Wave Front Set for Solutions to Schrödinger Equations

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Abstract

In this note, we discuss the wave front set for solutions to Schrödinger equation with variable coefficients. It is well-known that the propagation speed of the wave front set of solutions to Schrödinger equation is infinite, and hence we cannot expect the usual propagation theorem such as for the solutions to the wave equation. Instead, relations between the decay property of initial condition and the wave front set of solutions have been studied, which is generally called (microlocal) smoothing properties.

Here we propose a different formulation, which is closer to the "propagation of singularity theorem", at least in the spirit.

We consider a Schrödinger equation:

$$\frac{d}{dt}u(t) = -iHu(t), \qquad u(0) = u_0 \in L^2(\mathbb{R}^d)$$

on $L^2(\mathbb{R}^d)$, where $d \geq 1$, and H is the Schrödinger operator defined by

$$H = \frac{1}{2}\sum_{i,j=1}^{d} D_j a_{jk}(x) D_k + V(x), \qquad D_j = -i\frac{\partial}{\partial x_j}.$$

We suppose the coefficients $\{a_{ij}(x)\}$ and the potential $V(x)$ satisfy the following conditions:

Assumption A. $a_{ij}(x), V(x) \in C^\infty(\mathbb{R}^d;\mathbb{R})$ for $i,j = 1,\dots,d$, and there exist $\mu > 0$, and $C_\alpha > 0$ for each $\alpha \in \mathbb{Z}_+^d$ such that

$$|\partial_x^\alpha (a_{ij}(x) - \delta_{ij})| \leq C_\alpha \langle x\rangle^{-\mu-|\alpha|},$$
$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle x\rangle^{2-\mu-|\alpha|}, \qquad x \in \mathbb{R}^d.$$

Moreover, H is elliptic, i.e., $\det(a_{ij}(x)) \neq 0$ for each $x \in \mathbb{R}^d$.

Then it is well-known that H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d)$. We denote the unique self-adjoint extension by the same symbol H. Thus, by the Stone theorem, $u(t) = e^{-itH}u_0$ is the solution to the Schrödinger equation with the initial condition

$u(0) = u_0$. We will study how the wave front set of u_0 is described using the properties of $u(t)$, $t > 0$.

We denote the symbol of the kinetic energy part by $p(x, \xi)$, i.e.,

$$p(x,\xi) = \frac{1}{2}\sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j, \quad x, \xi \in \mathbb{R}^d.$$

We denote the solution to the Hamilton equation:

$$\frac{d}{dt}y(t) = \frac{\partial p}{\partial \xi}(y(t), \eta(t)), \quad \frac{d}{dt}\eta(t) = -\frac{\partial p}{\partial x}(y(t), \eta(t)) \tag{1}$$

with initial condition $y(0) = x$, $\eta(0) = \xi$ by $y(t; x, \xi)$ and $\eta(t; x, \xi)$.

Definition 1. $(x, \xi) \in \mathbb{R}^{2d}$ is said to be *forward nontrapping* if $|y(t; x, \xi)| \to +\infty$ as $t \to +\infty$.

Short-range case

We say H is a *short-range perturbation* of $H_0 = -\frac{1}{2}\Delta$ (or simply short-range type) if Assumption A is satisfied with $\mu > 1$. In this case, if (x, ξ) is forward nontrapping, then it is well-known that there exists $(x_+, \xi_+) \in \mathbb{R}^{2d}$ such that

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

Namely, the classical trajectory $y(t; x, \xi)$ approaches to the free motion $x_+ + t\xi_+$ as $t \to +\infty$. Note, by the conservation of energy, $|\xi_+|^2/2 = p(x, \xi)$. The map:

$$S : (x, \xi) \mapsto (x_+, \xi_+)$$

is the classical (inverse) wave operator.

We denote the wave front set of $u \in \mathcal{D}'(\mathbb{R}^d)$ by $WF(u) \subset \mathbb{R}^{2d}$.

Theorem 1 ([7]). *Suppose Assumption A with $\mu > 1$, and suppose $(x_0, \xi_0) \in \mathbb{R}^{2d}$ is forward nontrapping. Let $u(t) = e^{-itH}u_0$ with $u \in L^2(\mathbb{R}^d)$, and let $t_0 > 0$. Then*

$$(x_0, \xi_0) \in WF(u_0) \iff (x_+(x_0, \xi_0), \xi_+(x_0, \xi_0)) \in WF(e^{it_0H_0}u(t_0)).$$

Remark. Recently, Hassel and Wunsch [3] have obtained different characterization of the wave front set of solutions to Schrödinger equations using the quadratic scattering wave front set. The setting and the formulation are quite different, and the relationship is not clear to the author.

Now we discuss the relationship of our result and the microlocal smoothing properties. For a symbol $a(x, \xi) \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, we denote the Weyl quantization by

$$a^W(x, D_x)u(x) = (2\pi)^{-d} \int e^{i(x-y)\cdot\xi} a((x+y)/2, \xi)u(y)dyd\xi$$

where $u \in \mathcal{S}(\mathbb{R}^d)$. By the basic property of the Weyl quantization (see [4]), we have

$$e^{-itH_0} a^W(x, D_x) e^{itH_0} = a^W(x + tD_x, D_x),$$

where the right hand side is the Weyl quantization of $a(x + t\xi, \xi)$. We recall the wave front set is characterized as follows:

$$(x', \xi') \notin WF(e^{itH_0}u) \iff \begin{array}{c} \exists a \in S^0_{1,0} : \text{ elliptic at } (x', \xi') \text{ and} \\ a^W(x, D_x) e^{itH_0} u \in \mathcal{S}(\mathbb{R}^d), \end{array}$$

where $S^m_{\rho,\delta} = S(\langle\xi\rangle^m, \langle\xi\rangle^{2\delta} dx^2 + \langle\xi\rangle^{-2\rho} d\xi^2)$ is the usual pseudodifferential operator symbol class. The last condition of the RHS is equivalent to

$$e^{-itH_0} a^W(x, D_x) e^{itH_0} u = a^W(x - tD_x, D_x) u \in \mathcal{S}(\mathbb{R}^d)$$

since e^{-itH_0} is an isomorphism on $\mathcal{S}(\mathbb{R}^d)$. Thus, by combining this with Theorem 1, we learn that

$$(x_0, \xi_0) \in WF(u_0) \iff \begin{array}{l} \exists a \in S^0_{1,0} : \text{ elliptic at } (x_+(x_0, \xi_0), \xi_+(x_0, \xi_0)) \\ \text{and } a^W(x - t_0 D_x, D_x) u(t_0) \in \mathcal{S}(\mathbb{R}^d). \end{array}$$

Now we suppose that

$$\text{supp } a \in \{(x, \xi) \mid |x - x_+| < \delta, |\xi/|\xi| - \xi_+| < \delta\}$$

with small $\delta > 0$, then we can easily see that $a(x - t\xi, \xi)$ is supported in a small conic neighborhood of $(t\xi_+, \xi_+)$.

We denote $a \in S(1, dX^2/\langle X\rangle^2)$ with $X = (x, \xi)$ if $a \in C^\infty(\mathbb{R}^{2d})$ and for any $\alpha \in \mathbb{Z}^{2d}_+$,

$$|\partial^\alpha_X a(X)| \le C_\alpha \langle X\rangle^{-|\alpha|}, \qquad X \in \mathbb{R}^{2d}.$$

$a \in S(1, dX^2/\langle X\rangle^2)$ is called elliptic at $X_0 \in \mathbb{R}^{2d} \setminus 0$ if there exist a conic neighborhood Ω of X_0 and $\varepsilon > 0$ such that $|a(X)| \ge \varepsilon$ for $X \in \Omega$.

From the above discussion, we learn that if there exists $a \in S(1, dX^2/\langle x\rangle^2)$ that is elliptic at $(t_0\xi_+, \xi_+)$ and $a^W(x, D_x)u(t_0) \in \mathcal{S}(\mathbb{R}^d)$, then $(x_0, \xi_0) \notin WF(u)$. Now we introduce the following definition:

Definition 2. Let $u \in \mathcal{S}'(\mathbb{R}^d)$. We say $(x, \xi) \in \mathbb{R}^{2d} \setminus 0$ is not in the *homogeneous wave front set* of u if there exists $a \in S(1, dX^2/\langle X\rangle^2)$ such that a is elliptic at (x, ξ) and $a^W(x, D_x)u \in \mathcal{S}(\mathbb{R}^d)$. We denote $(x, \xi) \notin HWF(u)$ if this condition is satisfied, and denote the complement by $HWF(u)$.

Then the following claim follows from Theorem 1.

Corollary 2. *Suppose the conditions of Theorem 1. If* $(t_0\xi_+(x_0, \xi_0), \xi_+(x_0, \xi_0)) \notin HWF(u(t_0))$ *then* $(x_0, \xi_0) \notin WF(u_0)$. *In other words, if* $(x_0, \xi_0) \in WF(u_0)$ *then* $(t_0\xi_+(x_0, \xi_0), \xi_+(x_0, \xi_0)) \in HWF(u(t_0))$.

It is easy to see from the definition that if $u(x)$ decays rapidly in a conic neighborhood of $x' \in \mathbb{R}^d$, then $(x', \xi') \notin HWF(u)$ with any ξ'. Thus we also have the following immediate consequence of Corollary 2:

Corollary 3. *Let u, t_0, x_0, ξ_0, etc., as in Theorem 1. If $u(t_0)$ decays rapidly in a conic neighborhood of $\xi_+(x_0, \xi_0)$ then $(x_0, \xi_0) \notin WF(u_0)$.*

This result is essentially the same as the *micrilocal smoothing property* of Craig, Kappeler and Strauss [1]. Note that the condition of Corollary 3 is independent of the time t_0 (except for the sign), and instead the condition is more strict. We also note that Corollaries 2 and 3 do not contain reference to the asymptotic free motion: $x_+ + t\xi_+$, but only the asymptotic momentum ξ_+. Though these results are much weaker than Theorem 1 which characterizes the wave front set in nontrapping region, we can hope that such results can be extended to more general situation where the asymptotic free motion does not necessarily exist. This leads us to the study of the perturbation of *long-range* type.

Long-range case

We say H is long-range type if Assumption A is satisfied with $0 < \mu \leq 1$. Let (x_0, ξ_0) be forward-nontrapping. Then, in this case, $y(t; x_0, \xi_0)$ does not necessarily approach to a free motion. However, it is known that

$$\xi_+(x_0, \xi_0) := \lim_{t \to +\infty} \eta(t; x_0, \xi_0)$$

exists. In this case, we can prove the following extension of Corollary 2:

Theorem 4 ([6]). *Suppose Assumption A with $\mu > 0$, and suppose $(x_0, \xi_0) \in \mathbb{R}^{2d}$ is forward nontrapping. Let $t_0 > 0$. If $(t_0\xi_+, \xi_+) \notin HWF(u(t_0))$, then $(x_0, \xi_0) \notin WF(u_0)$. In other words, if $(x_0, \xi_0) \in WF(u_0)$, then $(t_0\xi_+, \xi_+) \in HWF(u(t_0))$.*

It seems this result is closely related to the result of Wunsch [8], though the formulation is quite different, and the assumption also differs considerably.

Naturally, we can obtain the microlocal smoothing property of [1] as a corollary of Theorem 4:

Corollary 5. *Suppose (x_0, ξ_0) is forward nontrapping. If $u(t)$ decays rapidly in a conic neighborhood of $\xi_+(x_0, \xi_0)$ for some $t > 0$, then $(x_0, \xi_0) \notin WF(u_0)$.*

The idea of Proof

At first we discuss the idea of Theorem 1. The basic idea is to use an Egorov-type theorem, i.e., the construction of asymptotic solutions to the Heisenberg equation. We consider the Heisenberg equation generated by H:

$$\frac{d}{dt}F(t) = -i[H, F(t)]$$

for an operator-valued function $F(t)$ with the initial condition:

$$F(0) = f_0^W(x, hD_x) \quad \text{with} \quad f_0 \in C_0^\infty(\mathbb{R}^{2d}), \quad f_0(x_0, \xi_0) > 0,$$

where $h > 0$ is a semiclassical parameter. The exact solution to this equation is $F(t) = e^{-itH} f_0^W(x, hD_x) e^{itH}$, and we try to compute the symbol of $F(t)$. At least formally, the principal symbol of $F(t)$ should be

$$\varphi_0(t; x, \xi) = f_0(T_{h^{-1}t}^{-1}(x, h\xi))$$

where

$$T_t : (x, \xi) \mapsto (y(t; x, \xi), \eta(t; x, \xi))$$

is the geodesic flow generated by $p(x, \xi) = \frac{1}{2} \sum a_{ij}(x) \xi_i \xi_j$. However, we observe that $\varphi_0(t; x, \xi)$ is not in a reasonable semiclassical symbol class, even for the case of free Hamiltonian. Instead of $F(t)$, we consider an operator conjugated by the free evolution:

$$G(t) = e^{itH_0} F(t) e^{-itH_0}.$$

Then $G(t)$ satisfies a time-dependent Heisenberg equation:

$$\frac{d}{dt} G(t) = -i[L(t), G(t)],$$

where

$$\begin{aligned} L(t) &= e^{itH_0}(H - H_0)e^{-itH_0} \\ &= \frac{1}{2} \sum_{j,k=1}^{d} D_j \big(a_{jk}^W(x + tD_x) - \delta_{jk}\big) D_k + V^W(x + tD_x). \end{aligned}$$

If we can compute the principal symbol of $G(t)$ (as a semiclassical pseudodifferential operator), and we have

$$\psi(t; x, \xi) \sim f_0(T_{h^{-1}t}^{-1}(x + th\xi, h\xi)), \quad \text{where} \quad G(t) = \psi^W(t; x, D_x).$$

We note $T_{h^{-1}t}^{-1}(x + t\xi', \xi')$ converges to $S^{-1}(x, \xi')$ as $h \to 0$ provided $t > 0$, where $S : (x, \xi) \mapsto (x_+, \xi_+)$ is the classical wave operator. Thus the principal symbol of $G(t)$ converges to a (semiclassical) symbol as $h \to 0$. In fact, by asymptotic expansion, we can prove that the total symbol of the asymptotic solution of the equation converges as $h \to 0$, and we obtain an asymptotic solution $G(t) \in OPS_{1,0}^1$. Namely, we have

$$\left\| G(t) - e^{-itH_0} e^{itH} F(0) e^{-itH} e^{-itH_0} \right\| = O(h^\infty)$$

and the principal symbol of $G(t)$ is $f_0(S^{-1}(x, h\xi))$. Now we can prove Theorem 1 using this and the characterization of the wave front set in terms of semiclassical pseudodifferential operators (cf. [2], [5]).

Now we tern to the proof of Theorem 4. We again consider the Heisenberg equation, but here we solve Heisenberg *inequality*:

$$\frac{d}{dt}F(t) \geq -i[H, F(t)]$$

up to small error as $h \longrightarrow 0$, with initial condition:

$$F(0) = f_0^W(x, hD_x) \quad \text{with} \quad f_0 \in C_0^\infty(\mathbb{R}^{2d}), f_0(x_0, \xi_0) > 0.$$

This idea is a variation of positive commutator methods used extensively by Doi, and goes back (at least) to the proof of propagation of singularity theorem by Hörmander.

Let $\psi(t; x, \xi)$ be the symbol of $F(t)$ and let ψ_0 be its principal symbol. Then ψ_0 should satisfy

$$\frac{D}{Dt}\psi_0(t; x, \xi) := \frac{\partial \psi_0}{\partial t} + \{p, \psi_0\} \geq 0,$$

where $\{\cdot, \cdot\}$ is the Poisson bracket. Let $\Psi(r) \in C^\infty(\mathbb{R})$ such that $0 \leq \Psi(r) \leq 1$, $\Psi(r) = 1$ if $r \leq 1/2$, and $\psi(r) = 0$ if $r \geq 1$. With suitably chosen constants $\delta_1, \delta_2 > 0, C_1$, we set

$$\psi_0(t; x, \xi) = \Psi\left(\frac{|x - y(t)|}{\delta_1 t}\right) \Psi\left(\frac{|\xi - \eta(t)|}{\delta_2 - C_1 t^{-\mu}}\right)$$

for $t >> 0$. Here we denote $y(t) = y(t; x_0, \xi_0)$, $\eta(t) = \eta(t; x_0, \xi_0)$. By direct computation, we can show $\frac{D}{Dt}\psi_0 \geq 0$ for sufficiently large $t \geq T_0$. Then we solve the equation $\frac{D}{Dt}\psi_0(t; x, \xi) = 0$ for $0 \leq t \leq T_0$ with the boundary conditon at $t = T_0$.

Next we construct an asymptotic solution to the operator inequality by iterating similar procedure. Then the inequality implies

$$\frac{d}{dt}\langle u(t), F(t)u(t)\rangle \geq -O(h^\infty)$$

as $h \longrightarrow 0$, and Theorem 4 follows by usnig the standard procedure as well as Theorem 1.

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