# Singularities for solutions to time dependent Schrödinger equations with sub-quadratic potential

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**Abstract.** In this article, 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 via wave packet transform (short time Fourier transform).

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## §1. Introduction

In this article, we consider the following initial value problem for the time dependent Schrödinger equations,

(1.1) 
$$\begin{cases} i\partial_t u + \frac{1}{2} \Delta u - V(t, x)u = 0, & (t, x) \in \mathbb{R} \times \mathbb{R}^n, \\ u(0, x) = u_0(x), & x \in \mathbb{R}^n, \end{cases}$$

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 (1.1) with a sub-quadratic potential V(t, x) by using the representation of the Schrödinger evolution operator obtained by the authors in [12] and [13] 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.

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 a non-negative constant  $\rho$  satisfying  $0 \leq \rho < 2$  such that for all multiindices  $\alpha$ 

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

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

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 the 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  $\varphi$  in the definition of wave packet transform *basic wave packet*. Wave packet transform is called short time Fourier transform by some authors([8]).

We write  $U_0(t) = e^{i(t/2)\Delta}$  for the evolution operator for the free Schrödinger operator. In the previous paper [12], we proved that the wave packet transform of the solution  $u(t, x) = U_0(t)u_0(x)$  to the free Schrödinger equation with the basic wave packet  $\varphi^{(t)}(x) = U_0(t)\varphi_0(x)$  may be expressed by using the wave packet transform of  $u_0$  with  $\varphi_0$  as follows:

(1.2) 
$$W_{\varphi^{(t)}}u(t,x,\xi) = e^{-\frac{i}{2}t|\xi|^2} W_{\varphi_0}u_0(x-\xi t,\xi),$$

where  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$ . We often use this convention  $\varphi^{(t)} = \varphi^{(t)}(x)$  and  $W_{\varphi^{(t)}}u(t,x,\xi) = W_{\varphi^{(t)}(\cdot)}[u(t,\cdot)](x,\xi)$  for simplicity, if no confusion is feared.

In order to state our results precisely, we prepare several notations. Let b be a real number with 0 < b < 1. For  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n)$ , we put  $(\varphi_0)_{\lambda}(x) = \lambda^{nb/2}\varphi_0(\lambda^b x)$  and  $\varphi_{\lambda}^{(t)}(x) = U_0(t)(\varphi_0)_{\lambda}(x)$  for  $\lambda \ge 1$ . 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  $\lambda \ge 1$  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

(1.3) 
$$\begin{cases} \dot{x}(s) &= \xi(s), \quad x(t) = x, \\ \dot{\xi}(s) &= -\nabla V(s, x(s)), \quad \xi(t) = \lambda \xi. \end{cases}$$

The following theorem is our main result.

**Theorem 1.2.** Assume Assumption 1.1. Take  $b = \min\left(\frac{2-\rho}{4}, \frac{1}{4}\right)$ . Let  $u_0(x) \in L^2(\mathbb{R}^n)$  and u(t,x) be the solution of (1.1) in  $C(\mathbb{R}; L^2(\mathbb{R}^n))$ . 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  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$ , there exists a constant  $C_{N,a,\varphi_0} > 0$  satisfying

(1.4) 
$$|W_{\varphi_{\lambda}^{(-t)}}u_0(x(0;t,x,\lambda\xi),\xi(0;t,x,\lambda\xi))| \le C_{N,a,\varphi_0}\lambda^{-N}$$

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 basic wave packet  $\varphi_{\lambda}^{(-t)}(x)$ . As previously stated,  $\varphi_{\lambda}^{(-t)}(x)$  depends on b.

**Remark 1.4.** In [13], 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. In [16], the authors give a partial answer to the problem which is discussed in this paper by the aid of characterization of wave front set by G. B. Folland and T. Ōkaji. Characterization of wave front set is discussed in Section 2.

**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 [24] shows that the fundamental solution of (1.1) has singularities everywhere.

**Corollary 1.6.** Assume Assumption 1.1 with  $\rho < 1$ . Take  $b = \min(\frac{1}{4}, 1 - \rho)$ . 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  $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$ , 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 [10]). It is proved in [11] 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 [17] 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 [22] and T. Sakurai [23] have treated the singularities of solutions to Schrödinger equations in the same way.

Since the Schrödinger operator  $i\partial_t + \frac{1}{2}\Delta$  commutes  $x + it\nabla$ , the solutions become smooth for t > 0 if the initial data decay at infinity. W. Craig,

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T. Kappeler and W. Strauss [2] have treated this type of smoothing property microlocally. They have shown for a solution of (1.1) 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], [18], [20], [21].

A. Hassell and J. Wunsch [9] and S. Nakamura [19] 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 (1.1),  $(x_0,\xi_0) \notin WF(u(t))$  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 give the characterization of wave front set in terms of wave packet transform.

**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, which is given in [15]. For fixed b with 0 < b < 1, we put  $\varphi_{\lambda}(x) = \lambda^{nb/2} \varphi(\lambda^b x)$ .

**Proposition 2.2.** Let  $(x_0, \xi_0) \in \mathbb{R}^n$  and  $u \in S'(\mathbb{R}^n)$ . The following conditions are equivalent.

- (i)  $(x_0, \xi_0) \notin WF(u)$
- (ii) There exist  $\varphi \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$ , a conic neighborhood V of  $(x_0, \xi_0)$  such that for all  $N \in \mathbb{N}$  and for all  $a \ge 1$  there exists a constant  $C_{N,a} > 0$  satisfying

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

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

(iii) There exist a conic neighborhood V of  $(x_0, \xi_0)$  such that for all  $N \in \mathbb{N}$ , for all  $a \ge 1$  and for all  $\varphi \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$  there exists a constant  $C_{N,a,\varphi} > 0$ satisfying

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

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

**Remark 2.3.** Characterization of wave front set by wave packet transform is firstly given by G. B. Folland [7]. Folland [7] has shown that the conclusion follows if the basic wave packet  $\varphi$  is an even and nonzero function in  $\mathcal{S}(\mathbb{R}^n)$ and b = 1/2. P. Gérard [6] has shown (i) is equivalent to (ii) in Proposition 2.2 with basic wave packet  $\varphi(x) = e^{-x^2}$  (Proof is also in J. M. Delort [3]). Ōkaji [20] has shown the same when  $\varphi$  satisfies  $\int x^{\alpha} \varphi(x) dx \neq 0$  for some multi-index  $\alpha$ .

**Remark 2.4.** Folland [7] and  $\overline{O}$ kaji [20] give the characterization for b = 1/2. In [15], we give the characterization for b = 1/2. Without any change of the proof, we can extend the characterization 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 (1.1) is transformed by the wave packet transform with the basic wave packet  $\varphi^{(t)}(x)$  to

$$(3.1) \begin{cases} \left(i\partial_t + i\xi \cdot \nabla_x - i\nabla_x V(t,x) \cdot \nabla_\xi - \frac{1}{2}|\xi|^2 - \widetilde{V}(t,x)\right) \times \\ W_{\varphi^{(t)}}u(t,x,\xi) = Ru(t,x,\xi), \\ W_{\varphi^{(0)}}u(0,x,\xi) = W_{\varphi_0}u_0(x,\xi), \end{cases}$$

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

$$Ru(t, x, \xi) = \sum_{|\alpha|=2} \frac{1}{\alpha!} \int \overline{\varphi^{(t)}(y-x)} \\ \times \left( \int_0^1 \partial^\alpha V(t, x+\theta(y-x))(1-\theta)d\theta \right) (y-x)^\alpha u(t, y) e^{-i\xi y} dy.$$

(For the deduction of (3.1), see [14].) Solving (3.1), we have the integral

equation

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

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

$$\begin{aligned} (3.2) \quad W_{\varphi_{\lambda}^{(t-t_{0})}}u(t,x(t;t_{0},x,\lambda\xi),\xi(t;t_{0},x,\lambda\xi)) \\ &= e^{-i\int_{0}^{t}\{\frac{1}{2}|\xi(s;t_{0},x,\lambda\xi)|^{2}+\widetilde{V}(s,x(s;t_{0},x,\lambda\xi))\}ds}W_{\varphi_{\lambda}^{(-t_{0})}}u_{0}(x(0;t_{0},x,\lambda\xi),\xi(0;t_{0},x,\lambda\xi)) \\ &\quad -i\int_{0}^{t}e^{-i\int_{s}^{t}\{\frac{1}{2}|\xi(s_{1},t_{0},x,\lambda\xi)|^{2}+\widetilde{V}(s_{1},x(s_{1};t_{0},x,\lambda\xi))\}ds_{1}} \\ &\quad \times Ru(s,x(s;t_{0},x,\lambda\xi),\xi(s;t_{0},x,\lambda\xi))ds, \end{aligned}$$

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

$$\begin{aligned} x(s;t,x(t;t_{0},x,\lambda\xi),\xi(t;t_{0},x,\lambda\xi)) &= x(s;t_{0},x,\lambda\xi),\\ \xi(s;t,x(t;t_{0},x,\lambda\xi),\xi(t;t_{0},x,\lambda\xi)) &= \xi(s;t_{0},x,\lambda\xi) \end{aligned}$$

and  $e^{\frac{i}{2}t\triangle}\varphi_{\lambda}^{(-t_0)}(x) = \varphi_{\lambda}^{(t-t_0)}(x)$ . We fix  $a \ge 1$ . Let  $V = K \times \Gamma$  be a neighborhood of  $(x_0, \xi_0)$  satisfying (1.4) for  $t = t_0, \lambda \ge 1, a^{-1} \le |\xi| \le a$  and  $(x,\xi) \in V$ . We only show the sufficiency here because the necessity is proved in the same way. To do so, it suffices to show that the following assertion  $P(\sigma, \varphi_0)$  holds for all  $\sigma \geq 0$  and for all  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}.$ 

 $P(\sigma, \varphi_0)$ : "There exists a positive constant  $C_{\sigma, a, \varphi_0}$  such that

$$(3.3) |W_{\varphi_{\lambda}^{(t-t_0)}}u(t, x(t; t_0, x, \lambda\xi), \xi(t; t_0, x, \lambda\xi))| \le C_{\sigma, a, \varphi_0} \lambda^{-\sigma}$$

for all  $x \in K$ , all  $\xi \in \Gamma$  with  $1/a \leq |\xi| \leq a$ , all  $\lambda \geq 1$  and  $0 \leq t \leq t_0$ . " 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  $\xi(t_0; t_0, x, \lambda\xi) = \lambda\xi$ . Hence from (3.3), we have immediately

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

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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 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 brevity.

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

First we show that  $P(0, \varphi_0)$  holds for all  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n)$ . Since  $u_0(x) \in L^2(\mathbb{R}^n)$ ,  $u(t, x) \in C(\mathbb{R}; L^2(\mathbb{R}^n))$ , Schwarz's inequality and the conservation of  $L^2$  norm of solutions of (1.1) show that

$$\begin{split} & \left| W_{\varphi_{\lambda}^{(t-t_{0})}} u(t, x(t; t_{0}, x, \lambda\xi), \xi(t; t_{0}, x, \lambda\xi)) \right| \\ & \leq \int |\varphi_{\lambda}^{(t-t_{0})}(y - x(t; t_{0}, x, \lambda\xi))| |u(t, y)| dy \\ & \leq \|\varphi_{\lambda}^{(t-t_{0})}(\cdot)\|_{L^{2}} \|u(t, \cdot)\|_{L^{2}} \\ & = \|\varphi_{\lambda}(\cdot)\|_{L^{2}} \|u_{0}(\cdot)\|_{L^{2}} = \|\varphi_{0}(\cdot)\|_{L^{2}} \|u_{0}(\cdot)\|_{L^{2}} \end{split}$$

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

Next we show that for a fixed  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$ ,  $P(\sigma + 2b, \varphi_0)$  holds under the assumption that  $P(\sigma, \varphi_0)$  holds for all  $\varphi_0 \in \mathcal{S}(\mathbb{R}^n) \setminus \{0\}$ . To do so, it suffices to show that for fixed  $\varphi_0$ , there exists a positive constant  $C_{a,\varphi_0}$  such that

$$(3.4) |Ru(s, x(s; t_0, x, \lambda\xi), \xi(s; t_0, x, \lambda\xi))| \le C_{a,\varphi_0} \lambda^{-(\sigma+2b)}$$

for all  $x \in K$ , all  $\xi \in \Gamma$  with  $1/a \leq |\xi| \leq a$ , all  $\lambda \geq 1$  and  $0 \leq s \leq t_0$ , since the first term of the right of (3.2) is estimated by  $C\lambda^{-(\sigma+2b)}$  from the condition on  $u_0$ .

Let L be an integer. Taylor's expansion of V(s, y) yields that

(3.5) 
$$Ru(s, x^*, \xi^*)$$
  
=  $\sum_{2 \le |\alpha| \le L-1} \frac{\partial_x^{\alpha} V(s, x^*)}{\alpha!} \int (y - x^*)^{\alpha} \overline{\varphi_{\lambda}^{(s-t_0)}(y - x^*)} u(s, y) e^{-iy\xi^*} dy + R_L,$ 

where

$$\begin{aligned} R_L(s, x^*, \xi^*) &= L \sum_{|\alpha|=L} \frac{1}{\alpha!} \frac{1}{\|\varphi_0\|_{L^2}^2} \\ &\times \iint \left( \int \left( \int_0^1 \partial_x^{\alpha} V(s, x^* - \theta(x^* - y))(1 - \theta)^{L-1} d\theta \right) (y - x^*)^{\alpha} \right. \\ &\times \overline{\varphi_{\lambda}^{(s-t_0)}(y - x^*)} \varphi_{\lambda}^{(s-t_0)}(y - z) e^{-iy(\xi^* - \eta)} dy \right) W_{\varphi_{\lambda}^{(s-t_0)}} u(s, z, \eta) dz d\eta. \end{aligned}$$

Here we use the inversion formula of the wave packet transform

$$W_{\varphi}^{-1}W_{\varphi}f(x) = f(x),$$

where

$$W_{\varphi}^{-1}g(x) = \frac{1}{(2\pi)^n \|\varphi\|_{L^2}^2} \iint g(y,\xi)\varphi(x-y)e^{ix\xi}d\xi dy$$

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

The strategy for the proof of (3.4) is the following. In Step 1, taking  $b = \frac{1}{4} \min(2 - \rho, 1)$  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 (3.5) by  $C\lambda^{-(\sigma+2b)}$ . In Step 2, taking L sufficiently large according to the value of  $\sigma$ , we likewise estimate the second term  $R_L$  of the right hand side of (3.5).

(Step1) We estimate the first term of the right hand side of (3.5). Recall that  $U_0(t) = e^{\frac{i}{2}t\Delta}$ . Since  $xU_0(t) = U_0(t)(x - it\partial_x)$ , we have

$$(y-x^*)^{\alpha}\varphi_{\lambda}^{(t^*)}(y-x^*) = U_0(t^*) \left[ (y-x^*-it^*\partial_y)^{\alpha}(\varphi_0)_{\lambda} \right] (y-x^*)$$
$$= \sum_{\substack{\beta+\gamma=\alpha\\\beta'\leq\beta,\gamma'\leq\gamma}} C_{\beta,\gamma,\beta',\gamma'} t^{*|\beta|} \lambda^{b(|\beta|-|\gamma|)} \varphi_{\lambda}^{(\beta',\gamma')}(t^*,y-x^*),$$

where  $\varphi^{(\beta,\gamma)}(x) = x^{\gamma} \partial_x^{\beta} \varphi_0(x)$  and  $\varphi^{(\beta,\gamma)}_{\lambda}(t,x) = U_0(t) \left(\varphi^{(\beta,\gamma)}\right)_{\lambda}(x)$ . The assumption of induction yields that

|(The first term of the right hand side of (3.5))||

$$\leq \sum_{2 \leq |\alpha| \leq L-1} \sum_{\substack{\beta+\gamma=\alpha\\\beta' \leq \beta, \gamma' \leq \gamma}} \frac{1}{\alpha!} |\partial_x^{\alpha} V(s, x^*)| C_{\beta, \gamma, \beta', \gamma'} |t^*|^{|\beta|} \lambda^{b(|\beta|-|\gamma|)} \\ \times \left| W_{\varphi_{\lambda}^{(\beta', \gamma')}(t^*, x)} u(s, x^*, \xi^*) \right|$$
$$\leq \sum_{2 \leq |\alpha| \leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} C(1+|x^*|)^{\rho-|\alpha|} C_{\beta, \gamma} |t^*|^{|\beta|} \lambda^{b(|\beta|-|\gamma|)} C \lambda^{-\sigma}.$$

Since

(3.6) 
$$x^* = x(s; t_0, x, \lambda\xi) = x + \int_{t_0}^s \dot{x}(s_1) ds_1$$
  
=  $x + (s - t_0)\lambda\xi - \int_{t_0}^s (s - s_1)\nabla_x V(s_1, x(s_1)) ds_1$ ,

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there exists a positive constant  $\lambda_0$  such that

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

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 (3.7)). Hence we have for  $\lambda^{-2b} \leq |t^*| \leq t_0$ 

|(The first term of the right hand side of (3.5))|

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

$$\leq C' \sum_{2 \leq |\alpha| \leq L-1} (1+|t^*|\lambda)^{\rho-|\alpha|} (|t^*|\lambda^b + \lambda^{-b})^{|\alpha|} \lambda^{-\sigma}$$

$$\leq C''' \sum_{2 \leq |\alpha| \leq L-1} (|t^*|\lambda)^{\rho-|\alpha|} (|t^*|\lambda^b)^{|\alpha|} \lambda^{-\sigma}$$

$$\leq C''' \sum_{2 \leq |\alpha| \leq L-1} (|t^*|)^{\rho} \lambda^{\rho-(1-b)|\alpha|} \lambda^{-\sigma} \leq C \lambda^{\rho+2b-2-\sigma} \leq C \lambda^{-2b-\sigma},$$

since  $2b = \frac{1}{2}\min(2-\rho, 1)$ . For  $|t^*| < \lambda^{-2b}$ , we have that

|(The first term of the right hand side of (3.5))|

$$\leq \sum_{2 \leq |\alpha| \leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} CC_{\beta,\gamma} |t^*|^{|\beta|} \lambda^{b(|\beta|-|\gamma|)} C \lambda^{-\sigma}$$
$$\leq \sum_{2 \leq |\alpha| \leq L-1} \sum_{\beta+\gamma=\alpha} \frac{1}{\alpha!} CC_{\beta,\gamma} \lambda^{-b(|\beta|+|\gamma|)} C \lambda^{-\sigma} = C' \lambda^{-2b-\sigma}$$

(Step 2) We estimate  $R_L$ . Let  $\psi_1, \psi_2$  be  $C^{\infty}$  functions 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 with 0 < d < b. 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

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

for j = 1, 2, we have

(3.8) 
$$R_L(s, x^*, \xi^*) = L \sum_{|\alpha|=L} \frac{1}{\alpha!} \frac{1}{(2\pi)^n \|\varphi_0\|_{L^2}^2} \sum_{j=1}^2 I_{\alpha,j}(s, x^*, \xi^*, \lambda).$$

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

(3.9) 
$$|I_{\alpha,j}(s,x^*,\xi^*,\lambda)| \le C_{\sigma,a,\varphi_0}\lambda^{-\sigma-2b}$$

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  $I_{\alpha,1}$ , integration by parts and the fact that  $(1 - \Delta_y)e^{iy(\xi-\eta)} = (1 + |\xi - \eta|^2)e^{iy(\xi-\eta)}$  yield that

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

We take d' such that 0 < d' < d. Since  $|y - x^*| \leq 2(1 + \lambda |t^*|)\lambda^{-d}$  if  $\psi_1\left(\frac{\lambda^d |y - x^*|}{1 + \lambda |t^*|}\right) \neq 0$ , the estimate (3.7) shows that for  $|t^*| \geq \lambda^{d'-1}$  and  $\lambda \geq \lambda_0$  with some  $\lambda_0 \geq 1$ , we obtain

$$\begin{aligned} &|\partial_x^{\alpha} V(s, x^* + \theta(y - x^*))||(y - x^*)^{\alpha}| \\ &\leq C(1 + |x^* + \theta(y - x^*)|)^{\rho - L}(1 + \lambda |t^*|)^L \lambda^{-dL} \\ &\leq C(1 + |x^*| - |y - x^*|)^{\rho - L}(1 + \lambda |t^*|)^L \lambda^{-dL} \\ &\leq C(1 + \lambda |t^*|)^{\rho} \lambda^{-dL}. \end{aligned}$$

Simple calculation yields that

$$\|\partial_y^{\beta}\varphi_{\lambda}^{(t^*)}(y-x^*)\|_{L^2} \le C\lambda^{b|\beta|}, \quad \left|\partial_y^{\beta}\left\{\psi_1\left(\frac{\lambda^d|y-x^*|}{1+\lambda|t^*|}\right)\right\}\right| \le C\lambda^{d|\beta|}.$$

Hence we have

(3.10) 
$$|I_{\alpha,1}(s,x^*,\xi^*,\lambda)| \le C\lambda^{-dL}\lambda^{2N+\rho}.$$

For  $|t^*| \leq \lambda^{d'-1}$ , we have  $|y - x^*| \leq C(1 + \lambda |t^*|)\lambda^{-d} \leq C\lambda^{d'-d}$ , which shows that  $|I_{\alpha,1}| \leq C\lambda^{-(d-d')L}\lambda^{2N+\rho}$ . Hence (3.9) with j = 1 holds if we take L sufficiently large.

Finally we estimate  $I_{\alpha,2}$ . Since  $xU_0(t) = U_0(t)(x - it\nabla_x)$ ,  $\partial_{x_j}U_0(t) = U_0(t)\partial_{x_j}$ ,  $x\varphi_\lambda(x) = \lambda^{-b}(x\varphi)_\lambda(x)$  and  $\nabla\varphi_\lambda(x) = \lambda^{b}(\nabla\varphi)_\lambda(x)$ , we have for any integer M and any multi-index  $\alpha$ 

$$(1+|x|^2)^M \partial_x^{\alpha} \varphi_{\lambda}^{(t)}(x)$$
  
= $U_0(t) \left[ (1+|x-it\nabla|^2)^M \partial_x^{\alpha} \varphi_{0,\lambda}(x) \right]$   
= $U_0(t) \left[ \sum_{|\beta+\gamma| \le 2M} C_{\beta,\gamma}(\lambda^b t)^{|\gamma|} \lambda^{-b(|\beta|-|\alpha|)} (x^{\beta} \partial_x^{\alpha+\gamma} \varphi_0)_{\lambda} \right]$   
 $\le \sum_{|\beta+\gamma| \le 2M} C_{\beta,\gamma}(\lambda^b t)^{|\gamma|} \lambda^{-b(|\beta|-|\alpha|)} U_0(t) \left[ (x^{\beta} \partial_x^{\alpha+\gamma} \varphi_0)_{\lambda} \right].$ 

Hence we have for  $M, N \in \mathbb{N}$ ,

Since  $|y - x^*| \ge \lambda^{-d}(1 + \lambda |t^*|)$  if  $\psi_2(\lambda^d |y - x^*|/(1 + |t^*|\lambda)) \ne 0$ , we have

with M = m + n + 1 and N = n + 1

$$\begin{split} |I_{\alpha,2}| &\leq \sum_{|\alpha_1 + \dots + \alpha_4| \leq 2N} \sum_{|\alpha| \leq |\beta + \gamma| \leq 2M + |\alpha|} \sum_{\alpha'_3 \leq \alpha_3} C|t^*|^{|\gamma|} \lambda^{b(|\gamma| + |\alpha_1|)} \lambda^{b(|\alpha_2| - |\beta|)} \\ &\times (1 + \lambda^{-2d} (1 + \lambda|t^*|)^2)^{-m} \| (1 + |y|^2)^{-n-1}) \|_{L^2_y} \| (1 + |\eta|^2)^{-n-1}) \|_{L^2_\eta} \\ &\times (1 + \lambda|t^*|)^{-|\alpha_3|} \lambda^{d|\alpha_3|} \| y^{\beta - \alpha_2} \partial_y^{\alpha_1 + \gamma} \varphi_0 \|_{L^2_y} \| \partial_z^{\alpha_3} \varphi_0 \|_{L^2_z} \| W_{\varphi_\lambda^{(t^*)}} u(s, z, \eta) \|_{L^2_{z, \eta}} \end{split}$$

For  $0 \le t \le \lambda^{-2b}$ , we have  $|t^*|\lambda^b \le \lambda^{-b}$ . Hence we obtain

$$\begin{split} |I_{\alpha,2}| &\leq \sum_{|\alpha_1 + \dots + \alpha_4| \leq 2N} \sum_{L \leq |\beta + \gamma| \leq 2M + L} \sum_{\alpha'_3 \leq \alpha_3} C\lambda^{-b(|\gamma| + |\beta| - |\alpha_1| - |\alpha_2|)} \lambda^{d|\alpha_3|} \\ &\leq C\lambda^{-b(L-2N)} = C\lambda^{-b(L-2(n+1))} \leq C\lambda^{-2b-\sigma}, \end{split}$$

 $\begin{array}{l} \text{if we take } L \geq N+2n+4+\sigma/b.\\ \text{For } \lambda^{-2b} \leq t \leq t_0, \text{ we have} \end{array}$ 

$$\begin{aligned} |I_{\alpha,2}| \\ &\leq \sum_{|\alpha_1 + \dots + \alpha_4| \leq 2N} \sum_{L \leq |\beta + \gamma| \leq 2M+L} C(1 + \lambda^{-2d}(1 + \lambda|t^*|)^2)^{-m} \\ &\times (\lambda^b |t^*|)^{|\gamma| - |\alpha_2|} \lambda^{b(|\alpha_1| - |\beta|)} \lambda^{d|\alpha_3|} \\ &\leq C(1 + (\lambda^{1-d-2b})^2)^{-m} \lambda^{b(2M+2N+L)} \\ &\leq C\lambda^{-2m(1-d-2b)} \lambda^{b(2m+4(n+1)+L)} \\ &\leq C\lambda^{-2m(1-d-2b)} \lambda^{b(4(n+1)+L)}. \end{aligned}$$

Since  $1-d-2b > 1-4b \ge 0$ , we have  $|I_{\alpha,2}| \le C\lambda^{-2b-\sigma}$ , if we take *m* sufficiently large. This shows (3.9) with j = 2 for  $x \in K$ ,  $\xi \in \Gamma$  with  $1/a \le |\xi| \le a$  and  $\lambda \ge 1$  and  $0 \le s \le t_0$ .

Proof of Corollary 1.6. (3.6) shows that

(3.11) 
$$x(0;t,x,\lambda\xi) = x - \lambda t\xi + \delta_1(\lambda)$$

where  $|\delta_1(\lambda)| \leq C\lambda^{\rho-1}$  uniformly in  $V \cap \{\xi \in \mathbb{R}^n | a^{-1} \leq |\xi| \leq a\}$  for  $\lambda \geq 1$ . In the same way as for (3.11), we have

(3.12) 
$$\xi(0; t, x, \lambda\xi) = \lambda\xi + \delta_2(\lambda)$$

where  $\delta_2(\lambda)$  has the same property of  $\delta_1(\lambda)$ . Roughly speaking, we show that

$$(3.13) \quad W_{\varphi_{\lambda}^{(t^*)}} u_0(x - \lambda t\xi + \delta_1(\lambda), \lambda\xi + \delta_2(\lambda)) = W_{\varphi_{\lambda}^{(t^*)}} u_0(x - \lambda t\xi, \lambda\xi) + (\text{lower order term}).$$

We have

$$W_{\varphi_{\lambda}^{(t^*)}} u_0(x - \lambda t\xi + \delta_1(\lambda), \lambda\xi + \delta_2(\lambda))$$
  
=  $\int \varphi_{\lambda}^{(t^*)} (y - (x - \lambda\xi t + \delta_1(\lambda))) u_0(y) e^{-iy(\lambda\xi + \delta_2(\lambda))} dy$ 

By Taylor's expansion, we have with an integer L

$$\begin{split} \varphi_{\lambda}^{(t^*)}(y - (x - \lambda\xi t + \delta_1(\lambda))) &= \varphi_{\lambda}^{(t^*)}(y - (x - \lambda\xi t)) \\ &+ \sum_{1 \le |\alpha| \le L} \frac{1}{\alpha!} \partial_x^{\alpha} \left( \varphi_{\lambda}^{(t^*)}(y - (x - \lambda\xi t)) \right) (-\delta_1(\lambda))^{\alpha} \\ &+ \sum_{|\alpha| = L+1} \frac{1}{\alpha!} r_{\alpha} \left( -\delta_1(\lambda) \right)^{\alpha}, \end{split}$$

where  $r_{\alpha} = \frac{L+1}{\alpha!} \int_0^1 (1-\theta)^L \partial_y^{\alpha} \varphi_{\lambda}^{(t^*)}(y - (x - \lambda \xi t) - \theta \delta_1(\lambda))$  and

$$e^{-y(\lambda\xi+\delta_2(\lambda))} = e^{-y\lambda\xi} \left(1 + \sum_{1 \le |\alpha|} \frac{1}{\alpha!} \left(-iy\delta_1(\lambda)\right)^{\alpha}\right),$$

from which we obtain

$$\begin{split} W_{\varphi_{\lambda}^{(t^{*})}} u_{0}(x - \lambda t\xi + \delta_{1}(\lambda), \lambda\xi + \delta_{2}(\lambda)) &= \\ W_{\varphi_{\lambda}^{(t^{*})}} u_{0}(x - \lambda t\xi, \lambda\xi) \\ &+ \sum_{1 \leq |\alpha| \leq L} \sum_{1 \leq |\beta|} \lambda^{b|\alpha|} \frac{(-\delta_{1})^{\alpha}}{\alpha!} \frac{(-\delta_{2})^{\beta}}{\beta!} W_{(\partial_{x}^{\alpha} \varphi)_{\lambda}^{(t^{*})}} \left[ y^{\beta} u(y) \right] (x - \lambda t\xi, \lambda\xi) \\ &+ \sum_{|\alpha| = L+1} \sum_{1 \leq |\beta|} \lambda^{b|\alpha|} \frac{(-\delta_{1})^{\alpha}}{\alpha!} \frac{(-\delta_{2})^{\beta}}{\beta!} \int R_{\alpha} y^{\beta} u(y) e^{-iy\lambda\xi} dy. \end{split}$$

Taking *L* large, the above equality implies that  $W_{(\partial_x^{\alpha}\varphi)_{\lambda}^{(t^*)}} \left[y^{\beta}u(y)\right] (x(0;t,x,\lambda\xi), \xi(0;t,x,\lambda\xi))$  and  $W_{(\partial_x^{\alpha}\varphi)_{\lambda}^{(t^*)}} \left[y^{\beta}u(y)\right] (x - \lambda t\xi,\lambda\xi)$  have the same order of with respect to  $\lambda$  uniformly in  $V \cap \{\xi \in \mathbb{R}^n | a^{-1} \leq |\xi| \leq a\}$  for  $\lambda \geq 1$ , since  $|\delta_1(\lambda)|, |\delta_2(\lambda)| \leq \lambda^{\rho-1}, W_{(\partial_x^{\alpha}\varphi)_{\lambda}^{(t^*)}} \left[y^{\beta}u(y)\right] (x - \lambda t\xi,\lambda\xi)$  is the same order of  $W_{\varphi_{\lambda}^{(t^*)}}u_0(x - \lambda t\xi,\lambda\xi)$  with respect to  $\lambda$  and the order of  $\int R_{\alpha}y^{\beta}u(y)e^{-iy\lambda\xi}dy$  with respect to  $\lambda$  is estimated above by some constant. This completes the proof.

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#### §A. Proof of the estimate (3.7)

In this appendix, we give the proof of the estimate (3.7). We fix p. We show the estimate (A.1) below 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 (3.6) 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  $N \ge 0$ . Then we have the solution x(s) of (3.6) as  $x(s) = \lim_{N\to\infty} x^{(N)}(s)$ . We show that there exists a positive constant  $\lambda_0 \ge 1$  such that

(A.1) 
$$\frac{1}{2a}|t^*|\lambda \le |x^{(N)}(s)| \le 2a|t^*|\lambda, \qquad (N=0,1,2,\ldots)$$

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 (A.1) by induction with respect to N.

Obviously (A.1) holds for N = 0.

Assuming that (A.1) holds for N, we have

$$\begin{split} x^{(N+1)}(s)| &\geq |x + (s - t_0)\lambda\xi| - \left|\int_{t_0}^s |s - s_1||\nabla_x V(s_1, x^{(N)}(s_1))| ds_1\right| \\ &\geq |t^*|\lambda|\xi| - |x| - \int_s^{t_0} |s - s_1|C(1 + |x^{(N)}(s_1)|)^{\rho - 1} ds_1 \\ &\geq |t^*|\lambda|\xi| - |x| - C\int_s^{t_0} |s - s_1|(1 + 2(|t_0 - s_1|\lambda|\xi|)^{\rho - 1}) ds_1 \\ &\geq |t^*|\lambda|\xi| - |x| - C|t^*|^2 - C\lambda^{\rho - 1}|\xi|^{\rho - 1}|t^*|^{\rho + 1} \\ &\geq |t^*|\lambda|\xi| \left(1 - \frac{|x|}{|t^*|\lambda|\xi|} - C\frac{|t_0|}{\lambda|\xi|} - C|t_0|^{\rho}\lambda^{\rho - 2}|\xi|^{\rho - 2}\right) \\ &\geq |t^*|\lambda|\xi| \left(1 - \frac{a|x|}{\lambda^{\rho}} - C\frac{a|t_0|}{\lambda} - C\frac{a^{2-\rho}|t_0|^{\rho}}{\lambda^{2-\rho}}\right). \end{split}$$

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

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 (A.1) holds for N.

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