Remarks on Fundamental Solutions to Schrödinger Equation with Variable Coefficients (Semiclassical Proof)

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1. Introduction.

Problem:
H : Schrödinger operator with variable coefficients,
$H_0 = -\frac{1}{2}\triangle$: 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: $W_\pm = \operatorname*{s-lim}_{t\to\pm\infty} e^{itH}e^{-itH_0}$ 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):

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

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

Classical flow: The classical hamiltonians are:

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

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

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

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

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

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

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).

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 $w_\pm$. (Note $e^{-itH} = e^{-itH_0} W(t)$.)

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

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

Wave operators:

Assumption (C):

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

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

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

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. (Semiclassical) 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 $u \in \mathcal{S}'(\mathbb{R}^m)$, $\widehat{u} \in L^2_{loc}(\mathbb{R}^m)$, we set

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

and define

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

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.,

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

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,

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

(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

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

(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

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

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 $S : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ be a homogeneous canonical diffeomorphism, and let Λ_S as above.
Suppose $a \in C_0^\infty(T^*\mathbb{R}^n \setminus 0)$, and set $a^h(x,\xi) = a(x, h\xi)$. We set

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

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 $a_1, a_2, \ldots, a_N \in C_0^\infty(T^*\mathbb{R}^n \setminus 0)$,

$$\left\| Ad_S(a_1^h) Ad_S(a_2^h) \cdots Ad_S(a_N^h) U \right\|_{\mathcal{B}(L^2)} = O(h^N), \;\; h \to 0.$$

Remark: If $S = Id$, then $Ad_S(a^h)U = [a(x, hD_x), U]$ 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 $a \in C_0^\infty(T^*\mathbb{R}^n \setminus 0)$ there is $b(h;\cdot) \in C_0^\infty(T^*\mathbb{R}^n \setminus 0)$, uniformly bounded in h, such that

$$Ua(x, hD_x)U^{-1} = (a \circ S^{-1})(x, hD_x) + h \cdot b(h; x, hD_x) + O(h^\infty),$$

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,N2].
We recall the result in the form we need here.

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

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

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

We consider the evolution:

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

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 $L(t) - \ell^W(t, x, D_x) \in \mathrm{OPS}^0_{1,0}(\mathbb{R}^n)$.
(Note $\ell = O(|\xi|^{2-\mu})$ as $|\xi| \to \infty$, for each $t \neq 0$, locally in x.)

Note $\ell(t,x,\xi)$ generates the evolution

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

i.e., $\dot{z}(t) = \{\ell(t), \xi(t)\}$, $\dot{\xi}(t) = -\{\ell(t), z(t)\}$ where $(z(t), \xi(t)) = w(t)(x_0, \xi_0)$.
For $a \in C_0^\infty(T^*\mathbb{R}^d \setminus 0)$, we set

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

$A(t)$ satisfies the Heisenberg equation

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

Then it is natural to expect

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

as $h \to 0$. (Note $\frac{d}{dt} a_0(x, \cdot) = -\{\ell(t), a_0(t, \cdot)\}$ with $a_0(0, \cdot) = a$)

In fact, we can construct an asymptotic solution:

$$a(h;t,x,\xi) \sim \sum_{j=0}^{\infty} h^j a_j(h;t,x,\xi), \quad a_j(h;t,\cdot,\cdot) \in C_0^\infty(T*\mathbb{R}^n \setminus 0),$$

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

$$\frac{\partial}{\partial t}\tilde{A}(t) + i[L(t), \tilde{A}(t)] = O(h^\infty),$$

where $\tilde{A}(t) = a^W(h;t,x,hD_x)$ and $\tilde{A}(0) = a^W(x,hD_x)$.
(Here $a_j(h;t,\cdot)$ are uniformly bounded as $h \to 0$.)
Hence $A(t) - \tilde{A}(t) = O(h^\infty)$, and in particular

$$A(t) - (a \circ w(t)^{-1})^W(x,D_x) = hb^W(h;t,x,hD_x) + O(h^\infty),$$

where $b \in C_0^\infty(T^*\mathbb{R}^n \setminus 0)$, and it is uniformly bounded as $h \to 0$.

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

$$a \circ w(t)^{-1} - a \circ w_\pm^{-1} = O(h^{\mu-1}).$$

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

$$A(t) - (a \circ w_\pm^{-1})(x, D_x) = h\tilde{b}^W(h;t,x,hD_x) + O(h^\infty)$$

with $\tilde{b}(h;t,x,\xi) \in C_0^\infty(T^*\mathbb{R}^n \setminus 0)$, uniformly bounded.
The condition of Corollary 4 follows from this with $U = W(t)$, $S = w_\pm$ where $\pm t > 0$. $\square$

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 not homogeneous in ξ. So the 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. The results can be extended to Schrödinger equations with *"long-range"* perturbations (cf. [N2]). Then we have

$$e^{-itH} = e^{-iS(t,D_x)}W(t),$$

where $S(t,\xi)$ is a solution to the Hamilton-Jacobi equation, and $W(t)$ is an FIO.

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

4. Extension to Schrödinger equations in exterior regions? (Open. We need to develop semiclassical analysis with boundaries.)

5. Applications to Strichartz estimates, and other smoothing estimates? (maybe possible with combining scaling argument in x-variables.)

6. Trapping cases? (Some results, e.g., Burq, Nonnenmacher, Zworski, .., but known to be difficult.)