

Propagation of Singularities for Schrödinger Equations with Modestly Long Range Type Potentials

by

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Abstract

In a previous paper by the second author [11], we discussed a characterization of the microlocal singularities for solutions to Schrödinger equations with long range type perturbations, using solutions to a Hamilton–Jacobi equation. In this paper we show that we may use Dollard type approximate solutions to the Hamilton–Jacobi equation if the perturbation satisfies somewhat stronger conditions. As applications, we describe the propagation of microlocal singularities for $e^{itH_0}e^{-itH}$ when the potential is asymptotically homogeneous as $|x| \rightarrow \infty$, where H is our Schrödinger operator, and H_0 is the free Schrödinger operator, i.e., $H_0 = -\frac{1}{2}\Delta$. We show $e^{itH_0}e^{-itH}$ shifts the wave front set if the potential V is asymptotically homogeneous of order 1, whereas $e^{itH}e^{-itH_0}$ is smoothing if V is asymptotically homogeneous of order $\beta \in (1, 3/2)$.

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§1. Introduction

We consider a Schrödinger operator with variable coefficients on \mathbb{R}^d , $d \geq 1$:

$$H = -\frac{1}{2} \sum_{m,n=1}^d \frac{\partial}{\partial x_m} a_{mn}(x) \frac{\partial}{\partial x_n} + V(x) \quad \text{on } L^2(\mathbb{R}^d).$$

We assume that the coefficients satisfy long range type conditions in the following sense:

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Assumption A. $a_{mn}, V \in C^\infty(\mathbb{R}^d; \mathbb{R})$ and $\mu > 0$. For any multi-index $\alpha \in \mathbb{Z}_+^d$, there is $C_\alpha > 0$ such that

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

for $x \in \mathbb{R}^d$, where $\partial_x = \partial/\partial x$ and $\langle x \rangle = (1 + |x|^2)^{1/2}$. Moreover $(a_{mn}(x))_{m,n=1}^d$ is a positive symmetric matrix for each $x \in \mathbb{R}^d$.

Then it is well-known that H is a self-adjoint operator with domain $H^2(\mathbb{R}^d)$, the Sobolev space of order 2. We consider solutions to the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(t) = H\psi(t), \quad \psi(0) = \psi_0 \in L^2(\mathbb{R}^d).$$

By the Stone theorem, the solution is given by $\psi(t) = e^{-itH}\psi_0 \in L^2(\mathbb{R}^d)$. It is also well-known that the singularities of the solution propagate with infinite speed, and hence the *propagation of singularities theorem* analogous to the one for solutions to the wave equation cannot hold. In [11], it is proved that the wave front set of $e^{-itH}\psi_0$ can be described in terms of the wave front set of $e^{-i\Phi(t, D_x)}\psi_0$, where $\Phi(t, \xi)$ is a solution to the Hamilton–Jacobi equation

$$\frac{\partial \Phi}{\partial t}(t, \xi) = p\left(\frac{\partial \Phi}{\partial \xi}(t, \xi), \xi\right), \quad t \in \mathbb{R}, \xi \in \mathbb{R}^d,$$

and

$$p(x, \xi) = \frac{1}{2} \sum_{m,n=1}^d a_{mn}(x) \xi_m \xi_n + V(x), \quad x, \xi \in \mathbb{R}^d,$$

is the symbol of the Schrödinger operator H .

The purpose of this paper is to show that if $\mu > 1/2$, we may employ a Dollard type approximate solution, or a modifier,

$$\Phi_D(t, \xi) = \int_0^t p(s\xi, \xi) ds,$$

to characterize the microlocal singularities of the solution. One advantage of using the Dollard type modifier is that it is easy to compute, and hence we can describe the propagation explicitly for several cases. In particular, if $V(x)$ is asymptotically homogeneous of order $\beta \in [1, 3/2)$, we give an explicit characterization of the wave front set of $e^{-itH}\psi_0$ in terms of $e^{-i\Phi_D(t, D_x)}\psi_0$.

Now we state our main result. Let $\exp(tH_k)$ be the Hamilton flow generated by $k(x, \xi) = \frac{1}{2} \sum_{m,n=1}^d a_{mn}(x) \xi_m \xi_n$, i.e.,

$$(x(t), \xi(t)) = \exp(tH_k)(x_0, \xi_0)$$

if $(x(t), \xi(t))$ is the solution to the Hamilton equation

$$x'(t) = \frac{\partial k}{\partial \xi}(x(t), \xi(t)), \quad \xi'(t) = -\frac{\partial k}{\partial x}(x(t), \xi(t)), \quad x(0) = x_0, \quad \xi(0) = \xi_0.$$

Under Assumption A, it is well-known that $\exp(tH_k)$ is a diffeomorphism in \mathbb{R}^d for any $t \in \mathbb{R}$. We assume all the trajectories are *nontrapping* in the following sense:

Assumption B. Let $(x(t), \xi(t)) = \exp(tH_k)(x_0, \xi_0)$ with $\xi_0 \neq 0$. Then $|x(t)| \rightarrow \infty$ as $t \rightarrow \pm\infty$.

Remark 1. We may assume this nontrapping condition only for (x_0, ξ_0) we are looking at, but we assume the global nontrapping condition to simplify the notation.

As mentioned above, we suppose Assumption A holds with $\mu > 1/2$. For later applications, it is convenient to suppose V is decomposed into a *long range part* and a *short range part*.

Assumption C. $a_{mn}(x)$ and $V(x)$ satisfy Assumption A with $\mu > 1/2$. Moreover, $V(x) = V^{(L)}(x) + V^{(S)}(x)$, where $V^{(L)}$ satisfies Assumption A with $\mu > 1/2$, and $V^{(S)}$ satisfies

$$|\partial_x^\alpha V^{(S)}(x)| \leq C_\alpha \langle x \rangle^{2-\nu-|\alpha|}, \quad x \in \mathbb{R}^d,$$

with $\nu > 1$ and $C_\alpha > 0$.

Under these conditions, we can show the existence of the classical (long range) scattering. We set

$$(1.1) \quad p^{(L)}(x, \xi) = k(x, \xi) + V^{(L)}(x),$$

$$(1.2) \quad \Phi(t, \xi) = \int_0^t p^{(L)}(s\xi, \xi) ds, \quad \Psi(t, \xi) = \int_0^t k(s\xi, \xi) ds.$$

Proposition 1. Let $(x_0, \xi_0) \in \mathbb{R}^d \times (\mathbb{R}^d \setminus \{0\})$, and define $(x(t), \xi(t)) = \exp(tH_k)(x_0, \xi_0)$. Then

$$x_\pm = \lim_{t \rightarrow \pm\infty} (x(t) - \nabla_\xi \Psi(t, \xi)), \quad \xi_\pm = \lim_{t \rightarrow \pm\infty} \xi(t)$$

exist. If we write

$$W_\pm^{\text{cl}} : (x_\pm, \xi_\pm) \mapsto (x_0, \xi_0),$$

then W_\pm^{cl} are diffeomorphisms in $\mathbb{R}^d \times (\mathbb{R}^d \setminus \{0\})$.

We prove Proposition 1 in Section 2.

The next theorem is our main result. We denote the wave front set of $u \in \mathcal{S}'(\mathbb{R}^d)$ by $\text{WF}(u)$. We write $D_x = -i\partial/\partial x$, and $F(D_x)$ denotes the Fourier multiplier with symbol $F(\xi)$.

Theorem 2. *Suppose Assumptions B and C hold. Then for any $u \in L^2(\mathbb{R}^d)$,*

$$\text{WF}(e^{i\Phi(t, D_x)} e^{-itH} u) = (W_{\pm}^{\text{cl}})^{-1}(\text{WF}(u)) \quad \text{for } \pm t > 0.$$

By replacing u by $e^{itH} u$, we obtain the following corollary:

Corollary 3. *Under the same assumptions as in Theorem 2,*

$$\text{WF}(e^{-itH} u) = W_{\mp}^{\text{cl}}(\text{WF}(e^{-i\Phi(t, D_x)} u)) \quad \text{for } \pm t > 0.$$

In other words, $(x_0, \xi_0) \in \text{WF}(e^{-itH} u)$ if and only if $(x_{\mp}, \xi_{\mp}) \in \text{WF}(e^{-i\Phi(t, D_x)} u)$ when $\pm t > 0$.

In the remainder of this Introduction, we consider the case where $V(x)$ is asymptotically homogeneous as $|x| \rightarrow \infty$. Here we suppose $a_{mn}(x) = \delta_{mn}$ for the sake of simplicity, though this is not really necessary. In this case, $\Psi(t, \xi) = \frac{t}{2} |\xi|^2$, Assumption B is satisfied, and the classical wave map W_{\pm}^{cl} is the identity map: $(x_{\pm}, \xi_{\pm}) = (x, \xi)$.

We first suppose $V(x)$ is homogeneous of order 1, i.e.,

$$(1.3) \quad V^{(L)}(x) = |x|V^{(L)}(\hat{x}) \quad \text{if } |x| \geq 1,$$

where $\hat{x} = x/|x| \in S^{d-1}$. This condition implies $\partial_x V^{(L)}(x) = \partial_x V^{(L)}(\hat{x})$ if $|x| \geq 1$, i.e., $\partial_x V^{(L)}(x)$ depends only on the direction \hat{x} of x . We set

$$S_{\sigma}^{\pm}(x, \xi) = (x \mp \sigma \partial_x V^{(L)}(\pm \hat{\xi}), \xi), \quad \sigma \in \mathbb{R}, x, \xi \in \mathbb{R}^d, \xi \neq 0.$$

Then S_{σ}^{\pm} is the Hamilton flow generated by $V^{(L)}(\pm \xi)$: $S_{\sigma}^{\pm} = \exp(\pm \sigma H_{V^{(L)}(\pm \xi)})$, if $|\xi| \geq 1$.

Theorem 4. *Suppose Assumption C holds, $a_{ij}(x) = \delta_{ij}$, (1.3) holds, and let $u \in L^2(\mathbb{R}^d)$. Then*

$$\text{WF}(e^{itH_0} e^{-itH} u) = S_{(-t^2/2)}^{\pm}(\text{WF}(u)), \quad \pm t > 0,$$

and hence

$$\text{WF}(e^{-itH} u) = S_{t^2/2}^{\pm}(\text{WF}(e^{-itH_0} u)).$$

Theorem 4 implies that the wave front set of the solution shifts according to the Hamilton flow generated by $V^{(L)}(\xi)$ if the metric is flat and the potential is asymptotically homogeneous of order 1.

We now turn to the case when $V(x)$ is asymptotically homogeneous of order $\beta \in (1, 3/2)$. In this case, the behavior of the singularities is quite different. Since the quantization of $\exp(\sigma H_V(\xi))$, $e^{-i\sigma V(D_x)}$, has diffusive properties similar to the free Schrödinger evolution group, we expect the vanishing of the singularities for $e^{itH_0} e^{-itH} u$ if u decays rapidly as $|x| \rightarrow \infty$. In fact, we can prove the following:

Theorem 5. *Suppose Assumptions B, C hold and*

$$V^{(L)}(x) = |x|^\beta V^{(L)}(\hat{x}) \quad \text{for } |x| \geq 1,$$

with $\beta \in (1, 3/2)$. Suppose moreover that $\nabla V^{(L)}(\hat{x}) \neq 0$ for $\hat{x} \in S^{d-1}$. If $e^{-itH_0}u \in L^{2,\infty}(\mathbb{R}^d) := \{f \in L^2(\mathbb{R}^d) \mid \langle x \rangle^m f(x) \in L^2(\mathbb{R}^d) \text{ for any } m\}$, then $e^{-itH}u \in C^\infty(\mathbb{R}^d)$ whenever $t \neq 0$.

Thus we observe that the propagation of singularities for e^{-itH} depends drastically on the growth rate of the potential at infinity.

Singularities of solutions to Schrödinger equations have been studied by many mathematicians, mostly the smoothing properties, with a view to applications to nonlinear problems. An explicit characterization of the wave front set of solutions was obtained relatively recently by Hassel and Wunsch [2], Nakamura [10], [11], Ito and Nakamura [4] and Martinez, Nakamura and Sordani [8], [9] under different conditions. We note that closely related results had been obtained for perturbed harmonic oscillators (with constant principal part; see Ōkaji [12], Doi [1] and the references therein), which case does not require the scattering-theoretical framework (see also Mao and Nakamura [6] for nonconstant principal part cases).

We call a Schrödinger operator satisfying Assumption A with $\mu > 1$ of *short range type*, though the potential $V(x)$ may be unbounded as $|x| \rightarrow \infty$, and not necessarily short range in the sense of scattering theory. The previous works cited above concern short range cases, except [11], [9]. We call a Schrödinger operator satisfying Assumption A with $\mu \in (0, 1]$ of *long range type*. In order to describe the microlocal singularities of solutions, we need to employ the framework of long range scattering theory (for the classical flow). In [11], a solution to the Hamilton–Jacobi equation at high energy is constructed for that purpose, but the construction is rather long and not easily computed. In this paper we use a simpler Dollard type modifier (see, e.g., [13, Section XI.9]) to characterize the microlocal singularities, and we hope this construction clarifies the analysis of [11].

The result for the asymptotically homogeneous case, Theorem 4, is closely related to the work of Doi [1], and Theorem 4 may be considered as a direct analogue of his result in our setting.

We also remark that we can actually prove that $e^{i\Phi(t, D_x)}e^{-itH}$ is a Fourier integral operator (in a slightly generalized sense) using the method of Ito and Nakamura [5], which we do not discuss in this paper.

The paper is organized as follows: We discuss the scattering theory for the classical mechanical flow in Section 2. We prove Theorem 2 in Section 3, mostly following the argument of [11]. We prove properties of our main examples, i.e., Theorems 4 and 5, in Section 4.

Throughout this paper, we use the following notation: We mainly work in $L^2(\mathbb{R}^d)$, and $\|\cdot\|$ denotes the L^2 -norm unless otherwise specified. We write $\langle x \rangle = (1 + |x|^2)^{1/2}$, which is standard in microlocal analysis. $\mathbb{Z}_+ = \{0, 1, 2, \dots\}$ denotes the set of nonnegative integers, and \mathbb{Z}_+^d is the set of multi-indices. For $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{Z}_+^d$, we denote $|\alpha| = \sum_j \alpha_j$. $S_{1,0}^m$ denotes the standard pseudodifferential operator symbol class, i.e., $a \in S_{1,0}^m$ means $a \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that for any $\alpha, \beta \in \mathbb{Z}_+^d$ and $K \Subset \mathbb{R}^d$,

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leq C_{\alpha\beta} \langle \xi \rangle^{m-|\beta|}, \quad x \in K, \xi \in \mathbb{R}^d$$

with some $C_{\alpha\beta} > 0$. $\mathcal{S}(\mathbb{R}^d)$ denotes the set of Schwartz functions. We denote various constants by C , which may change from line to line.

§2. Classical mechanics and high energy asymptotics

Here we consider the existence of the scattering theory and the high energy asymptotics for the classical mechanical flow. We denote

$$\begin{aligned} (x(t; x_0, \xi_0), \xi(t; x_0, \xi_0)) &= \exp(tH_p)(x_0, \xi_0), \\ (y(t; x_0, \xi_0), \eta(t; x_0, \xi_0)) &= \exp(tH_k)(x_0, \xi_0). \end{aligned}$$

We first prove Proposition 1. In the following, we always suppose Assumptions A, B hold with $1/2 < \mu < 1$ without loss of generality.

Proof of Proposition 1. We fix $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, $\xi_0 \neq 0$. It is well-known that

$$(2.1) \quad |y(t; x_0, \xi_0)| \geq c|t| - C, \quad t \in \mathbb{R},$$

with some $c, C > 0$ if (x_0, ξ_0) is nontrapping (see, e.g., [10, Lemma 2], [11, Proposition 2.1]). By the Hamilton equation, we have

$$(2.2) \quad \begin{aligned} \left| \frac{d}{dt} \eta_j(t; x, x_0) \right| &= \left| \frac{1}{2} \sum_{m,n=1}^d \frac{\partial a_{mn}}{\partial x_j}(y(t)) \eta_m(t) \eta_n(t) \right| \\ &\leq C \langle t \rangle^{-1-\mu}, \quad t \in \mathbb{R}. \end{aligned}$$

Here we have used the fact that $|\eta(t)|$ is bounded uniformly in t by energy conservation: $k(x(t), \xi(t)) = k(x_0, \xi_0)$. This implies the existence of

$$\xi_\pm = \lim_{t \rightarrow \pm\infty} \eta(t; x_0, \xi_0) = \xi_0 + \int_0^{\pm\infty} \frac{d\eta}{dt}(t; x_0, \xi_0) dt.$$

Moreover, (2.2) also implies

$$(2.3) \quad |\eta(t) - \xi_\pm| = \left| \int_t^{\pm\infty} \frac{d\eta}{dt}(t; x_0, \xi_0) dt \right| \leq C \langle t \rangle^{-\mu}, \quad \pm t > 0.$$

Similarly, we have

$$\begin{aligned} \left| \frac{d}{dt}(y_j(t) - t\eta_j(t)) \right| &= \left| \sum_m (a_{jm}(y(t)) - \delta_{jm})\eta_m(t) + \frac{t}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(y(t))\eta_m(t)\eta_n(t) \right| \\ &\leq C\langle t \rangle^{-\mu}, \quad t \in \mathbb{R}, \end{aligned}$$

and hence

$$(2.4) \quad |y(t) - t\eta(t)| \leq C\langle t \rangle^{1-\mu}, \quad t \in \mathbb{R}.$$

We compute $\frac{d}{dt}(y(t) - \partial_\xi \Psi(t, \eta(t)))$ as follows. We have

$$\begin{aligned} \frac{\partial \Psi}{\partial \xi_j}(t, \xi) &= \int_0^t \left(s \frac{\partial k}{\partial x_j}(s\xi, \xi) + \frac{\partial k}{\partial \xi_j}(s\xi, \xi) \right) ds \\ &= \int_0^t \left(\frac{s}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(s\xi)\xi_m\xi_n + \sum_m a_{jm}(s\xi)\xi_m \right) ds, \end{aligned}$$

and so

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial \Psi}{\partial \xi_j}(t, \eta(t)) \right) &= \frac{t}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(t\eta)\eta_m\eta_n + \sum_m a_{jm}(t\eta)\eta_m \\ &\quad + \sum_i \int_0^t \left(\frac{s^2}{2} \sum_{m,n} \frac{\partial^2 a_{mn}}{\partial x_j \partial x_i}(s\eta)\eta_m\eta_n + s \sum_m \frac{\partial a_{mi}}{\partial x_j}(s\eta)\eta_m \right. \\ &\quad \left. + s \sum_m \frac{\partial a_{jm}}{\partial x_i}(s\eta)\eta_m + a_{ji}(s\eta) \right) ds \times \frac{d\eta_i}{dt}. \end{aligned}$$

We remark that the η in the integrand is $\eta(t)$, not $\eta(s)$. We also note that the last term can be rewritten as

$$\begin{aligned} \sum_i \int_0^t a_{ji}(s\eta(t)) \frac{d\eta_i}{dt}(t) ds &= t \frac{d\eta_j}{dt}(t) + \sum_i \int_0^t (a_{ji}(s\eta) - \delta_{ji}) ds \times \frac{d\eta_i}{dt}(t) \\ &= -\frac{t}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(y(t))\eta_m(t)\eta_n(t) + O(\langle t \rangle^{-2\mu}) \end{aligned}$$

by using (2.2). Combining these with Assumption A, we have

$$\begin{aligned} \frac{d}{dt} \left(y_j(t) - \frac{\partial \Psi}{\partial \xi_j}(t, \eta(t)) \right) &= -\frac{t}{2} \sum_{m,n} \left(\frac{\partial a_{mn}}{\partial x_j}(y(t)) - \frac{\partial a_{mn}}{\partial x_j}(t\eta(t)) \right) \eta_m(t)\eta_n(t) \\ &\quad + \sum_m (a_{jm}(y(t)) - a_{jm}(t\eta(t)))\eta_m(t) + O(\langle t \rangle^{-2\mu}). \end{aligned}$$

Using Assumption A again with (2.4), we obtain

$$\left| \frac{d}{dt} \left(y(t) - \frac{\partial \Psi}{\partial \xi}(t, \eta(t)) \right) \right| \leq C\langle t \rangle^{-2\mu}, \quad t \in \mathbb{R}.$$

Since $2\mu > 1$, this implies the existence of

$$x_{\pm} = \lim_{t \rightarrow \pm\infty} \left(y(t) - \frac{\partial \Psi}{\partial \xi}(t, \eta(t)) \right).$$

The assertion that W_{\pm}^{cl} is a diffeomorphism can be proved by standard ODE methods, once we have integrability. \square

In the proof of Theorem 2, we actually consider the high energy asymptotics of $(x(t), \xi(t))$ for fixed t . If $V = 0$, i.e., for $(y(t), \eta(t))$, we have the scaling property

$$(y(t; x_0, \lambda \xi_0), \eta(t; x_0, \lambda \xi_0)) = (y(\lambda t; x_0, \xi_0), \lambda \eta(\lambda t; x_0, \xi_0))$$

for any $\lambda > 0$. Hence we deduce that

$$\lim_{\lambda \rightarrow \infty} \frac{1}{\lambda} \eta(t; x_0, \lambda \xi_0) = \lim_{\lambda \rightarrow \infty} \eta(\lambda t; x_0, \xi_0) = \xi_{\pm}$$

if $\pm t > 0$. Since

$$\Psi(t, \lambda \xi) = \int_0^t k(s\lambda \xi, \lambda \xi) ds = \int_0^{\lambda t} \lambda^2 k(\sigma \xi, \xi) \frac{d\sigma}{\lambda} = \lambda \Psi(\lambda t, \xi),$$

we have

$$\frac{\partial \Psi}{\partial \xi}(t, \lambda \xi) = \frac{\partial \Psi}{\partial \xi}(\lambda t, \xi).$$

Using this, we also infer that

$$\begin{aligned} \lim_{\lambda \rightarrow \infty} \left(y(t; x_0, \lambda \xi_0) - \frac{\partial \Psi}{\partial \xi}(t, \eta(t; x_0, \lambda \xi_0)) \right) \\ = \lim_{\lambda \rightarrow \infty} \left(y(\lambda t; x_0, \xi_0) - \frac{\partial \Psi}{\partial \xi}(\lambda t, \eta(t; x_0, \xi_0)) \right) = x_{\pm} \end{aligned}$$

if $\pm t > 0$. We have similar high energy asymptotics for $(x(t; x_0, \lambda \xi_0), \xi(t; x_0, \lambda \xi_0))$ if we replace $\Psi(t, \xi)$ by $\Phi(t, \xi)$:

Theorem 6. *Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, $\xi_0 \neq 0$, and set $(x(t; x_0, \lambda \xi_0), \xi(t; x_0, \lambda \xi_0)) = \exp(tH_p)(x_0, \lambda \xi_0)$ as above. Then*

$$\begin{aligned} x_{\pm} &= \lim_{\lambda \rightarrow \infty} \left(x(t; x_0, \lambda \xi_0) - \frac{\partial \Phi}{\partial \xi}(t, \eta(t; x_0, \lambda \xi_0)) \right), \\ \xi_{\pm} &= \lim_{\lambda \rightarrow \infty} \frac{1}{\lambda} \xi(t; x_0, \lambda \xi_0) \end{aligned}$$

if $\pm t > 0$, where $(x_0, \xi_0) = W_{\pm}^{cl}(x_{\pm}, \xi_{\pm})$. The convergence is locally uniform with all derivatives.

Proof. The proof is similar to that of Proposition 1, but slightly more involved. We fix $T > 0$ and consider $(x(t; x_0, \lambda\xi_0), \xi(t; x_0, \lambda\xi_0))$ with $|t| \leq T$.

For $\lambda > 0$, we set

$$x^\lambda(t; x_0, \xi_0) = x\left(\frac{t}{\lambda}; x_0, \lambda\xi_0\right), \quad \xi^\lambda(t; x_0, \xi_0) = \frac{1}{\lambda}\xi\left(\frac{t}{\lambda}; x_0, \lambda\xi_0\right).$$

Then it is easy to check

$$(x^\lambda(t; x_0, \xi_0), \xi^\lambda(t; x_0, \xi_0)) = \exp(tH_{p^\lambda})(x_0, \xi_0),$$

where

$$p^\lambda(x, \xi) = \frac{1}{\lambda^2}p(x, \lambda\xi) = \frac{1}{2} \sum_{m,n=1}^d a_{mn}(x)\xi_m\xi_n + \frac{1}{\lambda^2}V(x).$$

We can show, just like (2.1),

$$(2.5) \quad |x^\lambda(t; x_0, \xi_0)| \geq c|t| - C, \quad |t| \leq \lambda T,$$

uniformly for $\lambda \geq \lambda_0 \gg 0$ [11, Proposition 2.6]. The constants in the following proof are independent of such large $\lambda \geq \lambda_0 \gg 0$. The proof of (2.5) relies on the idea that $\lambda^{-2}V(x)$ has significantly smaller effect than the kinetic energy part $k(x, \xi)$ if λ is sufficiently large. We refer to [11] for the complete proof.

Then, just like (2.2), we have

$$\begin{aligned} \left| \frac{d}{dt} \xi_j^\lambda(t) \right| &= \left| \frac{1}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(x^\lambda) \xi_m^\lambda \xi_n^\lambda + \frac{1}{\lambda^2} \frac{\partial V}{\partial x_j}(x^\lambda) \right| \\ &\leq C\langle t \rangle^{-1-\mu} + C\lambda^{-2}\langle t \rangle^{1-\mu} \leq C\langle t \rangle^{-1-\mu} \end{aligned}$$

if $|t| \leq \lambda T$. On the other hand, by the continuity of solutions to linear ODEs with respect to coefficients, we obtain

$$\exp(tH_{p^\lambda})(x_0, \xi_0) \rightarrow \exp(tH_k)(x_0, \xi_0) \quad \text{as } \lambda \rightarrow \infty$$

for each fixed $t \in \mathbb{R}$. The convergence also holds for derivatives. Then we can apply the dominated convergence theorem to show

$$\xi^\lambda(\lambda t) = \xi_0 + \int_0^{\lambda t} \frac{d\xi^\lambda}{dt}(s) ds \rightarrow \xi_0 + \int_0^{\pm\infty} \frac{d\eta}{dt}(s) ds = \xi_\pm$$

as $\lambda \rightarrow \infty$, where $0 < \pm t \leq T$. This proves the second statement of the theorem.

We also have (just like (2.3)),

$$|\xi^\lambda(t) - \xi_\pm| \leq C\langle t \rangle^{-\mu}, \quad 0 < \pm t \leq \lambda T.$$

Then we compute

$$\begin{aligned} & \left| \frac{d}{dt} \left(x_j^\lambda(t) - t\xi_j^\lambda(t) \right) \right| \\ &= \left| \sum_m (a_{jm}(x^\lambda) - \delta_{jm})\xi_m^\lambda + \frac{t}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(x^\lambda)\xi_m^\lambda\xi_n^\lambda + \frac{t}{\lambda^2} \frac{\partial V}{\partial x_j}(x^\lambda) \right| \\ &\leq C\langle t \rangle^{-\mu} + C\lambda^{-2}\langle t \rangle^{2-\mu} \\ &\leq \langle t \rangle^{-\mu} \quad \text{if } |t| \leq \lambda T, \end{aligned}$$

and hence

$$(2.6) \quad |x^\lambda(t) - t\xi^\lambda(t)| \leq C\langle t \rangle^{1-\mu}, \quad |t| \leq \lambda T.$$

We set

$$\Phi^\lambda(t, \xi) = \int_0^t \left(k(s\xi, \xi) + \frac{1}{\lambda^2} V^{(L)}(s\xi) \right) ds$$

so that

$$\frac{\partial \Phi^\lambda}{\partial \xi}(\lambda t, \xi) = \frac{\partial \Phi}{\partial \xi}(t, \lambda \xi).$$

Then we have

$$\frac{\partial \Phi^\lambda}{\partial \xi_j}(t, \xi) = \int_0^t \left(\frac{s}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(s\xi)\xi_m\xi_n + \frac{s}{\lambda^2} \frac{\partial V^{(L)}}{\partial x_j}(s\xi) + \sum_m a_{jm}(s\xi)\xi_m \right) ds,$$

and so

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial \Phi^\lambda}{\partial \xi_j}(t, \xi^\lambda(t)) \right) &= \frac{t}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(t\xi^\lambda)\xi_m^\lambda\xi_n^\lambda + \frac{t}{\lambda^2} \frac{\partial V^{(L)}}{\partial x_j}(t\xi^\lambda) + \sum_m a_{jm}(t\xi^\lambda)\xi_m^\lambda \\ &\quad + \sum_i \int_0^t \left(\frac{s^2}{2} \sum_{m,n} \frac{\partial^2 a_{mn}}{\partial x_i \partial x_j}(s\xi^\lambda)\xi_m^\lambda\xi_n^\lambda + s \sum_m \frac{\partial a_{mi}}{\partial x_j}(s\xi^\lambda)\xi_m^\lambda \right. \\ &\quad \left. + \frac{s^2}{\lambda^2} \frac{\partial^2 V^{(L)}}{\partial x_i \partial x_j}(s\xi^\lambda) + s \sum_m \frac{\partial a_{jm}}{\partial x_i}(s\xi^\lambda)\xi_m^\lambda + a_{ji}(s\xi^\lambda) \right) ds \times \frac{d\xi_i^\lambda}{dt}. \end{aligned}$$

We recall

$$\begin{aligned} \frac{dx_j^\lambda}{dt}(t) &= \sum_m a_{jm}(x^\lambda(t))\xi_m^\lambda(t), \\ \frac{d\xi_j^\lambda}{dt}(t) &= -\frac{1}{2} \sum_{m,n} \frac{\partial a_{mn}}{\partial x_j}(x^\lambda(t))\xi_m^\lambda(t)\xi_n^\lambda(t) - \frac{1}{\lambda^2} \frac{\partial V^{(L)}}{\partial x_j}(x^\lambda(t)) - \frac{1}{\lambda^2} \frac{\partial V^{(S)}}{\partial x_j}(x^\lambda(t)). \end{aligned}$$

Combining these, we obtain, as in the proof of Proposition 1,

$$\begin{aligned} & \frac{d}{dt} \left(x_j^\lambda(t) - \frac{\partial \Phi^\lambda}{\partial \xi_j}(t, \xi^\lambda(t)) \right) \\ &= -\frac{t}{2} \sum_{m,n} \left(\frac{\partial a_{mn}}{\partial x_j}(x^\lambda) - \frac{\partial a_{mn}}{\partial x_j}(t\xi^\lambda) \right) \xi_m^\lambda \xi_n^\lambda - \frac{t}{\lambda^2} \left(\frac{\partial V^{(L)}}{\partial x_j}(x^\lambda) - \frac{\partial V^{(L)}}{\partial x_j}(t\xi^\lambda) \right) \\ & \quad + \sum_m (a_{jm}(x^\lambda) - a_{jm}(t\xi^\lambda)) \xi_m^\lambda + O(\langle t \rangle^{-2\mu} + \lambda^{-2} \langle t \rangle^{2-2\mu} + \lambda^{-2} \langle t \rangle^{2-\nu}). \end{aligned}$$

We recall (2.6), and using Assumption C, we have

$$\left| \frac{d}{dt} \left(x^\lambda(t) - \frac{\partial \Phi^\lambda}{\partial \xi}(t, \xi^\lambda(t)) \right) \right| \leq C \langle t \rangle^{-2\mu'}$$

if $|t| \leq \lambda T$, where $\mu' = \min(\mu, \nu/2) > 1/2$. Then, again observing

$$\frac{d}{dt} x^\lambda(t) \rightarrow \frac{d}{dt} y(t), \quad \frac{d}{dt} \left(\frac{\partial \Phi^\lambda}{\partial \xi}(t, \xi^\lambda(t)) \right) \rightarrow \frac{d}{dt} \left(\frac{\partial \Psi}{\partial \xi}(t, \eta(t)) \right)$$

as $\lambda \rightarrow \infty$ for each t , and using the dominated convergence theorem, we conclude that

$$x^\lambda(\lambda t) - \frac{\partial \Phi^\lambda}{\partial \xi}(\lambda t, \xi^\lambda(\lambda t)) \rightarrow x_\pm \quad \text{as } \lambda \rightarrow \infty,$$

if $0 < \pm t \leq T$. The first statement of the theorem follows immediately from this. The last claim can be proved using standard ODE methods. \square

Now we prepare several estimates for the next section.

Lemma 7. *Let $T > 0$. Then for any $\alpha \in \mathbb{Z}_+^d$ there is $C_\alpha > 0$ such that*

$$|\partial_\xi^\alpha (\Phi(t, \xi) - \frac{1}{2}t|\xi|^2)| \leq C_\alpha |t| \langle \xi \rangle^{2-\mu-|\alpha|}, \quad \xi \in \mathbb{R}^d, |t| \leq T.$$

In particular,

$$|\partial_\xi^\alpha (\partial_\xi \Phi(t, \xi) - t\xi)| \leq C_\alpha |t| \langle \xi \rangle^{1-\mu-|\alpha|}, \quad \xi \in \mathbb{R}^d, |t| \leq T.$$

Proof. We suppose $t \geq 0$. By the definition, we have

$$\Phi(t, \xi) - \frac{1}{2}t|\xi|^2 = \frac{1}{2} \int_0^t \sum_{m,n=1}^d (a_{mn}(s\xi) - \delta_{mn}) \xi_m \xi_n ds + \int_0^t V^{(L)}(s\xi) ds,$$

and hence

$$\begin{aligned}
 & \left| \partial_\xi^\alpha (\Phi(t, \xi) - \frac{1}{2}t|\xi|^2) \right| \\
 & \leq \frac{1}{2} \int_0^t \sum_{m,n} |\partial_\xi^\alpha \{ (a_{mn}(s\xi) - \delta_{mn}) \xi_m \xi_n \}| ds + \int_0^t |\partial_\xi^\alpha (V^{(L)}(s\xi))| ds \\
 & \leq C \sum_{j=0}^{|\alpha|} \int_0^t s^j \langle s\xi \rangle^{-\mu-j} |\xi|^{2-(|\alpha|-j)} ds + C \int_0^t s^{|\alpha|} \langle s\xi \rangle^{2-\mu-|\alpha|} ds \\
 & = C \sum_{j=0}^{|\alpha|} \int_0^{t|\xi|} \sigma^j \langle \sigma \rangle^{-\mu-j} |\xi|^{1-|\alpha|} d\sigma + C \int_0^{t|\xi|} \sigma^{|\alpha|} \langle \sigma \rangle^{2-\mu-|\alpha|} |\xi|^{-1-|\alpha|} d\sigma \\
 & \leq C \int_0^{t|\xi|} \langle \sigma \rangle^{-\mu} d\sigma \cdot |\xi|^{1-|\alpha|} + C \int_0^{t|\xi|} \langle \sigma \rangle^{2-\mu} d\sigma \cdot |\xi|^{-1-|\alpha|} \\
 & \leq C |t\xi| \langle t|\xi| \rangle^{-\mu} |\xi|^{1-|\alpha|} + C |t\xi| \langle t|\xi| \rangle^{2-\mu} |\xi|^{-1-|\alpha|} \\
 & \leq C |t| \langle \xi \rangle^{2-\mu-|\alpha|} \quad \text{if } |t| \leq T, |\xi| \geq 1.
 \end{aligned}$$

The case $t < 0$ is handled similarly. □

We then set

$$z(t; x_0, \xi_0) = x(t; x_0, \xi_0) - \partial_\xi \Phi(t; \xi(t; x_0, \xi_0)),$$

and consider the time evolution

$$t \mapsto (z(t; x_0, \xi_0), \xi(t; x_0, \xi_0)), \quad |t| \leq T.$$

We recall

$$x_\pm = \lim_{\lambda \rightarrow \infty} z(t; x_0, \lambda \xi_0) \quad \text{when } 0 < \pm t \leq T,$$

and in particular $\{z(t; x_0, \lambda \xi_0) \mid |t| \leq T, \lambda \geq \lambda_0\}$ is bounded in \mathbb{R}^d , provided λ_0 is sufficiently large. We set

$$\ell(t; z, \xi) = p(z + \partial_\xi \Phi(t, \xi), \xi) - \frac{\partial \Phi}{\partial t}(t, \xi).$$

Then we can show that $(z(t), \xi(t))$ is the Hamilton flow generated by the time-dependent Hamiltonian $\ell(t; z, \xi)$:

Lemma 8. $(z(t), \xi(t)) = (z(t; x_0, \xi_0), \xi(t; x_0, \xi_0))$ is the solution to

$$\frac{dz}{dt}(t) = \frac{\partial \ell}{\partial \xi}(t; z(t), \xi(t)), \quad \frac{d\xi}{dt} = -\frac{\partial \ell}{\partial z}(t; z(t), \xi(t)),$$

with the initial condition $z(0) = x_0, \xi(0) = \xi_0$.

Proof. The second equation and the initial conditions are easy to confirm. By the definitions, we have

$$\frac{\partial \ell}{\partial \xi_j}(t; z, \xi) = \frac{\partial p}{\partial \xi_j}(z + \partial_\xi \Phi, \xi) + \sum_{m=1}^d \frac{\partial^2 \Phi}{\partial \xi_j \partial \xi_m} \frac{\partial p}{\partial x_m}(z + \partial_\xi \Phi, \xi) - \frac{\partial^2 \Phi}{\partial \xi_j \partial t},$$

and

$$\frac{dz_j}{dt}(t) = \frac{dx_j}{dt} - \frac{\partial^2 \Phi}{\partial \xi_j \partial t} - \sum_{m=1}^d \frac{\partial^2 \Phi}{\partial \xi_j \partial \xi_m} \frac{d\xi_m}{dt}.$$

On the other hand, by the Hamilton equation for $(x(t), \xi(t))$, we have

$$\frac{dx_j}{dt} = \frac{\partial p}{\partial \xi_j}(z + \partial_\xi \Phi, \xi), \quad \frac{d\xi_m}{dt} = -\frac{\partial p}{\partial x_m}(z + \partial_\xi \Phi, \xi),$$

and we deduce the first equation of the lemma by combining them. □

By the definition, we easily see that

$$\frac{\partial \Phi}{\partial t}(t, \xi) = p^{(L)}(t\xi, \xi),$$

and hence we can write

$$\begin{aligned} \ell(t; z, \xi) &= p(z + \partial_\xi \Phi(t, \xi), \xi) - p^{(L)}(t\xi, \xi) \\ &= \frac{1}{2} \sum_{m,n=1}^d (a_{mn}(z + \partial_\xi \Phi(t, \xi)) - a_{mn}(t\xi)) \xi_m \xi_n \\ &\quad + (V^{(L)}(z + \partial_\xi \Phi(t, \xi)) - V^{(L)}(t\xi)) + V^{(S)}(z + \partial_\xi \Phi(t, \xi)). \end{aligned}$$

Combining this with Lemma 7, we obtain:

Lemma 9. *Let $K \subset \mathbb{R}^d$ be a bounded domain, and $\alpha, \beta \in \mathbb{Z}_+^d$. Then there is $C_{K\alpha\beta} > 0$ such that*

$$|\partial_z^\alpha \partial_\xi^\beta \ell(t; z, \xi)| \leq C_{K\alpha\beta} \langle \xi \rangle^{1-\gamma-|\beta|}, \quad z \in K, \xi \in \mathbb{R}^d, |t| \leq T,$$

where $\gamma = \min(2\mu - 1, \nu - 1) > 0$.

§3. Proof of the main theorem

The proof of Theorem 2 is analogous to the proof of [11, Theorem 1.2], given the estimates on the classical flow in Section 2. We sketch it for completeness, and give a somewhat formal proof.

For a symbol $a \in S_{1,0}^m$, we quantize it using the Weyl calculus [3, Section 18.5]:

$$a^W(x, D_x)u(x) = (2\pi)^{-d} \iint e^{i(x-y)\cdot\xi} a\left(\frac{x+y}{2}, \xi\right) u(y) dy d\xi, \quad u \in \mathcal{S}(\mathbb{R}^d).$$

By direct computations, it is easy to see that

$$\begin{aligned} p^W(x, D_x) &= -\frac{1}{8} \sum_{m,n} \left(\frac{\partial^2}{\partial x_m \partial x_n} a_{mn}(x) + 2 \frac{\partial}{\partial x_m} a_{mn}(x) \frac{\partial}{\partial x_n} + a_{mn}(x) \frac{\partial^2}{\partial x_m \partial x_n} \right) + V(x) \\ &= H - \frac{1}{8} \sum_{m,n} \frac{\partial^2 a_{mn}}{\partial x_m \partial x_n}(x), \end{aligned}$$

where $p(x, \xi) = \frac{1}{2} \sum a_{mn}(x) \xi_m \xi_n + V(x)$. Hence, replacing V in $p(x, \xi)$ by $V + \frac{1}{8} \sum \frac{\partial^2 a_{mn}}{\partial x_m \partial x_n}(x)$, we may consider $H = p^W(x, D_x)$.

We are interested in the behavior of

$$v(t) = e^{i\Phi(t, D_x)} e^{-itH} u_0, \quad t \in \mathbb{R}.$$

For $u_0 \in \mathcal{S}(\mathbb{R}^d)$, we can differentiate $v(t)$ in t to get

$$\frac{d}{dt} v(t) = ie^{i\Phi(t, D_x)} \left(\frac{\partial \Phi}{\partial t}(t, D_x) - H \right) e^{-itH} u_0 = -iL(t)v(t),$$

where

$$L(t) = e^{i\Phi(t, D_x)} H e^{-i\Phi(t, D_x)} - \frac{\partial \Phi}{\partial t}(t, D_x).$$

We note

$$\begin{aligned} e^{i\Phi(t, D_x)} x e^{-i\Phi(t, D_x)} &= \mathcal{F}^* [e^{i\Phi(t, \xi)} i \partial_\xi e^{-i\Phi(t, \xi)}] \mathcal{F} \\ &= \mathcal{F}^* [i \partial_\xi + \partial_\xi \Phi(t, \xi)] \mathcal{F} = x + \partial_\xi \Phi(t, D_x), \end{aligned}$$

where \mathcal{F} is the Fourier transform. Hence, we expect

$$e^{i\Phi(t, D_x)} p^W(x, D_x) e^{-i\Phi(t, D_x)} \sim p^W(x + \partial_\xi \Phi(t, D_x), D_x)$$

in some sense. In fact, combining Lemma 7 with [11, Lemma 3.1], we obtain

Lemma 10. $e^{i\Phi(t, D_x)} H e^{-i\Phi(t, D_x)}$ is a pseudodifferential operator with symbol in $S_{1,0}^2$. Moreover, if we set $\tilde{p}(t, x, \xi) = p(x + \partial_\xi \Phi(t, \xi), \xi)$, then

$$e^{i\Phi(t, D_x)} H e^{-i\Phi(t, D_x)} - \tilde{p}^W(t, x, D_x) = r^W(t, x, D_x)$$

with $r \in S_{1,0}^0$, i.e., for any $\alpha, \beta \in \mathbb{Z}_+^d$ and $K \Subset \mathbb{R}^d$, there is $C_{\alpha\beta K} > 0$ such that

$$|\partial_x^\alpha \partial_\xi^\beta r(t, x, \xi)| \leq C_{\alpha\beta K} \langle \xi \rangle^{-|\beta|}, \quad x \in K, \xi \in \mathbb{R}^d, |t| \leq T.$$

Thus, by recalling the definition of $\ell(t; x, \xi)$ in Section 2, we find that the principal symbol of $L(t)$ is given by $\ell(t; x, \xi)$. This is consistent with the fact that

$e^{i\Phi(t, D_x)} e^{-itH}$ is the quantization of the classical flow $(x_0, \xi_0) \mapsto (z(t), \xi(t))$, of which $\ell(t; x, \xi)$ is the Hamiltonian.

In order to analyze microlocal singularities, we use the semiclassical characterization of the wave front set: Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, $\xi_0 \neq 0$, and $u \in \mathcal{S}'(\mathbb{R}^d)$. Then $(x_0, \xi_0) \notin \text{WF}(u)$ if and only if there is $a \in C_0^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ such that $a(x_0, \xi_0) \neq 0$ and

$$(3.1) \quad \|a^W(x, \lambda^{-1}D_x)u\| \leq C_N \lambda^{-N}, \quad \lambda \gg 0,$$

with any $N \in \mathbb{Z}_+$ (see, e.g., [7, Section 2.9]).

Let $(x_0, \xi_0) \in \mathbb{R}^d \times \mathbb{R}^d$, $\xi_0 \neq 0$, be fixed, and suppose $a_0 \in C_0^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ is supported in a small neighborhood of (x_0, ξ_0) , for example, $B_\delta(x_0, \xi_0) = \{(x, \xi) \mid |x - x_0|^2 + |\xi - \xi_0|^2 < \delta^2\}$. We set

$$A(t) = e^{i\Phi(t, D_x)} e^{-itH} A_0 e^{itH} e^{-i\Phi(t, D_x)}, \quad A(0) = A_0 = a_0^W(x, \lambda^{-1}D_x),$$

and consider the time evolution of $A(t)$. In the weak sense on $\mathcal{S}(\mathbb{R}^d)$, we can compute the derivative of $A(t)$ in t , and obtain the Heisenberg equation

$$(3.2) \quad \frac{d}{dt} A(t) = -i[L(t), A(t)], \quad A(0) = a_0^W(x, \lambda^{-1}D_x).$$

We construct an asymptotic solution to this equation as $\lambda \rightarrow \infty$, using a Egorov type argument. The corresponding transport equation is given by

$$\frac{\partial}{\partial t} a(t, x, \xi) = -\{\ell, a\}(t, x, \xi) = -\sum_{m=1}^d \left(\frac{\partial \ell}{\partial \xi_m} \frac{\partial a}{\partial x_m} - \frac{\partial \ell}{\partial x_m} \frac{\partial a}{\partial \xi_m} \right)$$

with initial condition $a(0, x, \xi) = a_0(x, \lambda^{-1}\xi)$. We denote

$$\Sigma_t : (x_0, \xi_0) \mapsto (z(t), \xi(t)), \quad a_0^\lambda(x, \xi) = a_0(x, \lambda^{-1}\xi).$$

Then the solution to the transport equation is given by

$$\tilde{a}_0(t; x, \xi) = (a_0^\lambda \circ \Sigma_t^{-1})(x, \xi),$$

and $\tilde{a}_0(t, \cdot, \cdot)$ is supported in $\Sigma_t(\text{supp}(a_0^\lambda))$. We note that a_0^λ is bounded in $S_{1,0}^0$, uniformly in $\lambda \in [1, \infty)$. This also implies that $\tilde{a}_0(t, \cdot, \cdot)$ is uniformly bounded in $S_{1,0}^0$, provided $|t| \leq T$. Combining this observation with Lemma 9, we infer that

$$-i[L(t), A_0(t)] + \{\ell, \tilde{a}_0\}^W(x, D_x) = r_0^W(t; x, D_x)$$

with $r_0 \in S_{1,0}^{-1}$ uniformly in λ . Moreover, by the asymptotic expansion, $r_0(t; \cdot, \cdot)$ is supported in $\Sigma_t(\text{supp}(a_0^\lambda))$ modulo $O(\lambda^{-\infty})$ terms.

Following the standard Egorov type argument together with the scaling argument of Section 2, we can construct an asymptotic solution $\tilde{a}(t; x, \xi)$ with the following properties (see [11, Proposition 3.2]):

- (i) $\tilde{a}(0; x, \xi) = a_0^\lambda(x, \xi) = a_0(x, \lambda^{-1}\xi)$.
- (ii) $\tilde{a}(t; \cdot, \cdot)$ is supported in $\Sigma_t(\text{supp}(a_0^\lambda))$.
- (iii) For any $\alpha, \beta \in \mathbb{Z}_+^d$, there is $C_{\alpha\beta} > 0$ such that

$$|\partial_x^\alpha \partial_\xi^\beta \tilde{a}(t; x, \xi)| \leq C_{\alpha\beta} \lambda^{-|\beta|}, \quad |t| \leq T, \quad x, \xi \in \mathbb{R}^d, \quad \lambda \geq 1.$$

- (iv) The principal symbol of $\tilde{a}(t; x, \xi)$ is given by $a_0^\lambda \circ \Sigma_t^{-1}$, i.e.,

$$|\partial_x^\alpha \partial_\xi^\beta (\tilde{a}(t; x, \xi) - (a_0^\lambda \circ \Sigma_t^{-1})(x, \xi))| \leq C_{\alpha\beta} \lambda^{-1-|\beta|}$$

for $|t| \leq T, x, \xi \in \mathbb{R}^d$, and $\lambda \geq 1$.

- (v) $\tilde{A}(t) = \tilde{a}^W(t; x, D_x)$ satisfies the Heisenberg equation (3.2) asymptotically, i.e.,

$$\left\| \frac{d}{dt} \tilde{A}(t) + i[L(t), \tilde{A}(t)] \right\| \leq C_N \lambda^{-N}, \quad \lambda \geq 1,$$

for any $N \in \mathbb{Z}_+$ with some $C_N > 0$.

These properties imply

$$\left\| \frac{d}{dt} (e^{itH} e^{-i\Phi(t, D_x)} \tilde{A}(t) e^{i\Phi(t, D_x)} e^{-itH}) \right\| \leq C_N \lambda^{-N}, \quad |t| \leq T,$$

and hence

$$(3.3) \quad \left\| e^{itH} e^{-i\Phi(t, D_x)} \tilde{A}(t) e^{i\Phi(t, D_x)} e^{-itH} - a_0^W(x, \lambda^{-1} D_x) \right\| \leq C_N \lambda^{-N}$$

if $|t| \leq T$. This is equivalent to

$$(3.4) \quad \left\| \tilde{A}(t) - e^{i\Phi(t, D_x)} e^{-itH} a_0^W(x, \lambda^{-1} D_x) e^{itH} e^{-i\Phi(t, D_x)} \right\| \leq C_N \lambda^{-N}.$$

On the other hand, if we write

$$\begin{aligned} \Sigma_t^\lambda(x, \xi) &= (z(\lambda^{-1}t; x, \lambda\xi), \lambda^{-1}\xi(\lambda^{-1}t; x, \lambda\xi)) \\ &= (x^\lambda(t; x, \xi) - \partial_\xi \Phi^\lambda(t, \xi^\lambda(t; x, \xi)), \xi^\lambda(t; x, \xi)), \end{aligned}$$

then

$$(a_0^\lambda \circ \Sigma_t^{-1})(x, \lambda\xi) = (a_0 \circ (\Sigma_{\lambda t}^\lambda)^{-1})(x, \xi).$$

We note that $(\Sigma_{\lambda t}^\lambda)^{-1}$ converges to W_\pm^{cl} as $\lambda \rightarrow \infty$ when $\pm t > 0$ locally uniformly, with all derivatives (Theorem 6). Hence $(a_0^\lambda \circ \Sigma_t^{-1})(x, \lambda\xi)$ converges to $(a_0 \circ W_\pm^{\text{cl}})(x, \xi)$ uniformly in (x, ξ) with all derivatives, and the support of $(a_0^\lambda \circ \Sigma_t^{-1})(x, \lambda\xi)$ also converges to the support of $a_0 \circ W_\pm^{\text{cl}}$. This implies that

$(a_0^\lambda \circ \Sigma_t^{-1})^W(x, D_x)$ converges to $(a_0 \circ W_\pm^{\text{cl}})^W(x, \lambda^{-1} D_x)$ as $\lambda \rightarrow \infty$ including their microlocal support properties.

If $(x_0, \xi_0) \notin \text{WF}(u_0)$, and a_0 is supported in a small neighborhood of (x_0, ξ_0) such that (3.1) holds, then (3.3) implies

$$\|\tilde{A}(t)e^{i\Phi(t;D_x)}e^{-itH}u_0\| \leq C_N\lambda^{-N}.$$

Since the principal symbol of $\tilde{A}(t)$ is $(a_0^\lambda \circ \Sigma_t^{-1})(x, \xi)$, which is very close to $(a_0 \circ W_\pm^{\text{cl}})(x, \lambda\xi)$, this implies $(W_\pm^{\text{cl}})^{-1}(x_0, \xi_0) \notin \text{WF}(e^{i\Phi(t;D_x)}e^{-itH}u_0)$.

Similarly, if $(W_\pm^{\text{cl}})^{-1}(x_0, \xi_0) \notin \text{WF}(e^{i\Phi(t;D_x)}e^{-itH}u_0)$, then we deduce that $(x_0, \xi_0) \notin \text{WF}(u_0)$ using (3.4).

The above formal argument can be easily justified as in [11, Section 3.2], and Theorem 2 is proved. □

§4. Asymptotically homogeneous potentials

Here we consider the case of $a_{mn}(x) = \delta_{mn}$, and $V(x)$ asymptotically homogeneous of order $\beta \in [1, 3/2)$.

Proof of Theorem 4. Suppose $V^{(L)}(x) = |x|V^{(L)}(\hat{x})$, $\hat{x} = x/|x|$, if $|x| \geq 1$, and let $t > 0$. Then if $|\xi| \geq t^{-1}$, we have

$$\begin{aligned} \int_0^t V^{(L)}(s\xi)ds &= \int_0^t s|\xi|V^{(L)}(\hat{\xi})ds + \int_0^{1/|\xi|} (V^{(L)}(s\xi) - s|\xi|V^{(L)}(\hat{\xi})) ds \\ &= \frac{t^2}{2}|\xi|V^{(L)}(\hat{\xi}) + R(t, \xi). \end{aligned}$$

Here $R(t, \xi)$ can be computed as

$$R(t, \xi) = \int_0^1 (V^{(L)}(\sigma\hat{\xi}) - \sigma V^{(L)}(\hat{\xi}))|\xi|^{-1} d\sigma,$$

and hence for any $\alpha \in \mathbb{Z}_+^d$,

$$|\partial_\xi^\alpha R(t, \xi)| \leq C_\alpha |\xi|^{-1-|\alpha|}, \quad |\xi| \geq t^{-1}.$$

Hence, if we set

$$F(t, \xi) = \int_0^t V^{(L)}(s\xi) ds - \frac{t^2}{2}V^{(L)}(\xi),$$

then for any fixed $t \neq 0$, $F(t, \xi) \in S_{1,0}^{-1}$, i.e., for any $\alpha \in \mathbb{Z}_+^d$,

$$|\partial_\xi^\alpha F(t, \xi)| \leq C_\alpha \langle \xi \rangle^{-1-|\alpha|}, \quad \xi \in \mathbb{R}^d.$$

This implies $e^{iF(t,\xi)} \in S_{1,0}^0$, and it is obviously elliptic. In particular,

$$\text{WF}(e^{iF(t,D_x)}u) = \text{WF}(u), \quad u \in L^2(\mathbb{R}^d).$$

Now we note

$$\Phi(t, \xi) = \frac{t}{2}|\xi|^2 + \int_0^t V^{(L)}(s\xi) ds = \frac{t}{2}|\xi|^2 + \frac{t^2}{2}V^{(L)}(\xi) + F(t, \xi).$$

Combining these with Theorem 2, we find that

$$\begin{aligned} \text{WF}(u) &= \text{WF}(e^{i\Phi(t, D_x)} e^{-itH} u) = \text{WF}(e^{iF(t, D_x)} e^{i(t^2/2)V^{(L)}(D_x)} e^{itH_0} e^{-itH} u) \\ &= \text{WF}(e^{i(t^2/2)V^{(L)}(D_x)} e^{itH_0} e^{-itH} u). \end{aligned}$$

Since $V^{(L)}(\xi)$ is homogeneous of order 1, $e^{i(t^2/2)V^{(L)}(D_x)}$ is a Fourier integral operator with the associated canonical transform

$$S_{t^2/2}^+ : (x, \xi) \mapsto \left(x - \frac{t^2}{2} \partial_x V^{(L)}(\hat{\xi}), \xi \right)$$

and hence

$$(4.1) \quad \text{WF}(e^{i(t^2/2)V^{(L)}(D_x)} v) = S_{t^2/2}^+(\text{WF}(v))$$

(see, e.g., [3, Chapter XXV], [14, Section VIII.5]). Thus we have

$$\text{WF}(u) = S_{t^2/2}^+(\text{WF}(e^{itH_0} e^{-itH} u)),$$

which is equivalent to

$$\text{WF}(e^{itH_0} e^{-itH} u) = S_{(-t^2/2)}^+(\text{WF}(u)).$$

If $t < 0$, then

$$\int_0^t V^{(L)}(s\xi) ds = - \int_0^{|t|} V^{(L)}(-s\xi) ds,$$

and we replace $V^{(L)}(\hat{\xi})$ by $V^{(L)}(-\hat{\xi})$, and we change the direction of the shift to obtain $S_{t^2/2}^-$ in the statement. \square

Remark 2. The property (4.1) can also be proved using the propagation of singularities for hyperbolic equations. In fact, $e^{i\sigma V^{(L)}(D_x)} u_0$ is the solution to the hyperbolic evolution equation

$$\frac{\partial}{\partial \sigma} u(\sigma) = iV^{(L)}(D_x)u(\sigma), \quad u(0) = u_0,$$

and the claim (4.1) follows, for example, from the Egorov theorem (see, e.g., [14, Section VIII.2]).

Proof of Theorem 5. We suppose $t > 0$, and $V^{(L)}(x) = |x|^\beta V^{(L)}(\hat{\xi})$ for $|x| \geq 1$ with $1 < \beta < 3/2$. By the same computation as in the proof of Theorem 4,

$$\int_0^t V^{(L)}(s\xi) ds = \frac{t^{1+\beta}}{1+\beta} |\xi|^\beta V^{(L)}(\hat{\xi}) + R(t, \xi)$$

with

$$|\partial_\xi^\alpha R(t, \xi)| \leq C_\alpha |\xi|^{-1-|\alpha|}, \quad |\xi| \geq t^{-1},$$

for any $\alpha \in \mathbb{Z}_+^d$. Thus,

$$\Phi(t, \xi) = \frac{t}{2} |\xi|^2 + \frac{t^{1+\beta}}{1+\beta} V^{(L)}(\xi) + F(t, \xi)$$

with $F(t, \xi) \in S_{1,0}^{-1}$, and hence

$$\text{WF}(u) = \text{WF}(e^{i\sigma V^{(L)}(D_x)} e^{itH_0} e^{-itH} u)$$

where $\sigma = \frac{t^{1+\beta}}{1+\beta}$. This implies

$$(4.2) \quad \text{WF}(e^{itH} u) = \text{WF}(e^{i\sigma V^{(L)}(D_x)} e^{itH_0} u).$$

Since $V(\xi)$ is homogeneous of order $\beta > 1$, we can prove $e^{i\sigma V^{(L)}(D_x)}$ has the diffusivity property:

Lemma 11. *Let $N \in \mathbb{Z}_+$ and let $\sigma \neq 0$. Then there is C_N such that*

$$(4.3) \quad \|\langle x \rangle^{-N} e^{i\sigma V^{(L)}(D_x)} u\|_{H^s} \leq C_N \|\langle x \rangle^N u\|, \quad u \in L^{2,\infty}(\mathbb{R}^d),$$

where $s = (\beta - 1)N$. In particular, $e^{i\sigma V^{(L)}(D_x)} u \in C^\infty(\mathbb{R}^d)$ if $u \in L^{2,\infty}(\mathbb{R}^d)$.

Proof. For simplicity, we write $V^{(L)}(\xi) = V(\xi)$ and $\Lambda = V(D_x)$ in this proof. By direct computation of the Fourier transform, we have

$$x_j e^{i\sigma \Lambda} u = -\sigma (\partial_{\xi_j} V)(D_x) e^{i\sigma \Lambda} u + e^{i\sigma \Lambda} (x_j u),$$

and this implies

$$\langle x \rangle^{-1} (\partial_{\xi_j} V)(D_x) e^{i\sigma \Lambda} u = -\sigma^{-1} \{x_j \langle x \rangle^{-1} e^{i\sigma \Lambda} u - \langle x \rangle^{-1} e^{i\sigma \Lambda} (x_j u)\} \in L^2(\mathbb{R}^d).$$

By the assumption, we also have

$$\sum_{j=1}^d |\partial_{\xi_j} V(\xi)| \geq c |\xi|^{\beta-1}, \quad |\xi| \geq 1,$$

with some $c > 0$, so that $\langle x \rangle^{-1} e^{i\sigma \Lambda} u \in H^{\beta-1}(\mathbb{R}^d)$, and its norm is bounded by $\|\langle x \rangle u\|$. This proves (4.3) with $N = 1$. Similarly,

$$x_j^2 e^{i\sigma \Lambda} u = \sigma^2 (\partial_{\xi_j} V(D_x))^2 e^{i\sigma \Lambda} u + 2\sigma (\partial_{\xi_j} V)(D_x) e^{i\sigma \Lambda} (x_j u) + e^{i\sigma \Lambda} (x_j^2 u).$$

This implies $\langle x \rangle^{-2} ((\partial_{\xi_j} V)(D_x))^2 e^{i\sigma \Lambda} u \in L^2(\mathbb{R}^d)$ since we already know that $\langle x \rangle^{-1} (\partial_{\xi_j} V)(D_x) e^{i\sigma \Lambda} u \in L^2(\mathbb{R}^d)$. Summing up these estimates in j shows that $\langle x \rangle^{-2} e^{i\sigma \Lambda} u \in H^{2(\beta-1)}(\mathbb{R}^d)$, and we obtain (4.3) for $N = 2$. Iterating this procedure, we deduce (4.3) for any N . \square

The conclusion of Theorem 5 for $t < 0$ now follows from (4.2) and Lemma 11. The case $t > 0$ is proved similarly. \square

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References

- [1] S. Doi, Singularities of solutions of Schrödinger equations for perturbed harmonic oscillators, in *Hyperbolic problems and related topics*, Grad. Ser. Anal., Int. Press, Somerville, MA, 2003, 185–199. [Zbl 1047.35007](#) [MR 2056850](#)
- [2] A. Hassell and J. Wunsch, The Schrödinger propagator for scattering metrics, *Ann. of Math.* **162** (2005), 487–523. [Zbl 1126.58016](#) [MR 2178967](#)
- [3] L. Hörmander, *The analysis of linear partial differential operators I–IV*, Springer, New York, 1983–1985. [Zbl 0521.35001\(I\)](#) [Zbl 0521.35002\(II\)](#) [Zbl 0601.35001\(III\)](#) [Zbl 0612.35001\(IV\)](#) [MR 0717035\(I\)](#) [MR 0705278\(II\)](#) [MR 0781536\(III\)](#) [MR 0781537\(IV\)](#)
- [4] K. Ito and S. Nakamura, Singularities of solutions to the Schrödinger equation on scattering manifold, *Amer. J. Math.* **131** (2009), 1835–1865. [Zbl 1186.35004](#) [MR 2567509](#)
- [5] ———, Remarks on the fundamental solution to Schrödinger equation with variable coefficients, *Ann. Inst. Fourier (Grenoble)* **62** (2012), 1091–1121. [Zbl 1251.35102](#) [MR 3013818](#)
- [6] S. Mao and S. Nakamura, Wave front set for solutions to perturbed harmonic oscillators, *Comm. Partial Differential Equations* **34** (2009), 506–519. [Zbl 1178.35013](#) [MR 2530707](#)
- [7] A. Martinez, *An introduction to semiclassical and microlocal analysis*, Springer, 2002. [Zbl 0994.35003](#) [MR 1872698](#)
- [8] A. Martinez, S. Nakamura and V. Sordani, Analytic wave front for solutions to Schrödinger equations, *Adv. Math.* **222** (2009), 1277–1307. [Zbl 1180.35016](#) [MR 2554936](#)
- [9] ———, Analytic wave front set for solutions to Schrödinger equations II—Long range perturbations, *Comm. Partial Differential Equations* **35** (2010), 2279–2309. [Zbl 1214.35055](#) [MR 2763356](#)
- [10] S. Nakamura, Wave front set for solutions to Schrödinger equations, *J. Funct. Anal.* **256** (2009), 1299–1309. [Zbl 1155.35014](#) [MR 2488342](#)
- [11] ———, Semiclassical singularity propagation property for Schrödinger equations, *J. Math. Soc. Japan* **61** (2009), 177–211. [Zbl 1176.35045](#) [MR 2272875](#)
- [12] T. Ōkaji, Propagation of wave packets and its applications, in *Partial differential equations and spectral theory* (Clausthal, 2000), Oper. Theory Adv. Appl. 126, Birkhäuser, Basel, 2001, 239–243. [Zbl 1001.35031](#) [MR 1946675](#)
- [13] M. Reed and B. Simon, *The methods of modern mathematical physics. Volume III. Scattering theory*, Academic Press, 1979. [Zbl 0405.47007](#) [MR 0529429](#)
- [14] M. Taylor, *Pseudodifferential operators*, Princeton Univ. Press, 1981. [Zbl 0453.47026](#) [MR 0618463](#)