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Remark on wave front sets of solutions to Schrödinger equation of a free particle and a harmonic oscillator

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Abstract. In this paper, we determine the wave front sets of solutions to the Schrödinger equations of the Schrödinger evolution operator of a free particle and of a harmonic oscillator by using the representation of the Schrödinger evolution operator of a free particle introduced by Kato, Kobayashi and Ito (2011) and a new representation of the evolution operator of a harmonic oscillator via wave packet transform (short time Fourier transform).

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§1. Introduction

In this paper, we consider the following initial value problems of the Schrödinger equations of a free particle and of a harmonic oscillator,

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

and

$$\begin{cases} i\partial_t u + \frac{1}{2}\triangle u - \frac{1}{2}|x|^2 u = 0, & (t,x) \in \mathbb{R} \times \mathbb{R}^n, \\ u(0,x) = u_0(x), & x \in \mathbb{R}^n, \end{cases} \tag{1.2}$$

where $i = \sqrt{-1}$, $u : \mathbb{R} \times \mathbb{R}^n \to \mathbb{C}$ and $\triangle = \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2} = \sum_{j=1}^n \partial_j^2$.

We shall determine the wave front sets of solutions to the Schrödinger equations of a free particle and of a harmonic oscillator by using the representation of the Schrödinger evolution operator of a free particle introduced in [14] and a new representation of the evolution operator of a harmonic oscillator via the wave packet transform which is defined by A. Córdoba and C. Fefferman [2]. 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 or windowed Fourier transform in several literatures([10]).

Let $\varphi \in \mathcal{S}(\mathbb{R}^n)\backslash\{0\}$ 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 φ as follows:

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

Transforms with Gaussian function similar to the above are used by many researchers. In 1946, D. Gabor has used discrete version of windowed Fourier transform with Gaussian function to apply to telecommunication([9]). Such transforms are used in some other situation([1], [15], [16]).

In the sequel, we call the function φ a window function (or window).

In the previous paper [14], we give a representation of the Schrödinger evolution operator of a free particle, which is the following:

$$W_{\varphi(t)} u(t,x,\xi) = e^{-\frac{i}{2}t|\xi|^2} W_{\varphi_0} u_0(x-\xi t, \xi), \tag{1.3}$$

where $\varphi(t) = \varphi(t,x) = e^{i\frac{t}{2}\triangle}\varphi_0(x)$ with $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n)$ 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. In the following, we fix $\varphi_0(x) = e^{-|x|^2/2}$. We put

$$\varphi^{(t)}(x) = \frac{1}{(1+it)^{n/2}} \exp\left(-\frac{1}{2(1+it)}|x|^2\right) = e^{i\frac{t}{2}\triangle}\varphi_0(x)$$

and $\varphi_\lambda^{(t)}(x) = \varphi^{(\lambda t)}(\lambda^{1/2}x)$ for $\lambda \geq 1$. For (x_0,ξ_0), we call a subset $V = K \times \Gamma$ of $\mathbb{R}^{2n}$ a conic neighborhood of (x_0,ξ_0) if K is a neighborhood of x_0 and Γ is a conic neighborhood of ξ_0 (i.e. $\xi \in \Gamma$ and $\alpha > 0$ implies $\alpha\xi \in \Gamma$). The following theorems are our main results.

Theorem 1.1. *Let $u_0(x) \in \mathcal{S}'(\mathbb{R}^n)$ and $u(t,x)$ be a solution of* (1.1). *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,ξ_0) such that for all $N \in \mathbb{N}$ and for all $a \geq 1$ there exists a constant $C_{N,a} > 0$ satisfying*

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

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

Remark 1.2. $W_{\varphi_\lambda^{(-t)}} u_0(x,\xi)$ is the wave packet transform of $u_0(x)$ with a window function $\varphi_\lambda^{(-t)}(x)$.

For $x, \xi \in \mathbb{R}^n$, $t \in \mathbb{R}$ and $\lambda \geq 1$, we put

$$\begin{cases} x(t,\lambda) &= x\cos t - \lambda\xi \sin t, \\ \xi(t,\lambda) &= \lambda\xi\cos t + x\sin t, \end{cases}$$

$\varphi_{0,\lambda}(x) = \lambda^{n/4}\varphi_0(\lambda^{1/2}x) = \lambda^{n/4}e^{-\lambda|x|^2/2}$ and $\varphi_\lambda(t) = e^{i\lambda nt}\varphi_{0,\lambda}$. For a solution of (1.2), we have a new representation

$$(1.4)\quad W_{\varphi_\lambda(t)}u(t,x,\xi) = e^{-\frac{i}{2}\int_0^t (|\xi(s-t,\lambda)|^2 - |x(s-t,\lambda)|^2)ds} W_{\varphi_{0,\lambda}} u_0(x(t,\lambda),\xi(t,\lambda)),$$

which is proved in Section 4. By using the representation (1.4), we have the following theorem.

Theorem 1.3. *Let $u_0(x) \in \mathcal{S}'(\mathbb{R}^n)$ and $u(t,x)$ be a solution of (1.2). 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,ξ_0) such that for all $N \in \mathbb{N}$ and for all $a \geq 1$ there exists a constant $C_{N,a} > 0$ satisfying*

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

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, D. Iagolnitzer and L. Hörmander have treated the singularities of functions by this idea independently around 1970. Wave front set is introduced by L. Hörmander in 1970 (see [12]). It is proved in [13] 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 [23] and T. Sakurai [25] 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 [3] have treated this smoothing property microlocally. They have shown for a solution of (1.1) that for a point $x_0 \neq 0$ and a conic neighborhood Γ 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 Γ' 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 [5], [6], [7], [18], [19], [21], [22], [27].

A. Hassell and J. Wunsch [11] and S. Nakamura [20] 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) and $h>0$ $(x_0,\xi_0) \notin WF(u(t))$ if and only if there exists a C_0^∞ 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.

This paper is organized as follows: In Section 2, we give a proof of the representation of (1.3). In Section 3, we prove Theorem 1.1. In Section 4, we prove Theorem 1.3.

§2. Representation of the Schrödinger evolution operator of a free particle

In this section, we recall a proof of the representation (1.3), which is given in [14]. We transform (1.1) via the wave packet transform with respect to the space variable x with window function $\varphi(t,x)$, where $\varphi(t,x) = e^{\frac{i}{2}t\triangle}\varphi_0(x)$ with $\varphi_0(x) \in \mathcal{S}(\mathbb{R}^n)\backslash\{0\}$. By integration by parts, we have

$$
\begin{aligned}
&W_{\varphi(t)}(\triangle u)(t,x,\xi)\\
&= \int \overline{\varphi(t,y-x)}\triangle u(y)e^{-iy\xi}dy\\
&= \int \triangle\overline{\varphi(t,y-x)}u(y)e^{-iy\xi}dy + \int(-2i\xi\cdot\nabla_y)\overline{\varphi(t,y-x)}u(y)e^{-iy\xi}dy\\
&\qquad\qquad\qquad\qquad\qquad\qquad - |\xi|^2 W_{\varphi(t,x)}u(t,x,\xi)\\
&= W_{\triangle\varphi(t)}u(t,x,\xi) + 2i\xi\cdot\nabla_x W_{\varphi(t)}u(t,x,\xi) - |\xi|^2 W_{\varphi(t)}u(t,x,\xi).
\end{aligned}
$$

Since $W_{\varphi(t)}(i\partial_t u)(t,x,\xi) = i\partial_t W_{\varphi(t)}u(t,x,\xi) + W_{i\partial_t\varphi(t)}u(t,x,\xi)$, (1.1) is transformed to

$$
\begin{cases}
(i\partial_t + i\xi\cdot\nabla_x - \frac{1}{2}|\xi|^2)W_{\varphi(t)}u(t,x,\xi) = 0,\\
W_{\varphi(0)}u(0,x,\xi) = W_{\varphi_0}u_0(x,\xi).
\end{cases}
\tag{2.1}
$$

Solving (2.1), we have the representation (1.3). Using the inverse of wave packet transform $W_{\varphi(t)}^{-1}$ for a function $F(x,\xi)$ on $\mathbb{R}^n\times\mathbb{R}^n$ which is defined by

$$
W_{\varphi(t)}^{-1}\left[F(\cdot,\cdot)\right](x) = \frac{1}{\|\varphi(t,\cdot)\|_{L^2}^2}\iint_{\mathbb{R}^{2n}}\varphi(t,x-y)F(y,\xi)e^{ix\xi}dy\,đ\xi,
$$

we have

$$u(t,x) = W^{-1}_{\varphi(t)}\left[e^{-\frac{i}{2}t|\xi|^2} W_{\varphi_0} u_0(x-\xi t,\xi)\right].$$

§3. Proof of Theorem 1.1

In this section, we give a proof of Theorem 1.1. In order to demonstrate Theorem 1.1, we introduce the definition of wave front set $WF(u)$ and the characterization of wave front set by G. B. Folland [8].

Definition 3.1 (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 $a(x)$ in $C_0^\infty(\mathbb{R}^n)$ with $a(x_0) \neq 0$ and a conic neighborhood Γ of ξ_0 such that for all $N \in \mathbb{N}$ there exists a constant $C_N > 0$ satisfying

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

for all $\xi \in \Gamma$.

To prove Theorem 1.1, we use the following characterization of the wave front set by G. B. Folland [8]. Let $\varphi \in \mathcal{S}$ with $\varphi(0) \neq 0$ and $\hat{\varphi}(0) \neq 0$. We put $\varphi_\lambda(x) = \lambda^{n/4}\varphi(\lambda^{1/2}x)$.

Proposition 3.2 (G. B. Folland [8, Theorem 3.22] and T. Ōkaji [21, Theorem2.2])**.** *For $f \in \mathcal{S}'(\mathbb{R}^n)$, we have $(x_0,\xi_0) \notin WF(f)$ if and only if there exist a neighborhood K of x_0 and a conic neighborhood Γ of ξ_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 $\lambda \ge 1$, $a^{-1} \le |\xi| \le a$, $x \in K$ and $\xi \in \Gamma$.

Remark 3.3. Folland [8] has shown that the conclusion follows if the window function φ is an even and nonzero function in $\mathcal{S}(\mathbb{R}^n)$. In Ōkaji [21], the proof of Proposition 3.2 is given. The wave front set can be characterized by F. B. I. transform in almost the same way. (See J.-M. Delort [4] and references therein.)

Proof of Theorem 1.1. Putting $\varphi_\lambda^{(-t)}$ into φ_0 in the equality (1.3), we have

$$W_{\varphi_{0,\lambda}} u(t,x,\lambda\xi) = e^{-\frac{i}{2}t|\xi|^2} W_{\varphi_\lambda^{(-t)}} u_0(x-\lambda\xi t,\lambda\xi),$$

since $e^{\frac{i}{2}t\triangle}\varphi_\lambda^{(-t)} = e^{\frac{i}{2}t\triangle}e^{-\frac{i}{2}t\triangle}\varphi_{0,\lambda} = \varphi_{0,\lambda}$. Hence we have

$$\left|W_{\varphi_{0,\lambda}} u(t,x,\lambda\xi)\right| = |W_{\varphi_\lambda^{(-t)}} u_0(x-\lambda\xi t,\lambda\xi)|. \tag{3.1}$$

This equality (3.1) and Proposition 3.2 yield the conclusion of Theorem 1.1. □

§4. Schrödinger equation of a harmonic oscillator

In this section, we consider the Schrödinger equation of a harmonic oscillator (1.2). Let

$$\begin{cases} i\partial_t\varphi + \frac{1}{2}\triangle\varphi - \frac{1}{2}|x|^2\varphi = 0, & (t,x) \in \mathbb{R}\times\mathbb{R}^n, \\ \varphi(0,x) = \varphi_0(x), & x \in \mathbb{R}^n. \end{cases}$$

By using the wave packet transform with a window $\varphi(t,x)$ with respect to space variable x, (1.2) is transformed to

$$\begin{cases} (i\partial_t + i\xi\cdot\nabla_x - ix\cdot\nabla_\xi - \frac{1}{2}(|\xi|^2 - |x|^2))W_{\varphi(t)}u(t,x,\xi) = 0, \\ W_{\varphi(0)}u(0,x,\xi) = W_{\varphi_0}u_0(x,\xi). \end{cases} \tag{4.1}$$

Solving this first order partial differential equation (4.1), we have

$$W_{\varphi(t)}u(t,x,\xi) = e^{-\frac{i}{2}\int_0^t(|\xi(t-s)|^2-|x(t-s)|^2)ds}W_{\varphi_0}u_0(x(t),\xi(t)),$$

where

$$\begin{cases} x(t) & = x\cos t - \xi\sin t, \\ \xi(t) & = \xi\cos t + x\sin t. \end{cases}$$

If $\varphi_0(x) = \exp(-|x|^2/2)$, then $\varphi(t,x) = e^{int/2}\varphi_0(x)$. Hence we have

$$|W_{\varphi_0}u(t,x,\xi)| = |W_{\varphi(t)}u(t,x,\xi)| = |W_{\varphi_0}u_0(x(t),\xi(t))|. \tag{4.2}$$

Replacing φ_0 to $\varphi_{0,\lambda}$ in (4.2), Proposition 3.2 yields Theorem 1.3.

§5. Further study

Our method in this paper is applicable to the Schrödinger equation with electric potential. Consider the following Schrödinger equation with the potential $V(t,x)$:

$$\begin{cases} i\partial_t u = -\frac{1}{2}\triangle u + V(t,x)u, & (t,x)\in\mathbb{R}\times\mathbb{R}^n, \\ u(0,x) = u_0(x), & x\in\mathbb{R}^n. \end{cases} \tag{5.1}$$

For $\rho < 2$, we put the following assumption on $V(t,x) \in C^\infty(\mathbb{R}^{n+1})$:

Assumption 5.1. For all multi-indices α, there exists a constant $C_\alpha > 0$ such that

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

for all $x \in \mathbb{R}^n$ and all $t \le 0$.

Remark 5.2. In one space dimension, if $V(t,x) = V(x)$ is super-quadratic in the sense that $V(x) \geq C(1+|x|)^{2+\epsilon}$ with $\epsilon > 0$, K. Yajima [26] shows that the fundamental solution of (5.1) has singularities everywhere.

We transform (5.1) via the wave packet transform in the same way as in Section 2 to get

$$
\begin{cases}
\left(i\partial_t + i\xi\cdot\nabla_x - \nabla_x V(t,x)\cdot\nabla_\xi - \frac{1}{2}|\xi|^2 - \widetilde{V}(t,x)\right)\times \\
\qquad\qquad\qquad\qquad W_{\varphi(t)}u(t,x,\xi) = Ru(t,x,\xi), \\
W_{\varphi(0)}u(0,x,\xi) = W_{\varphi_0}u_0(x,\xi),
\end{cases}
\tag{5.2}
$$

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

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

with $V_{jk}(t,x,y) = \int_0^1 \partial_j\partial_k V(t, x+\theta(y-x))(1-\theta)d\theta$. Solving (5.2), we have

(5.3)

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

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

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

From the assumption, $|V_{jk}(t,x,y)|$ is estimated by $C(1+|x|)^{\rho-2}$ if $|x-y|$ is small. Hence we may get the same result as Theorem 1.1 for this case. The proof would be given in our forthcoming paper.

We can transform the initial value problem (5.2) to the integral equation (5.3) formally if the potential function $V(t,x)$ is continuous in t and continuously differentiable in x. So we expect that our method can be applied to nonlinear equations such as: $i\partial_t u + \frac{1}{2}\triangle u = \lambda|u|^{p-1}u$, where λ is a real number and $p > 1$.

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