xi_j}\right]$$

and their Hamilton flows are denoted by $\exp(tH_k)$ and $\exp(tH_p)$. We write:

$$(y(t,x,\xi), \eta(t,x,\xi)) = \exp(tH_k)(x,\xi), \quad t \in \mathbb{R}, (x,\xi) \in T^*\mathbb{R}^n.$$

1.4 Nontrapping condition:

Our main geometrical assumption is the global nontrapping condition:

Assumption B: For any $(x,\xi) \in T^*\mathbb{R}^n$, $\xi \ne 0$, $|y(t,x,\xi)| \to \infty$ as $t \to \pm\infty$.

1.5   Classical scattering:

Under Assumptions A and B,

$$z_{\pm} = \lim_{t \to \pm\infty} (y(t,x) - t\eta(t,x,\xi)), \quad \xi_{\pm} = \lim_{t \to \pm\infty} \eta(t,x,\xi)$$

exist. Moreover,

$$|y(t,x,\xi) - (z_{\pm} + t\xi_{\pm})| \to 0 \quad \text{as } t \to \pm\infty.$$

We write:

$$(z_{\pm}, \xi_{\pm}) = w_{\pm}(x,\xi) = \lim_{t \to \pm\infty} \exp(-tH_{p_0}) \circ \exp(tH_k),$$

where $p_0 = \frac{1}{2}|\xi|^2$. Note $w_{\pm}$ is homogeneous in ξ:

$$w_{\pm}(x, \lambda\xi) = (z_{\pm}(x,\xi), \lambda\xi_{\pm}(x,\xi)).$$

since $k(x,\xi)$ is homogeneous in ξ (scaling property).

1.6   Main result:

Theorem 1: Suppose Assumptions A and B with $\mu = 2$. Then for $t \in \mathbb{R}_{\pm}$,

$$W(t) = e^{itH_0}e^{-itH}$$

are FIOs associated to $w_{\pm}$.

1.7   Application to the propagation of singularities:

We note

$$e^{-itH} = e^{-itH_0}W(t)$$

and

$$\mathrm{WF}(W(t)u) = w_{\pm}(\mathrm{WF}(u))$$

where $\mathrm{WF}(\cdot)$ denotes the wave front set. This implies

$$\mathrm{WF}(e^{-itH_0}u) = \mathrm{WF}(W(-t)e^{-itH}u) = w_{\mp}(\mathrm{WF}(e^{-itH}u))$$

and hence

$$\mathrm{WF}(e^{-itH}u) = w_{\mp}^{-1}(\mathrm{WF}(e^{-itH_0}u)).$$

1.8 Wave operators:

In order to study wave operators, we need to assume stronger assumption on V:

Assumption (C):

$$|\partial_x^\alpha(a_{jk}(x) - \delta_{jk})| \leq C_\alpha \langle x \rangle^{-\mu-|\alpha|}, \quad |\partial_x^\alpha V(x)| \leq C_\alpha \langle x \rangle^{-\mu-|\alpha|}$$

for any $\alpha \in \mathbb{Z}_+^n$ with some $\mu > 1$ (a_{jk} and V are both short range).

Theorem 2. Suppose Assumption B and C. Then

$$W_\pm = \operatorname*{s-lim}_{t \to \pm\infty} e^{itH} e^{-itH_0}$$

exist and are FIOs associated to $w_\pm^{-1}$.

2 Beals-type characterization of FIOs.

2.1 Standard definition of FIOs:

We first recall the definition of FIOs (following Hörmander).

Definition: (Besov space: $B_2^{\sigma,\infty}(\mathbb{R}^m)$) Let $\sigma \in \mathbb{R}$. For $u \in \mathcal{S}'(\mathbb{R}^m)$, $\hat{u} \in L_{loc}^2(\mathbb{R}^m)$, we set

$$\|u\|_{B_2^{\sigma,\infty}} = \left(\int_{|\xi|\leq 1} |\hat{u}(\xi)|^2 d\xi\right)^{1/2} + \sup_{j\geq 0}\left(\int_{2^j\leq|\xi|\leq 2^{j+1}} \left|2^{\sigma j}\hat{u}(\xi)\right|^2 d\xi\right)^{1/2}$$

and define

$$B_2^{\sigma,\infty}(\mathbb{R}^m) = \left\{u \in \mathcal{S}'(\mathbb{R}^m) \mid \|u\|_{B_2^{\sigma,\infty}} < \infty\right\}.$$

Definition: (Lagrangian submanifolds) $\Lambda \subset T^*\mathbb{R}^m \setminus 0$ is called a *Lagrangian submanifold*, if Λ is an m-dimensional C^∞-submanifold in $\mathbb{R}^m$, and is conic, i.e.,

$$(x,\xi) \in \Lambda \implies (x,\lambda\xi) \in \Lambda \quad (\lambda > 0).$$

Moreover the pull-back of $\omega_0 = dx \wedge d\xi$ to Λ vanishes, i.e., $i^*\omega_0 = 0$.

Definition: (Lagrangian distribution) Let $\Lambda \subset T^*\mathbb{R}^m \setminus 0$ be a conic Lagrangian submanifold, and let $u \in \mathcal{S}'(\mathbb{R}^m)$, $\sigma \in \mathbb{R}$. u is called a *Lagrangian distribution* of order σ associated to Λ, or equivalently, $u \in I^\sigma(\mathbb{R}^m, \Lambda)$, if for any $p_1, p_2, \ldots, p_N \in S^1$ such that the principal symbol of p_j vanishes on Λ,

$$p_1(x, D_x)p_2(x, D_x)\cdots p_N(x, D_x)u \in B_{2,loc}^{-\sigma-m/4,\infty}(\mathbb{R}^m).$$

(S^m is the classical symbol class.)

Remark: If $u \in I^\sigma(\mathbb{R}^m, \Lambda)$, then there exist $N \leq m$, $\Psi(x, \theta)$ which is homogeneous in θ and $a(x, \theta) \in S_{1,0}^{\sigma + m/4 - N/2}(\mathbb{R}^m \times \mathbb{R}^N)$ such that

$$u(x) = (2\pi)^{-m/4 - N/2} \int_{\mathbb{R}^N} e^{i\Psi(x,\theta)} a(x, \theta) d\theta$$

where $\Psi(x, \theta)$ is related to Λ by

$$\Lambda = \left\{ (x, \partial_x \Psi(x, \theta)) \in T^*\mathbb{R}^m \mid \partial_\theta \Psi(x, \theta) = 0 \right\}.$$

(Typically $N = m/2$, and hence $a \in S_{1,0}^\sigma(\mathbb{R}^m)$.)

Definition: (Fourier integral operator) Let $U : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}'(\mathbb{R}^n)$ and let u be its distribution kernel. Let $S : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ be a canonical transform which is homogeneous of order 1 in ξ. Let

$$\Lambda_S = \{ (y, x, \eta, -\xi) \mid (y, \eta) = S(x, \xi) \} \subset T^*\mathbb{R}^{2n}.$$

U is called a *Fourier integral operators* of order $\sigma \in \mathbb{R}$ associated to S if $u \in I^\sigma(\Lambda_S, \mathbb{R}^{2n})$.

2.2   Beals-type characterization:

Let $S : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ be a homogeneous canonical diffeomorphism, and let Λ_S as above. Suppose $a \in S_{1,0}^1(\mathbb{R}^n)$ is supported in compact set in x, and supported away from $\{\xi = 0\}$. For such a, we set

$$Ad_S(a)U = (a \circ S^{-1})(x, D_x) U - U a(x, D_x)$$

Theorem 3. Let S and Ad_S be as above. Let $U \in \mathcal{L}(L_{cpt}^2(\mathbb{R}^n), L_{loc}^2(\mathbb{R}^n))$. U is an FIO of order 0 associated to S if and only if for any $a_1, a_2, \ldots, a_N \in S^1(\mathbb{R}^n)$ satisfying the above condition,

$$Ad_S(a_1) Ad_S(a_2) \cdots Ad_S(a_N) U \in \mathcal{L}(L_{cpt}^2(\mathbb{R}^n), L_{loc}^2(\mathbb{R}^n)).$$

Remark: If $S = Id$, then $Ad_S(a)U = [a(x, D_x), U]$ and the above result is (a variation of) the Beals characterization of pseudodifferential operators.

The following simple consequence of Theorem 3 is useful in applications.

Corollary 4. Let S and U as in Theorem 3. If U is invertible, and for any $a \in S^1(\mathbb{R}^n)$ there is $b \in S_{1,0}^0(\mathbb{R}^n)$ such that

$$U a(x, D_x) U^{-1} = (a \circ S^{-1})(x, D_x) + b(x, D_x),$$

then U is an FIO associated to S.

Remark: This result may be considered as a converse of the Egorov theorem.

3   Proof of Theorem 1.

Now we know that it is sufficient to show the Egorov theorem. It was essentially done in [N1] in semiclassical setting. We recall the result in the form we need here.

We use the notation: The Weyl quantization of a symbol a is

$$a^W(x, D_x)\psi(x) = (2\pi)^{-n} \iint e^{i(x-y)\cdot\xi} a(\tfrac{x+y}{2}, \xi)\psi(y)dyd\xi$$

for $\psi \in \mathcal{S}(\mathbb{R}^n)$.

We consider the evolution

$$\frac{\partial}{\partial t}W(t)\psi = -ie^{itH_0}(H - H_0)e^{-itH}\psi$$
$$= -ie^{itH_0}(H - H_0)e^{-itH_0}W(t)\psi = -iL(t)W(t)\psi.$$

We note $e^{itH_0}a^W(x, D_x)e^{-itH_0} = a^W(x - tD_x, D_x)$ and hence,

$$L(t) = -\frac{1}{2}\sum_{j,k=1}^n \frac{\partial}{\partial x_j}(a_{jk}^W(x - tD_x) - \delta_{jk})\frac{\partial}{\partial x_k} + V(x - tD_x).$$

In particular, if we set

$$\ell(t, x, \xi) = \frac{1}{2}\sum_{j,k=1}^n (a_{jk}(x - t\xi) - \delta_{jk})\xi_j\xi_k + V(x - t\xi),$$

then $L(t) - \ell^W(t, x, D_x) \in \mathrm{OPS}_{1,0}^0(\mathbb{R}^n)$. Note $\ell(t, x, \xi)$ generates the evolution

$$w(t) = \exp(-tH_{p_0}) \circ \exp(tH_p).$$

For $a \in S^1(\mathbb{R}^n)$, we set

$$A(t) = W(t)a^W(x, D_x)W(t)^{-1}.$$

$A(t)$ satisfies the Heisenberg equation

$$\frac{\partial}{\partial t}A(t) = -i[L(t), A(t)], \quad A(0) = a^W(x, D_x).$$

Then it is natural to expect

$$A(t) \sim a_0^W(t, x, D_x),$$

where $a_0(t, x, \xi) = (a \circ w(t)^{-1})(x, \xi)$. In fact, we can construct an asymptotic solution:

$$a(t, x, \xi) \sim \sum_{j=0}^\infty a_j(t, x, \xi), \quad a_j(t, \cdot, \cdot) \in S_{1,0}^{1-j}(\mathbb{R}^n)$$

solving transport equations along $w(t)$, so that

$$\frac{\partial}{\partial t}\tilde{A}(t) + i[L(t), \tilde{A}(t)] \in \mathrm{OPS}^{-\infty}(\mathbb{R}^n),$$

where $\tilde{A}(t) = a^W(t, x, D_x)$ and $\tilde{A}(0) = a^W(x, D_x)$. Hence $A(t) - \tilde{A}(t) \in \mathrm{OPS}^{-\infty}$, and in particular

$$A(t) - (a \circ w(t)^{-1})^W(x, D_x) \in \mathrm{OPS}^0_{1,0}(\mathbb{R}^n).$$

For $\pm t > 0$, we have

$$w(t, x, \xi) - w_\pm(x, \xi) = O(|\xi|^{1-\mu}) \quad \text{as } |\xi| \to \infty$$

by scattering relations. This implies

$$a \circ w(t)^{-1} - a \circ w_\pm^{-1} \in S^{2-\mu}_{1,0}(\mathbb{R}^n).$$

So far, we need only $\mu > 1$. If $\mu = 2$, then

$$A(t) - (a \circ w_\pm^{-1})(x, D_x) \in \mathrm{OPS}^0_{1,0}(\mathbb{R}^n)$$

and the condition of Corollary 4 follows from this with $U = W(t)$, $S = w_\pm$ where $\pm t > 0$. $\qquad\square$

4   The case $\mu \in (1, 2)$.

In the proof of Theorem 1, we used the assumption only at the last step. So it is natural to expect:

Theorem 5. Suppose Assumption A with $\mu \in (1, 2)$ and Assumption B. Then $W(t)$ is an FIO associated to $w(t)$.

The problem is that $w(t)$ is canonical, but is <u>not</u> homogeneous in ξ. So usual definition of FIOs does not apply. However, $w(t)$ is *asymptotically homogeneous* in the following sense: $w_\pm$ is homogeneous in ξ and

$$|\partial_x^\alpha \partial_\xi^\beta (w(t, x, \xi) - w_\pm(x, \xi))| \le C_{\alpha\beta}\langle\xi\rangle^{-\nu-|\beta|}$$

for any $\alpha, \beta \in \mathbb{Z}_+^n$, with some $\nu = \mu - 1 > 0$

We can define *asymptotically conic* manifolds, and if S is asymptotically homogeneous in the above sense, then we can show

$$\Lambda_S = \{(y, x, \eta, -\xi) \mid (y, \eta) = S(x, \xi)\} \in T^*\mathbb{R}^{2n}$$

is an *asymptotically conic Lagrangian manifold*. We can define

- *Lagrangian distribution associated to an asymptotically conic manifold;*

- *Fourier integral operators associated to an asymptotically homogeneous canonical transform.*

(We omit the precise definitions here.)
Theorem 5 makes sense using above definitions.   □

5   Other Remarks.

1. Theorem 2 does not require $\mu = 2$ to show $W_\pm$ are FIOs associated to $w_\pm^{-1}$. This is because (at least formally) $W_\pm^*$ is associated to $w_\pm = \lim_{t\to\pm\infty} w(t)$, and it is already homogeneous in ξ. Instead, we need precise time-dependence of estimates. Also, we cannot use Corollary 4 directly because $W_\pm$ is not invertible.

2. We believe the results can be extended to Schrödinger equations with *"long-range"* perturbations. (cf. [N2])

3. We also believe the results can be extended to Schrödinger equations on *"scattering manifolds"*. (cf. [IN1])

References

Here are several references closely related to our result. Our main result (Theorem 1) is analogous to the paper by Hassell and Wunsch, though the formulation, assumption, proof are quite different:

[**HW**] Hassell, A., Wunsch, J.: The Schrödinger propagator for scattering metrics. Ann. Math. **162**, 487-523 (2005).

In our proof, we use an Egorov type theorem, which is employed formerly in:

[**N1**] Nakamura, S.: Wave front set for solutions to Schrödinger equations. *J. Functional Analysis* **256**, 1299-1309 (2009)

[**N2**] Nakamura, S.: Semiclassical singularity propagation property for Schrödinger equations. *J. Math. Soc. Japan* **61** (1), 177-211 (2009)

[**IN1**] Ito, K., Nakamura, S.: Singularities of solutions to Schrödinger equation on scattering manifold. Preprint, Nov. 2007. To appear in *American J. Math.* (http://arxiv.org/abs/0711.3258)