

# **Remarks on Fundamental Solutions to Schrödinger Equation with Variable Coefficients**

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# 1. Introduction.

## Problem:

$H$  : Schrödinger operator with variable coefficients,  
 $H_0 = -\frac{1}{2}\Delta$  : Free Schrödinger operator.

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:  $W_{\pm} = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH}e^{-itH_0}$  is an FIO?

Answer: Yes (under certain assumptions).

**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):**

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

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

**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:

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

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

**Classical scattering:** Under Assumptions A and B,

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

exist. Moreover,

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

We write:

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

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

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

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

**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  $w_\pm$ .

**Application to the propagation of singularities:** We note  $e^{-itH} = e^{-itH_0}W(t)$  and

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

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

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

and hence

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

**Wave operators:**

**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

$$W_\pm = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0}$$

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

## Remark: Closely related results

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

[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>)

[IN2] Ito, K., Nakamura, S.: Remarks on the Fundamental Solution to Schrödinger Equation with Variable Coefficients. Preprint, Dec. 2009. (<http://arxiv.org/abs/0912.4939>)

## 2. Beals-type characterization 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

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

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  $\Lambda$  is an  $m$ -dimensional  $C^\infty$ -submanifold in  $\mathbb{R}^m$ , and is conic, i.e.,

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

Moreover the pull-back of  $\omega_0 = dx \wedge d\xi$  to  $\Lambda$  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  $\sigma$  associated to  $\Lambda$ , or equivalently,  $u \in I^\sigma(\mathbb{R}^m, \Lambda)$ , if for any  $p_1, p_2, \dots, p_N \in S^1$  such that the principal symbol of  $p_j$  vanishes on  $\Lambda$ ,

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

( $S^m$  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  $\theta$  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  $\Lambda$  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  $U : \mathcal{S}(\mathbb{R}^n) \rightarrow \mathcal{S}'(\mathbb{R}^n)$  and let  $u$  be its distribution kernel. Let  $S : T^*\mathbb{R}^n \rightarrow T^*\mathbb{R}^n$  be a canonical transform which is homogeneous of order 1 in  $\xi$ . 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  $u \in I^\sigma(\Lambda_S, \mathbb{R}^{2n})$ .

**Beals-type characterization:** Let  $S : T^*\mathbb{R}^n \rightarrow T^*\mathbb{R}^n$  be a homogeneous canonical diffeomorphism, and let  $\Lambda_S$  as above.

Suppose  $a \in S^1_{1,0}(\mathbb{R}^n)$  is supported in compact set in  $x$ , and supported away from  $\{\xi = 0\}$ . For such  $a$ , we set

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

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

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

**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

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

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

$$a^W(x, D_x)\psi(x) = (2\pi)^{-n} \iint e^{i(x-y)\cdot\xi} a\left(\frac{x+y}{2}, \xi\right) \psi(y) dy d\xi$$

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

We consider the evolution

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

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  $L(t) - \ell^W(t, x, D_x) \in \text{OPS}_{1,0}^0(\mathbb{R}^n)$ .

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

$$A(t) \sim a_0^W(t, x, D_x), \quad \text{where } a_0(t, x, \xi) = (a \circ w(t)^{-1})(x, \xi).$$

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

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

where  $\tilde{A}(t) = a^W(t, x, D_x)$  and  $\tilde{A}(0) = a^W(x, D_x)$ .

Hence  $A(t) - \tilde{A}(t) \in \text{OPS}^{-\infty}$ , and in particular

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

For  $\pm t > 0$ , we have

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

by scattering relations. This implies

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

So far, we need only  $\mu > 1$ .

If  $\mu = 2$ , then

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

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

## 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 not homogeneous in  $\xi$ . So usual definition of FIOs does not apply. However,  $w(t)$  is *asymptotically homogeneous* in the following sense:  $w_{\pm}$  is homogeneous in  $\xi$  and

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

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  $w_{\pm} = \lim_{t \rightarrow \pm\infty} w(t)$ , and it is already homogeneous in  $\xi$ .

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])