# Application of wave packet transform to Schrödinger equations

東京理科大学理学部 加藤 圭一(Keiichi Kato)

Department of Mathematics, Faculty of Science, Tokyo University of Science 東京理科大学理学部 伊藤 真吾 (Shingo Ito)

Department of Mathematics, Faculty of Science, Tokyo University of Science 山形大学理学部 小林 政晴 (Masaharu Kobayashi)

Department of Mathematical Sciences, Faculty of Science, Yamagata University

#### Abstract

In this note, we determine the wave front sets of solutions to time dependent Schrödinger equations with a sub-quadratic potential by using the representation of the Schrödinger evolution operator of a free particle introduced in [11] via wave packet transform (short time Fourier transform).

### 1 Introduction

In this note, we consider the following initial value problem of the time dependent Schrödinger equations,

$$\begin{cases} i\partial_t u + \frac{1}{2}\triangle u - V(t, x)u = 0, & (t, x) \in \mathbb{R} \times \mathbb{R}^n, \\ u(0, x) = u_0(x), & x \in \mathbb{R}^n, \end{cases}$$
(1)

where  $i = \sqrt{-1}$ ,  $u : \mathbb{R} \times \mathbb{R}^n \to \mathbb{C}$ ,  $\triangle = \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}$  and V(t, x) is a real valued function.

We shall determine the wave front sets of solutions to the Schrödinger equations (1) with a sub-quadratic potential V(t,x) by using the representation of the Schrödinger evolution operator of a free particle introduced in [11] via the wave packet transform which is defined by A. Córdoba and C. Fefferman [1]. In particular, we determine the location of all the singularities of the solutions from the information of the initial data. Wave packet transform is called short time Fourier transform in several literatures([7]).

We assume the following assumption on V(t,x).

**Assumption 1.1.** V(t,x) is a real valued function in  $C^{\infty}(\mathbb{R} \times \mathbb{R}^n)$  and there exists  $0 \le \rho < 2$  such that for all multi-indices  $\alpha$ ,

$$|\partial_x^{\alpha} V(t,x)| \le C(1+|x|)^{\rho-|\alpha|}$$

holds for some C > 0 and for all  $(t, x) \in \mathbb{R} \times \mathbb{R}^n$ .

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Let  $\varphi \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$  and  $f \in \mathcal{S}'(\mathbb{R}^n)$ . We define the wave packet transform  $W_{\varphi}f(x,\xi)$  of f with the wave packet generated by a function  $\varphi$  as follows:

$$W_{\varphi}f(x,\xi) = \int_{\mathbb{R}^n} \overline{\varphi(y-x)} f(y) e^{-iy\xi} dy, \quad x,\xi \in \mathbb{R}^n.$$

In the sequel, we call the function  $\varphi$  a window function (or window).

In the previous paper [11], we give a representation of the Schrödinger evolution operator of a free particle, which is the following:

$$W_{\varphi(t)}u(t,x,\xi) = e^{-\frac{i}{2}t|\xi|^2}W_{\varphi_0}u_0(x-\xi t,\xi), \tag{2}$$

where  $\varphi^{(t)} = \varphi^{(t)}(x) = e^{i(t/2)\triangle}\varphi_0(x)$  with  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n)\setminus\{0\}$  and  $W_{\varphi^{(t)}}u(t,x,\xi) = W_{\varphi^{(t)}(\cdot)}[u(t,\cdot)](x,\xi)$ . In the following, we often use this convention  $W_{\varphi^{(t)}}u(t,x,\xi) = W_{\varphi^{(t)}(\cdot)}[u(t,\cdot)](x,\xi)$  for simplicity.

In order to state our results precisely, we prepare several notations. Let  $b = (2 - \rho)/4$ . For  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n)$ , we put  $\varphi^{(t)}(x) = e^{i(t/2)\triangle}\varphi_0(x)$  and  $\varphi_{\lambda}^{(t)}(x) = \lambda^{nb/2}\varphi^{(\lambda^2bt)}(\lambda^b x)$  for  $\lambda \geq 1$ . For  $(x_0, \xi_0) \in \mathbb{R}^n \times \mathbb{R}^n \setminus \{0\}$ , we call a subset  $V = K \times \Gamma$  of  $\mathbb{R}^{2n}$  a conic neighborhood of  $(x_0, \xi_0)$  if K is a neighborhood of  $x_0$  and  $\Gamma$  is a conic neighborhood of  $\xi_0$  (i.e.  $\xi \in \Gamma$  and  $\alpha > 0$  implies  $\alpha \xi \in \Gamma$ ). For  $\lambda \geq 1$  and  $(x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n$ , let  $x(s; t, x, \lambda \xi)$  and  $\xi(s; t, x, \lambda \xi)$  be the solutions to

$$\begin{cases} \dot{x}(s) = \xi(s), & x(t) = x, \\ \dot{\xi}(s) = -\nabla V(s, x(s)), & \xi(t) = \lambda \xi. \end{cases}$$
 (3)

The following theorem is our main result.

**Theorem 1.2.** Let  $u_0(x) \in L^2(\mathbb{R}^n)$  and u(t,x) be a solution of (1) in  $C(\mathbb{R}; L^2(\mathbb{R}^n))$ . Then under the assumption 1.1,  $(x_0, \xi_0) \notin WF(u(t,x))$  if and only if there exists a conic neighborhood  $V = K \times \Gamma$  of  $(x_0, \xi_0)$  such that for all  $N \in \mathbb{N}$ , for all  $a \ge 1$  and for all  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n)$  satisfying  $\int x^{\alpha} \varphi_0(x) dx \neq 0$  for some multi-index  $\alpha$ , there exists a constant  $C_{N,a,\varphi_0} > 0$  satisfying

$$|W_{\varphi_{\lambda}^{(-t)}}u_0(x(0;t,x,\lambda\xi),\xi(0;t,x,\lambda\xi))| \le C_{N,a,\varphi_0}\lambda^{-N}$$

for  $\lambda \ge 1$ ,  $a^{-1} \le |\xi| \le a$  and  $(x, \xi) \in V$ .

**Remark 1.3.**  $W_{\varphi_{\lambda}^{(-t)}}u_0(x,\xi)$  is the wave packet transform of  $u_0(x)$  with a window function  $\varphi_{\lambda}^{(-t)}(x)$ .

**Remark 1.4.** In [12], the authors investigate the wave front sets of solutions to Schrödinger equations of a free particle and a harmonic oscillator via the wave packet transformation.

**Remark 1.5.** In one space dimension, if V(t,x) = V(x) is super-quadratic in the sense that  $V(x) \ge C(1+|x|)^{2+\epsilon}$  with some  $\epsilon > 0$ , K. Yajima [20] shows that the fundamental solution of (1) has singularities everywhere.

Corollary 1.6. If  $\rho < 1$ , then  $(x_0, \xi_0) \notin WF(u(t, x))$  if and only if there exists a conic neighborhood  $V = K \times \Gamma$  of  $(x_0, \xi_0)$  such that for all  $N \in \mathbb{N}$ , for all  $a \ge 1$  and for all  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n)$  satisfying  $\int x^{\alpha} \varphi_0(x) dx \neq 0$  for some multi-index  $\alpha$ , there exists a constant  $C_{N,a,\varphi_0} > 0$  satisfying

$$|W_{\varphi_{\lambda}^{(-t)}}u_0(x-\lambda t\xi,\lambda\xi)| \le C_{N,a,\varphi_0}\lambda^{-N}$$

for  $\lambda \geq 1$ ,  $a^{-1} \leq |\xi| \leq a$  and  $(x, \xi) \in V$ .

The idea to classify the singularities of generalized functions "microlocally" has been introduced firstly by M. Sato, J. Bros and D. Iagolnitzer and L. Hörmander independently around 1970. Wave front set is introduced by L. Hörmander in 1970 (see [9]). It is proved in [10] that the wave front set of solutions to the linear hyperbolic equations of principal type propagates along the null bicharacteristics.

For Schrödinger equations, R. Lascar [13] has treated singularities of solutions microlocally first. He introduced quasi-homogeneous wave front set and has shown that the quasi-homogeneous wave front set of solutions is invariant under the Hamilton-flow of Schrödinger equation on each plane t = constant. C. Parenti and F. Segala [18] and T. Sakurai [19] have treated the singularities of solutions to Schrödinger equations in the same way.

The Schrödinger operator  $i\partial_t + \frac{1}{2}\triangle$  commutes  $x + it\nabla$ . Hence the solutions become smooth for t > 0 if the initial data decay at infinity. W. Craig, T. Kappeler and W. Strauss [2] have treated this smoothing property microlocally. They have shown for a solution of (1) that for a point  $x_0 \neq 0$  and a conic neighborhood  $\Gamma$  of  $x_0$ ,  $\langle x \rangle^r u_0(x) \in L^2(\Gamma)$  implies  $\langle \xi \rangle^r \hat{u}(t,\xi) \in L^2(\Gamma')$  for a conic neighborhood of  $\Gamma'$  of  $x_0$  and for  $t \neq 0$ , though they have considered more general operators. Several mathematicians have shown this kind of results for Schrödinger operators [4], [5], [14], [16], [17].

A. Hassell and J. Wunsch [8] and S. Nakamura [15] determine the wave front set of the solution by means of the initial data. Hassell and Wunsch have studied the singularities by using "scattering wave front set". Nakamura has treated the problem in semi-classical way. He has shown that for a solution u(t,x) of (1),  $(x_0,\xi_0) \notin WF(u(t))$  if and only if there exists a  $C_0^{\infty}$  function  $a(x,\xi)$  in  $\mathbb{R}^{2n}$  with  $a(x_0,\xi_0) \neq 0$  such that  $||a(x+tD_x,hD_x)u_0|| = O(h^{\infty})$  as  $h \downarrow 0$ . On the other hand, we use the wave packet transform instead of the pseudo-differential operators.

#### 2 Preliminaries

In this section, we introduce the definition of wave front set WF(u) and the characterization of wave front set by G. B. Folland [6].

**Definition 2.1** (Wave front set). For  $f \in \mathcal{S}'(\mathbb{R}^n)$ , we say  $(x_0, \xi_0) \notin WF(f)$  if there exist a function  $\chi(x)$  in  $C_0^{\infty}(\mathbb{R}^n)$  with  $\chi(x_0) \neq 0$  and a conic neighborhood  $\Gamma$  of  $\xi_0$  such that for all  $N \in \mathbb{N}$  there exists a positive constant  $C_N$  satisfying

$$|\widehat{\chi f}(\xi)| \le C_N (1 + |\xi|)^{-N}$$

for all  $\xi \in \Gamma$ .

To prove Theorem 1.2, we use the following characterization of the wave front set by G. B. Folland [6]. Let  $\varphi \in \mathcal{S}(\mathbb{R}^n)$  satisfying  $\int x^{\alpha} \varphi(x) dx \neq 0$  for some multi-index  $\alpha$ . For fixed b with 0 < b < 1, we put  $\varphi_{\lambda}(x) = \lambda^{nb/2} \varphi(\lambda^b x)$ .

**Proposition 2.2** (G. B. Folland [6, Theorem 3.22] and T. Ōkaji [16, Theorem 2.2]). For  $f \in \mathcal{S}'(\mathbb{R}^n)$ , we have  $(x_0, \xi_0) \notin WF(f)$  if and only if there exist a conic neighborhood K of  $x_0$  and a conic neighborhood  $\Gamma$  of  $\xi_0$  such that for all  $N \in \mathbb{N}$  and for all  $a \geq 1$  there exists a constant  $C_{N,a} > 0$  satisfying

$$|W_{\varphi_{\lambda}}f(x,\lambda\xi)| \le C_{N,a}\lambda^{-N}$$

for  $\lambda \geq 1$ ,  $x \in K$  and  $\xi \in \Gamma$  with  $a^{-1} \leq |\xi| \leq a$ .

**Remark 2.3.** Folland [6] has shown that the conclusion follows if the window function  $\varphi$  is an even and nonzero function in  $\mathcal{S}(\mathbb{R}^n)$  and b=1/2. In  $\bar{O}$ kaji [16], the proof of Proposition 2.2 for b=1/2 is given.

**Remark 2.4.** Folland [6] and  $\bar{O}$ kaji [16] have proved for b = 1/2. It is easy to extend for 0 < b < 1.

# 3 Proofs of Theorem 1.2 and Corollary 1.6

In this section, we prove Theorem 1.2 and Corollary 1.6.

*Proof of Theorem 1.2.* The initial value problem (1) is transformed by the wave packet transform to

$$\begin{cases}
 \left(i\partial_t + i\xi \cdot \nabla_x - i\nabla_x V(t, x) \cdot \nabla_\xi - \frac{1}{2}|\xi|^2 - \widetilde{V}(t, x)\right) \times \\
 W_{\varphi^{(t)}} u(t, x, \xi) = Ru(t, x, \xi), \\
 W_{\varphi^{(0)}} u(0, x, \xi) = W_{\varphi_0} u_0(x, \xi),
\end{cases} (4)$$

where  $\widetilde{V}(t,x) = V(t,x) - \nabla_x V(t,x) \cdot x$  and

$$Ru(t,x,\xi) = \sum_{j,k} \int \overline{\varphi^{(t)}(y-x)} V_{jk}(t,x,y) (y_j - x_j) (y_k - x_k) u(t,y) e^{-i\xi y} dy$$

with  $V_{jk}(t,x,y) = \int_0^1 \partial_j \partial_k V(t,x+\theta(y-x))(1-\theta)d\theta$ . Solving (4), we have the integral equation

$$\begin{split} W_{\varphi^{(t)}}u(t,x,\xi) &= e^{-i\int_0^t \{\frac{1}{2}|\xi(s;t,x,\xi)|^2 + \tilde{V}(s,x(s;t,x,\xi))\}ds} W_{\varphi_0}u_0(x(0;t,x,\xi),\xi(0;t,x,\xi)) \\ &- i\int_0^t e^{-i\int_s^t \{\frac{1}{2}|\xi(s_1;t,x,\xi)|^2 + \tilde{V}(s_1,x(s_1;t,x,\xi))\}ds_1} Ru(s,x(s;t,x,\xi),\xi(s;t,x,\xi))ds, \end{split}$$

where  $x(s;t,x,\xi)$  and  $\xi(s;t,x,\xi)$  are the solutions of

$$\begin{cases} \dot{x}(s) &= \xi(s), \ x(t) = x, \\ \dot{\xi}(s) &= -\nabla_x V(s, x(s)), \ \xi(t) = \xi. \end{cases}$$

For fixed  $t_0$ , we have

$$W_{\varphi_{\lambda}^{(t-t_{0})}}u(t,x(t;t_{0},x,\lambda\xi),\xi(t;t_{0},x,\lambda\xi))$$

$$=e^{-i\int_{0}^{t}\{\frac{1}{2}|\xi(s;t_{0},x,\lambda\xi)|^{2}+\widetilde{V}(s,x(s;t_{0},x,\lambda\xi))\}ds}W_{\varphi_{\lambda}^{(-t_{0})}}u_{0}(x(0;t_{0},x,\lambda\xi),\xi(0;t_{0},x,\lambda\xi))$$

$$+i\int_{0}^{t}e^{-i\int_{s}^{t}\{\frac{1}{2}|\xi(s_{1},t_{0},x,\lambda\xi)|^{2}+\widetilde{V}(s_{1},x(s_{1};t_{0},x,\lambda\xi))\}ds_{1}}Ru(s,x(s;t_{0},x,\lambda\xi),\xi(s;t_{0},x,\lambda\xi))ds, \quad (5)$$

substituting  $(x(t;t_0,x,\lambda\xi),\xi(t;t_0,x,\lambda\xi))$  and  $\varphi_{\lambda}^{(-t_0)}(x)$  for  $(x,\xi)$  and  $\varphi_0(x)$  respectively. Here we use the fact that

$$x(s; t, x(t; t_0, x, \lambda \xi), \xi(t; t_0, x, \lambda \xi)) = x(s; t_0, x, \lambda \xi),$$
  
$$\xi(s; t, x(t; t_0, x, \lambda \xi), \xi(t; t_0, x, \lambda \xi)) = \xi(s; t_0, x, \lambda \xi)$$

and  $e^{\frac{i}{2}t\triangle}\varphi_{\lambda}^{(-t_0)}(x) = \varphi_{\lambda}^{(t-t_0)}(x)$ .

We only show the sufficiency here because the necessity is proved in the same way. To do so, we show that there exist a neighborhood K of  $x_0$  and a conic neighborhood  $\Gamma$  of  $\xi_0$  such that the following assertion  $P(\sigma,\varphi_0)$  holds for all  $\sigma \geq 0$  and for all  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n)$ satisfying  $\int x^{\alpha} \varphi_0(x) dx \neq 0$  for some  $\alpha$ .

 $P(\sigma, \varphi_0)$ : "For  $a \geq 1$  there exists a positive constant  $C_{\sigma,a,\varphi_0}$  such that

$$|W_{\varphi_{\lambda}^{(t-t_0)}}u(t, x(t; t_0, x, \lambda \xi), \xi(t; t_0, x, \lambda \xi))| \le C_{\sigma, a, \varphi_0} \lambda^{-\sigma}$$
(6)

for all  $x \in K$ , all  $\xi \in \Gamma$  with  $1/a \le |\xi| \le a$ , all  $\lambda \ge 1$  and  $0 \le t \le t_0$ . "

In fact, taking  $t = t_0$ , we have  $\varphi_{\lambda}^{(t_0 - t_0)} = (\varphi_0)_{\lambda}$ ,  $x(t_0; t_0, x, \lambda \xi) = x$  and  $\xi(t_0; t_0, x, \lambda \xi) = x$  $\lambda \xi$ . Hence from (6), we have immediately

$$|W_{(\varphi_0)}, u(t_0, x, \lambda \xi)| \leq C_{\sigma, a, \varphi_0} \lambda^{-\sigma}$$

for  $\lambda \geq 1$ ,  $x \in K$  and  $\xi \in \Gamma$  with  $1/a \leq |\xi| \leq a$ . This and Proposition 2.2 show the sufficiency.

We fix  $b = (2 - \rho)/4$ . We write  $x^* = x(s; t_0, x, \lambda \xi), \xi^* = \xi(s; t_0, x, \lambda \xi), t^* = s - t_0$  and  $\varphi_{\lambda}(x) = (\varphi_0)_{\lambda}(x)$  for simple description.

We show by induction with respect to  $\sigma$  that  $P(\sigma, \varphi_0)$  holds for all  $\sigma \geq 0$  and for all  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n)$  satisfying  $\int x^{\alpha} \varphi_0(x) dx \neq 0$  for some  $\alpha$ .

First we show that  $P(0,\varphi_0)$  holds for all  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n)$ . Since  $u_0(x) \in L^2(\mathbb{R}^n)$ ,  $u(t,x) \in \mathcal{S}(\mathbb{R}^n)$  $C(\mathbb{R}; L^2(\mathbb{R}^n))$ . Schwarz's inequality and conservativity for  $L^2$  norm of solutions of (1) show that

$$\begin{split} & \left| W_{\varphi_{\lambda}^{(t-t_0)}} u(t, x(t; t_0, x, \lambda \xi), \lambda \xi(t; t_0, x, \lambda \xi)) \right| \\ & \leq \int |\varphi_{\lambda}^{(t-t_0)} (y - x(t; t_0, x, \lambda \xi))| |u(t, y)| dy \\ & \leq \|\varphi_{\lambda}^{(t-t_0)} (\cdot)\|_{L^2} \|u(t, \cdot)\|_{L^2} \\ & = \|\varphi_{\lambda} (\cdot)\|_{L^2} \|u_0 (\cdot)\|_{L^2} = \|\varphi_0 (\cdot)\|_{L^2} \|u_0 (\cdot)\|_{L^2}. \end{split}$$

Hence  $P(0, \varphi_0)$  holds.

Next we show that for fixed  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n)$  satisfying  $\int x^{\alpha} \varphi_0(x) dx \neq 0$  for some  $\alpha$ ,  $P(\sigma + (2-\rho)/2, \varphi_0)$  holds under the assumption that  $P(\sigma, \varphi_0)$  holds for all  $\varphi_0$  satisfying  $\int x^{\alpha} \varphi_0(x) dx \neq 0$  for some  $\alpha$ . To do so, it suffices to show that for fixed  $\varphi_0$ , there exists a positive constant  $C_{a,\varphi_0}$  such that

$$|Ru(s, x(s; t_0, x, \lambda \xi), \xi(s; t_0, x, \lambda \xi))| \le C_{a,\varphi_0} \lambda^{-(\sigma + (2-\rho)/2)}$$
(7)

for all  $x \in K$ , all  $\xi \in \Gamma$  with  $1/a \le |\xi| \le a$ , all  $\lambda \ge 1$  and  $0 \le s \le t_0$ , since the first term of the right hand side of (5) is estimated by the condition on  $u_0$ .

Taylor's expansion of  $V(s, x^*, y)$  yields that

$$Ru(s, x^*, \xi^*, \lambda) = \sum_{2 \le |\alpha| \le L-1} \frac{\partial_x^{\alpha} V(s, x^*)}{\alpha!} \int (x^* - y)^{\alpha} \overline{\varphi_{\lambda}^{(s-t_0)}(y - x^*)} u(s, y) e^{-iy\xi^*} dy + R_L, \quad (8)$$

where

$$R_{L}(s, x^{*}, \xi^{*}, \lambda) = L \sum_{|\alpha|=L} \frac{1}{\alpha!} \frac{1}{\|\varphi_{0}\|_{L^{2}}^{2}} \times \iint \left( \int \left( \int_{0}^{1} \partial_{x}^{\alpha} V(s, x^{*} - \theta(x^{*} - y))(1 - \theta)^{L-1} d\theta \right) (x^{*} - y)^{\alpha} \times \overline{\varphi_{\lambda}^{(s-t_{0})}(y - x^{*})} \varphi_{\lambda}^{(s-t_{0})}(y - z) e^{-iy(\xi^{*} - \eta)} dy \right) W_{\varphi_{\lambda}^{(s-t_{0})}}u(s, z, \eta) dz d\eta.$$

Here we use the inversion formula of the wave packet transform

$$\frac{1}{\|\varphi\|_{L^2}^2} W_{\varphi}^{-1} W_{\varphi} f(x) = f(x),$$

where

$$W_{\varphi}^{-1}g(x) = \iint g(y,\xi)\varphi(y-x)e^{ix\xi}d\xi dy$$

for a smooth tempered function  $g(y,\xi)$  on  $\mathbb{R}^{2n}$ .

The strategy for the proof of (7) is the following. In Step 1, taking  $b = (2 - \rho)/4$  according to the value of  $\rho$  which is the order of increasing of V(t,x) with respect to x in the assumption 1.1, we estimate the first term of the right hand side of (8). In Step 2, taking L sufficiently large according to the value of  $\sigma$ , we estimate the second term  $R_L$  of the right hand side of (8).

(Step1) We estimate the first term of the right hand side of (8). Since

$$(x_j^* - y_j) \exp\left(-\frac{i|z - \lambda^b(y - x^*)|^2}{2t^*\lambda^{2b}}\right) = \left(\frac{\lambda^b t^*}{i} \partial_{z_j} + \frac{1}{\lambda^b} z_j\right) \exp\left(-\frac{i|z - \lambda^b(y - x^*)|^2}{2t^*\lambda^{2b}}\right),$$

we have

$$(x^* - y)^{\alpha} \exp\left(-\frac{i|z - \lambda^b(y - x^*)|^2}{2t^*\lambda^{2b}}\right) = \left(\frac{\lambda^b t^*}{i}\partial_z + \frac{1}{\lambda^b}z\right)^{\alpha} \exp\left(-\frac{i|z - \lambda^b(y - x^*)|^2}{2t^*\lambda^{2b}}\right).$$

Thus we have

$$\begin{split} &(x^*-y)^{\alpha}\overline{\varphi_{\lambda}^{(t^*)}(y-x^*)} \\ =& \overline{(2\pi\lambda^{2b}t^*i)^{-n/2}}\lambda^{nb/2}\int\left(\frac{\lambda^bt^*}{i}\partial_z+\frac{1}{\lambda^b}z\right)^{\alpha}\exp\left(-\frac{i|z-\lambda^b(y-x^*)|^2}{2t^*\lambda^{2b}}\right)\overline{\varphi_0(z)}dz \\ =& \overline{(2\pi\lambda^{2b}t^*i)^{-n/2}}\lambda^{nb/2}\int\exp\left(-\frac{i|z-\lambda^b(y-x^*)|^2}{2t^*\lambda^{2b}}\right)\left(\frac{\lambda^bt^*}{i}\partial_z+\frac{1}{\lambda^b}z\right)^{\alpha}\overline{\varphi_0(z)}dz \\ =& \sum_{\beta+\gamma=\alpha}C_{\beta,\gamma}t^{*|\beta|}\lambda^{b(|\beta|-|\gamma|)}\overline{\varphi_{\lambda}^{(\beta,\gamma)}(t^*,y-x^*)}, \end{split}$$

where  $\varphi^{(\beta,\gamma)}(x) = x^{\gamma} \partial_x^{\beta} \varphi_0(x)$  and  $\varphi_{\lambda}^{(\beta,\gamma)}(t,x) = e^{\frac{i}{2}t\triangle} \left(\varphi^{(\beta,\gamma)}\right)_{\lambda}(x)$ . Since  $\varphi^{(\beta,\gamma)}(x) = x^{\gamma} \partial_x^{\beta} \varphi_0(x)$  satisfying  $\int x^{\alpha} \varphi^{(\beta,\gamma)}(x) dx \neq 0$  for some  $\alpha$ , the assumption of induction yields that

|(The first term of the right hand side of (8))|

$$\leq \sum_{2\leq |\alpha|\leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} |\partial_x^{\alpha} V(s,x^*)| C_{\beta,\gamma} t^{*|\beta|} \lambda^{b(|\beta|-|\gamma|)} \left| W_{\varphi_{\lambda}^{(\beta,\gamma)}(t^*,x)} u(s,x^*,\xi^*) \right| \\ \leq \sum_{2\leq |\alpha|\leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} C(1+|x^*|)^{\rho-|\alpha|} C_{\beta,\gamma} t^{*|\beta|} \lambda^{b(|\beta|-|\gamma|)} C\lambda^{-\sigma}.$$

Since

$$x^* = x(s; t_0, x, \lambda \xi) = x + \int_{t_0}^{s} \dot{x}(s_1) ds_1$$
$$= x + (s - t_0) \lambda \xi - \int_{t_0}^{s} (s - s_1) \nabla_x V(s_1, x(s_1)) ds_1, \quad (9)$$

there exists a positive constant  $\lambda_0$  such that

$$|x^*| \ge \frac{1}{2a} |t^*| \lambda \tag{10}$$

for all  $\lambda \geq \lambda_0, \ \lambda^{-2b} \leq |t^*| \leq t_0, \ x \in K$  and  $\xi \in \Gamma$  with  $1/a \leq |\xi| \leq a$ . (see Appendix A for the proof of (10)). Hence we have for  $\lambda^{-2b} \leq |t^*| \leq t_0$ 

(The first term of the right hand side of (8))

$$\leq \sum_{2\leq |\alpha|\leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} C(1+|t^*|\lambda)^{\rho-|\alpha|} C_{\beta,\gamma} t^{*|\beta|} \lambda^{b(|\beta|-|\gamma|)} C \lambda^{-\sigma}$$

$$\leq C' \sum_{2\leq |\alpha|\leq L-1} \lambda^{\rho-|\alpha|+b|\alpha|-\sigma}$$

$$\leq C'' \lambda^{\rho-2+2b-\sigma} = C'' \lambda^{-(2-\rho)/2-\sigma},$$

since  $b = (2 - \rho)/4$ . For  $|t^*| < \lambda^{-2b}$ , we have which shows that

(The first term of the right hand side of (8))

$$\leq \sum_{2\leq |\alpha|\leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} CC_{\beta,\gamma} t^{*|\beta|} \lambda^{b(|\beta|-|\gamma|)} C\lambda^{-\sigma}$$

$$\leq \sum_{2\leq |\alpha|\leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} CC_{\beta,\gamma} \lambda^{-b(|\beta|+|\gamma|)} C\lambda^{-\sigma} = C'\lambda^{-(2-\rho)/2-\sigma}.$$

(Step 2) We estimate  $R_L$ . Let  $\psi_1, \psi_2$  be  $C^{\infty}$  function on  $\mathbb{R}$  satisfying

$$\psi_1(s) = \begin{cases} 1 & \text{for } s \le 1, \\ 0 & \text{for } s \ge 2, \end{cases}$$

$$\psi_2(s) = \begin{cases} 0 & \text{for } s \le 1, \\ 1 & \text{for } s \ge 2, \end{cases}$$

$$\psi_1(s) + \psi_2(s) = 1 & \text{for all } s \in \mathbb{R}.$$

Take d > 0 satisfying 1 - b < d < 1. Putting  $V_{\alpha}(s, x^*, y) = \int_0^1 \partial_x^{\alpha} V(s, x^* - \theta(x^* - y))(1 - \theta)^{L-1} d\theta$  and

$$\begin{split} I_{\alpha,j,k}(s,x^*,\xi^*,\lambda) \\ &= \iiint \psi_j \left( \frac{|y-x^*|}{(1+\lambda|t^*|)^{2b}\lambda^{d-1}} \right) \psi_k \left( \frac{|y-z|}{(1+\lambda|t^*|)^{2b}\lambda^{d-1}} \right) V_\alpha(s,x^*,y) (x^*-y)^\alpha \\ &\qquad \qquad \overline{\varphi_\lambda^{(t^*)}(y-x^*)} \varphi_\lambda^{(t^*)}(y-z) W_{\varphi_\lambda^{(t^*)}} u(s,z,\eta) e^{-iy(\xi^*-\eta)} dz d\eta dy \end{split}$$

for j, k = 1, 2, we have

$$R_L(s, x^*, \xi^*, \lambda) = L \sum_{|\alpha|=L} \frac{1}{\alpha!} \frac{1}{\|\varphi_0\|_{L^2}^2} \sum_{j,k=1}^2 I_{\alpha,j,k}(s, x^*, \xi^*, \lambda).$$
 (11)

We need to show that for j, k = 1, 2, there exists a positive constant  $C_{\sigma,a,\varphi_0}$  such that

$$|I_{\alpha,j,k}(s,x^*,\xi^*,\lambda)| \le C_{\sigma,a,\varphi_0} \lambda^{-\sigma - (2-\rho)/2} \tag{12}$$

for  $\lambda \geq 1$ ,  $x \in K$ ,  $\xi \in \Gamma$  with  $1/a \leq |\xi| \leq a$  and  $0 \leq s \leq t_0$ . For  $I_{\alpha,1,1}$ , integration by parts and the fact that  $(1 - \Delta_y)e^{iy(\xi - \eta)} = (1 + |\xi - \eta|^2)e^{iy(\xi - \eta)}$  yield that

$$\begin{split} I_{\alpha,1,1}(s,x^*,\xi^*,\lambda) &= \iiint \left(1 + |\xi - \eta|^2\right)^{-N} \\ &\times (1 - \triangle_y)^N \left[ \overline{\varphi_{\lambda}^{(t^*)}(y - x^*)} \varphi_{\lambda}^{(t^*)}(y - z) \psi_1 \left( \frac{|y - x^*|}{(1 + \lambda |t^*|)^{2b} \lambda^{d-1}} \right) \right. \\ &\times \psi_1 \left( \frac{|y - z|}{(1 + \lambda |t^*|)^{2b} \lambda^{d-1}} \right) V_{\alpha}(s,x^*,y) \right] W_{\varphi_{\lambda}^{(t^*)}} u(s,z,\eta) e^{-iy(\xi^* - \eta)} dy d\eta dz. \end{split}$$

We take d' = (1-d)/(4b), which satisfies 2bd' + d - 1 = (d-1)/2 < 0. Since  $|y - x^*| \le C(1+\lambda|t^*|)^{2b}\lambda^{d-1}$  in the support of  $\psi_1\left(\frac{|y-x^*|}{(1+\lambda|t^*|)^{2b}\lambda^{d-1}}\right)$  with respect to y, the estimate (10) shows that for  $|t^*| \ge \lambda^{d'-1}$ 

$$\begin{split} |\partial_x^{\alpha} V(s, x^* + \theta(y - x^*))||(x^* - y)^{\alpha}| &\leq C(1 + |x^* + \theta(y - x^*)|)^{\rho - L} (1 + \lambda |t^*|)^{2bL} \lambda^{(d-1)L} \\ &\leq C(1 + |x^*| - |y - x^*|)^{\rho - L} (1 + \lambda |t^*|)^{2bL} \lambda^{(d-1)L} \\ &\leq C(1 + \lambda |t^*|)^{\rho - (1 - 2b)L} \lambda^{(d-1)L}, \end{split}$$

from which we have

$$|I_{\alpha,1,1}(s, x^*, \xi^*, \lambda)| \le C\lambda^{(d-1)L}\lambda^l,\tag{13}$$

where l are positive numbers which are independent of L. Since d-1 < 0, (12) with j = k = 1 holds if we take L sufficiently large. For  $|t^*| \le \lambda^{d'-1}$ , we have  $|y - x^*| \le C(1 + \lambda |t^*|)^{2b} \lambda^{d-1} \le \lambda^{2bd'+d-1} \le \lambda^{(d-1)/2}$ , which shows (13) for some l.

Finally we estimate  $I_{\alpha,j,k}$  for j=2 or k=2. Before the estimate, we estimate  $\varphi_{\lambda}^{(t)}(x)=e^{it\triangle/2}\varphi_{\lambda}(x)$  in the domain  $D=\{(t,x)||x|\geq (1+|\lambda t|)^{2b}\lambda^{d-1}\}$ . Take a positive number  $\delta$  satisfying  $0<\delta< b+d-1$ . Note that in  $D, |\lambda^b x|\geq \lambda^b(1+|\lambda t|)^{2b}\lambda^{d-1}\geq \lambda^{b+d-1}$  and b+d-1>0.

For  $0 \le t \le \lambda^{-2b}$ , the fact that  $\varphi_1^{(t)}(x) \in C(\mathbb{R}; \mathcal{S}(\mathbb{R}^n))$  yields that for any integer N and any multi-index  $\alpha$ , we have in D

$$|\partial_x^{\alpha} \varphi_{\lambda}^{(t)}(x)| = |\partial_x^{\alpha} (\varphi_1^{(\lambda^{2b}t)}(\lambda^b x))| \le C_{N,\alpha} \lambda^{b(|\alpha|-N)} \langle x \rangle^{-N}.$$

For  $\lambda^{-2b} \leq t \leq t_0$ , we put  $\varphi_{\lambda}^{(t)}(x) = \varphi_{\lambda,1}^{(t)}(x) + \varphi_{\lambda,2}^{(t)}(x)$ , where

$$\varphi_{\lambda,j}^{(t)}(x) = \frac{1}{(2\pi i \lambda^{2b} t)^{n/2}} \int \psi_j\left(\frac{|y|}{\lambda^{\delta}}\right) e^{-i\frac{|\lambda^b x - y|^2}{2\lambda^{2b} t}} \varphi_0(y) dy$$

for j = 1, 2. In the support of  $\psi_2\left(\frac{|y|}{\lambda^{\delta}}\right)$ ,  $|y| \geq \lambda^{\delta}$  holds. Since  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n)$ , for any integer N we have

$$|\varphi_0(y)| \le C_N (1+|y|)^{-N-n-1} \le C_N (1+\lambda^{\delta})^{-N} (1+|y|)^{-n-1}.$$

The above estimates, the fact that

$$(1 - \triangle_y) \exp\left(-i\frac{|\lambda^b x - y|^2}{2\lambda^{2b}t}\right) = \left(1 + \frac{|y - \lambda^b x|^2}{(\lambda^{2b}t)^2} + i\frac{n}{\lambda^{2b}t}\right) \exp\left(-i\frac{|\lambda^b x - y|^2}{2\lambda^{2b}t}\right)$$

and integration by parts yield that for any integer N and multi-index  $\alpha$ ,

$$|\partial_x^{\alpha} \varphi_{\lambda,2}^{(t)}(x)| \le C_{N,\alpha} \lambda^{-N} (1+|x|)^{-n-1}$$

in D for  $\lambda \geq 1$ .

In the support of  $\psi_1\left(\frac{|y|}{\lambda^{\delta}}\right)$ ,  $|y| \leq 2\lambda^{\delta}$  holds. Hence

$$\begin{split} \frac{|\lambda^b x - y|}{2|t|\lambda^{2b}} &\geq \frac{1}{2|t|\lambda^{2b}} (|\lambda^b x| - |y|) \\ &\geq \frac{1}{2|t|\lambda^{2b}} \left( (1 + |\lambda t|)^{2b} \lambda^{d-1} \lambda^b - 2\lambda^\delta \right) \\ &\geq \frac{(1 + |\lambda t|)^{2b}}{2|t|\lambda^{2b}} \left( \lambda^{b+d-1} (1 - 2\lambda^{\delta+1-b-d}) \right) \\ &\geq C|t_0|^{2b-1} \lambda^{b+d-1} \end{split}$$

for some constant C > 0, since  $b \le 1/2$  and  $\delta + 1 - b - d < 0$ . This estimate as above, the fact that

$$(1 - \triangle_y) \exp\left(-i\frac{|\lambda^b x - y|^2}{2\lambda^{2b}t}\right) = \left(1 + \frac{|y - \lambda^b x|^2}{(\lambda^{2b}t)^2} + i\frac{n}{\lambda^{2b}t}\right) \exp\left(-i\frac{|\lambda^b x - y|^2}{2\lambda^{2b}t}\right)$$

and integration by parts yield that for any integer N and any multi-index  $\alpha$ 

$$|\partial_x^{\alpha} \varphi_{\lambda,1}^{(t)}(x)| \le C_{N,\alpha} \lambda^{-N} \langle x \rangle^{-n-1}$$

in D for  $\lambda \geq 1$ . The estimates as above show that

$$|\partial_x^{\alpha} \varphi_{\lambda}^{(t)}(x)| \le C_{N,\alpha} \lambda^{-N} \langle x \rangle^{-n-1}$$

in D for  $\lambda \geq 1$ ,  $0 \leq t \leq t_0$  and  $x \in \mathbb{R}^n$ . This estimate implies that for any integer N

$$\left| \int \psi_{2} \left( \frac{|y - x^{*}|}{(1 + \lambda |t^{*}|)^{2b} \lambda^{d-1}} \right) \psi_{k} \left( \frac{|y - z|}{(1 + \lambda |t^{*}|)^{2b} \lambda^{d-1}} \right) \right.$$

$$\left. V_{\alpha}(s, x^{*}, y) (x^{*} - y)^{\alpha} \overline{\varphi_{\lambda}^{(t^{*})} (y - x^{*})} \varphi_{\lambda}^{(t^{*})} (y - z) e^{-iy(\xi^{*} - \eta)} dy \right|$$

$$\leq C_{N} \lambda^{-N} (1 + |x^{*} - z|)^{-n-1} (1 + |\xi^{*} - \eta|)^{-n-1},$$

which shows (12) with j=2 and k=1,2 for  $x\in K,\,\xi\in\Gamma$  with  $1/a\leq |\xi|\leq a$  and  $\lambda\geq 1$  and  $0\leq s\leq t_0$ . In the same way as above, we have that (12) with j=1,k=2 holds for  $x\in K,\,\xi\in\Gamma$  with  $1/a\leq |\xi|\leq a$  and  $\lambda\geq 1$  and  $0\leq s\leq t_0$ .

Proof of Corollary 1.6. (9) shows that

$$x(0;t,x,\lambda\xi) = x - \lambda t\xi + O(\lambda^{\rho-1}). \tag{14}$$

In the same way as for (14), we have

$$\xi(0;t,x,\lambda\xi) = \lambda t\xi + O(\lambda^{\rho-1}). \tag{15}$$

Since  $\rho - 1 < 0$ , (14) and (15) show that Theorem 1.2 implies Corollary 1.6.

## A Proof of the estimate (10)

In this appendix, we give the proof of the estimate (10). We fix p. We show the estimate (16) for  $|t_0| \ge |t^*| \ge \lambda^{p-1}$ ,  $\lambda \ge \lambda_0$ ,  $x \in K$ ,  $\xi \in \Gamma$  with  $1/a \le |\xi| \le a$ .

*Proof.* The equation (9) can be solved by Picard's iteration method. We put  $x^{(0)}(s) = x + (s - t_0)\lambda\xi$  and we define

$$x^{(N+1)}(s) = x + (s - t_0)\lambda \xi - \int_{t_0}^{s} (s - s_1) \nabla_x V(s_1, x^{(N)}(s_1)) ds_1$$

for  $N \geq 0$ . Then we have the solution x(s) of (9) as  $x(s) = \lim_{N \to \infty} x^{(N)}(s)$ . We show that there exists a positive constant  $\lambda_0 \geq 1$  such that

$$\frac{1}{2a}|t^*|\lambda \le |x^{(N)}(s)| \le 2a|t^*|\lambda,\tag{16}$$

for  $\lambda \geq \lambda_0$ ,  $\lambda^{p-1} \leq |t^*| \leq t_0$ ,  $x \in K$  and  $\xi \in \Gamma$  with  $1/a \leq |\xi| \leq a$ . We only treat the case that  $1 \leq \rho < 2$ . We show (16) by induction with respect to N.

Obviously (16) holds for N = 0.

Assuming that (16) holds for N, we have

$$|x^{(N+1)}(s)| \ge |x + (s - t_0)\lambda\xi| - \left| \int_{t_0}^s |s - s_1| |\nabla_x V(s_1, x^{(N)}(s_1))| ds_1 \right|$$

$$\ge |t^*|\lambda|\xi| - |x| - \int_s^{t_0} |s - s_1| C(1 + |x^{(N)}(s_1)|)^{\rho - 1} ds_1$$

$$\ge |t^*|\lambda|\xi| - |x| - C \int_s^{t_0} |s - s_1| (1 + 2(|t_0 - s_1|\lambda|\xi|)^{\rho - 1}) ds_1$$

$$\ge |t^*|\lambda|\xi| - |x| - C|t^*|^2 - C\lambda^{\rho - 1} |\xi|^{\rho - 1} |t^*|^{\rho + 1}$$

$$\ge |t^*|\lambda|\xi| \left(1 - \frac{|x|}{|t^*|\lambda|\xi|} - C\frac{|t_0|}{\lambda|\xi|} - C|t_0|^\rho \lambda^{\rho - 2} |\xi|^{\rho - 2}\right)$$

$$\ge |t^*|\lambda|\xi| \left(1 - \frac{a|x|}{\lambda^p} - C\frac{a|t_0|}{\lambda} - C\frac{a^{2-\rho}|t_0|^\rho}{\lambda^{2-\rho}}\right).$$

Since p > 0 and  $2 - \rho > 0$ , there exists a constant  $\lambda_0 \ge 1$  such that

$$1 - \frac{a|x|}{\lambda^{p}} - C\frac{a|t_{0}|}{\lambda} - C\frac{a^{2-\rho}|t_{0}|^{\rho}}{\lambda^{2-\rho}} \ge \frac{1}{2}$$

for  $\lambda \geq \lambda_0$ . Hence we have  $|x^{(N+1)}(s)| \geq \frac{1}{2}|t^*|\lambda|\xi| \geq \frac{1}{2a}|t^*|\lambda$ .

In the same way as above, we can show that

$$|x^{(N+1)}(s)| \le 2|t^*|\lambda a$$

for  $\lambda \geq \lambda_0$ ,  $\lambda^{p-1} \leq |t^*| \leq t_0$ ,  $x \in K$  and  $\xi \in \Gamma$  with  $1/a \leq |\xi| \leq a$ , assuming that (16) holds for N.

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