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On the Schrödinger equation with potential in modulation spaces

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Abstract This work deals with Schrödinger equations with quadratic and sub-quadratic Hamiltonians perturbed by a potential. In particular we shall focus on bounded, but not necessarily smooth perturbations, following the footsteps of the preceding works (Cordero et al., Generalized metaplectic operators and the Schrödinger equation with a potential in the Sjöstrand class, 2013; Cordero et al., Propagation of the Gabor wave front set for Schrödinger equations with non-smooth potentials, 2013). To the best of our knowledge these are the pioneering papers which contain the most general results about the time–frequency concentration of the Schrödinger evolution. We shall give a representation of such evolution as the composition of a metaplectic operator and a pseudodifferential operator having symbol in certain classes of modulation spaces. About propagation of singularities, we use a new notion of wave front set, which allows the expression of optimal results of propagation in our context. To support this claim, many comparisons with the existing literature are performed in this work.

Keywords Fourier integral operators · Modulation spaces · Metaplectic operator · Short-time Fourier transform · Wiener algebra · Schrödinger equation

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1 Introduction

A wave packet is a function on $\mathbb{R}^d$ that is well-localized both in its time and frequency domain. Willing to decompose a function $f(x)$ into uniform wave packets, we are led to the following time–frequency concepts, at the basis of the time–frequency analysis: the linear operators of translation and modulation

$$T_y f(x) = f(x-y) \quad \text{and} \quad M_\xi f(x) = e^{2\pi i \xi x} f(x), \quad x, y, \xi \in \mathbb{R}^d,$$

whose composition is the time–frequency shift $\pi(z) = M_\xi T_y$, $z = (y, \xi) \in T^*\mathbb{R}^d = \mathbb{R}^{2d}$, called the phase-space (or time–frequency space).

Given $g \in \mathcal{S}(\mathbb{R}^d)\setminus\{0\}$, the so-called Gabor atom $\pi(z)g$ can then be considered a wave packet.

As elementary application of this decomposition, consider the Cauchy problem for the Schrödinger equation which describes the free particle:

$$\begin{cases} i\dfrac{\partial u}{\partial t} + \Delta u = 0 \\ u(0,x) = u_0(x), \end{cases} \tag{1}$$

with $x \in \mathbb{R}^d$, $d \geq 1$. The explicit formula for the solution is the Fourier multiplier

$$u(t,x) = e^{it\Delta} u_0(x) = (K_t * u_0)(x), \tag{2}$$

where[1]

$$K_t(x) = \frac{1}{(4\pi i t)^{d/2}} e^{i|x|^2/(4t)}. \tag{3}$$

Starting with the wave packet $u_0 = \pi(z)\varphi$, where $\varphi(x) = e^{-\pi|x|^2}$ is the Gaussian function, the computations developed in [10, Section 6] show that the solution $u(t,x) = e^{it\Delta}(\pi(z)\varphi)(x)$, $z = (z_1, z_2) \in \mathbb{R}^{2d}$, is given by

$$u(t,x) = (1+4\pi i t)^{-d/2} e^{-\frac{4\pi^2 t z_2(2z_1 + i z_2)}{1+4\pi i t}} M_{\frac{z_2}{1+4\pi i t}} T_{z_1} e^{-\frac{\pi}{1+4\pi i t}|x|^2}. \tag{4}$$

Then straightforward computations show there exist constant $C_t > 0$, $\epsilon_t > 0$, depending on t, such that

$$|\langle u, \pi(w)\varphi\rangle| \leq C e^{-\epsilon|w - \mathcal{A}_t z|^2} \tag{5}$$

where $\mathcal{A}_t z = (z_1 + 4\pi t z_2, z_2)$. So the evolution $e^{it\Delta}$ sends wave packets into wave packets and the phase-space concentration of the evolution is well-determined.

This simple example gives the intuition that the evolution of Schrödinger equations with Hamiltonians coming from classical mechanics can be still interpreted as trajectory of particles in phase-space. In fact (5) tells us that for a wave-packet initial datum,

[1] If $z \in \mathbb{C}$, with $\operatorname{Re} z \geq 0$, $z \neq 0$, we take as argument of $z^{1/2}$ that belonging to $[-\pi/4, \pi/4]$. We then define $z^{k/2} = (z^{1/2})^k$ if k is an integer.

the solution is highly concentrated along the trajectory of the corresponding classical system. In other terms, wave packets correspond to particles which roughly follow the classical trajectory in phase-space.

The natural concept in this order of ideas is the time–frequency representation called the short-time Fourier transform. Precisely, the short-time Fourier transform (STFT) of a function or distribution f on $\mathbb{R}^d$ with respect to a Schwartz window function $g \in \mathcal{S}(\mathbb{R}^d)\setminus\{0\}$ is defined by

$$V_g f(z) = \langle f, \pi(z)g\rangle = \int_{\mathbb{R}^d} f(v)\overline{g(v-z_1)}e^{-2\pi i v z_2}\, dv, \quad z=(z_1,z_2)\in\mathbb{R}^{2d}. \quad (6)$$

The time–frequency localization of f is obtained by comparison to wave packets $\pi(z)g$: f is localized near $z_0 \in \mathbb{R}^{2d}$ if $V_g f(z)$ is large for z near z_0 and decays off z_0. The formal theory of time–frequency localization leads to modulation spaces, introduced by Feichtinger in 1983 [17]. Namely, fix $g \in \mathcal{S}(\mathbb{R}^d)$, consider a weight function m on $\mathbb{R}^{2d}$ and $1 \le p \le \infty$. The modulation space $M^p_m(\mathbb{R}^d)$ is defined as the space of all tempered distribution $f \in \mathcal{S}'(\mathbb{R}^d)$ for which

$$\int_{\mathbb{R}^{2d}} |V_g f(z)|^p m(z)^p\, dz < \infty \quad (7)$$

(with obvious modifications for $p=\infty$, see Sect. 2 below). The measure of the time–frequency localization of f is done by computing a weighted L^p norm of the corresponding STFT $V_g f$. If $m=1$ (unweighted case), we simply write M^p in place of M^p_m. A preliminary question is then the following.

Does the Schrödinger evolution preserve modulation spaces?

A first positive answer for the evolution of the free particle in (1) is contained in the pioneering work [1] on boundedness on modulation spaces for Fourier multipliers:

$$\|e^{it\Delta}u_0\|_{M^p} \le C(1+|t|)^{d/2}\|u_0\|_{M^p}, \quad u_0 \in \mathcal{S}(\mathbb{R}^d).$$

The proof follows from (4), (5), by taking into account the t-dependence.

The study of nonlinear Schrödinger equations and other PDEs in modulation spaces has been widely developed by Wang and collaborators in many papers, see e.g., [43, 50, 51] and the recent textbook [52].

Here our attention is addressed to more general linear Schrödinger equations. Namely we show how time–frequency analysis can be successfully applied in the study of the Cauchy problem for linear Schrödinger equations of the type

$$\begin{cases} i\dfrac{\partial u}{\partial t} + Hu = 0 \\ u(0,x) = u_0(x), \end{cases} \quad (8)$$

with $t \in \mathbb{R}$ and the initial condition $u_0 \in \mathcal{S}(\mathbb{R}^d)$ or some larger space. We consider an operator H of the form

$$H = a^w + \sigma^w, \tag{9}$$

where a^w is the Weyl quantization of a real quadratic homogeneous polynomial on $\mathbb{R}^{2d}$ and σ^w is a pseudodifferential operator (in the Weyl form) with a rough symbol σ, belonging to a suitable modulation space. We recall that the Weyl quantization of a symbol $a(x, \xi)$ is correspondingly defined as

$$a^w f(x) = a^w(x, D) f = \iint_{\mathbb{R}^{2d}} e^{2\pi i (x-y)\xi} a\Big(\frac{x+y}{2}, \xi\Big) f(y) dy\, d\xi,$$

see [18,54]. The aim is to find conditions on the perturbation σ^w for which the evolution e^{itH} preserves modulation spaces. Estimates on modulation spaces for Schrödinger evolution operators e^{itH} are performed in the works [31–34]. In particular, the most general result is given in [34], where the authors study the operator $H = \Delta - V(t, x)$, the time–dependent potential $V(t, x)$ being smooth and quadratic or sub-quadratic. They obtain boundedness results for the propagator e^{itH} in the unweighted modulation spaces $M^{p,q}$, $1 \le p, q \le \infty$ (see definition in Sect. 2). In these papers the key idea is to consider, as window function to estimate the modulation space norm of the solution $e^{itH} u_0$, the Schwartz function $\varphi(t, \cdot) = e^{it\Delta}\varphi$, for a given $\varphi = \varphi(0, \cdot) \in \mathcal{S}(\mathbb{R}^d) \setminus \{0\}$, used to estimate the modulation norm of the initial datum u_0.

Related results in the L^p-theory are contained in [29,30]. Finally, more general Hamiltonians and potentials are studied in [7,13]. In particular the perturbation operators have symbols in the so-called Sjöstrand class $S_w = M^{\infty,1}(\mathbb{R}^{2d})$.

In what follows we shall present to the reader a proof, new in literature, of the boundedness of e^{itH} on modulation spaces when the perturbation σ^w belongs to the following scale of modulation spaces

$$S_w^s = M^\infty_{1\otimes v_s}(\mathbb{R}^{2d}), \quad v_s(z) = \langle z\rangle^s = (1 + |z|^2)^{s/2},\ z \in \mathbb{R}^{2d}, \tag{10}$$

with the parameter $s > 2d$ (See Theorem 5.1 in the sequel). Observe that

$$\bigcap_{s\ge 0} S_w^s = S^0_{0,0}, \tag{11}$$

where $S^0_{0,0}$ is the Hörmander class of all $\sigma \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ satisfying

$$|\partial^\alpha \sigma(z)| \le C_\alpha, \quad \alpha \in \mathbb{Z}_+^{2d},\ z = (x, \xi) \in \mathbb{R}^{2d}. \tag{12}$$

For $s \to 2d+$, the symbols in S_w^s have a smaller regularity. In particular, for $s > 2d$, $S_w^s \subset \mathcal{C}^0(\mathbb{R}^{2d})$, but the differentiability is lost in general as soon as $s \le 2d + 1$.

Finally, note that $\bigcup_{s>2d} S_w^s \subset S_w \subset \mathcal{C}^0(\mathbb{R}^{2d})$, with strict inclusions.

The representation of the evolution operator e^{ita^w} which is related to the unperturbed Schrödinger equation $\sigma^w = 0$ is already well understood since e^{ita^w} is then a metaplectic operator. To benefit of non-expert readers, we shall study in detail this case in the next Sect. 5. We recall that metaplectic operators quantize linear symplectic transformations of the phase-space and arise as intertwining operators of the Schrödinger representation of the Heisenberg group.

If we consider the perturbed problem ($\sigma^w \neq 0$), a natural question is as follows:

What is the representation of e^{itH} in presence of perturbations?

An answer in the case $\sigma^w = \sigma_t(x)$, that is, the potential is a multiplication by a smooth function $\sigma_t \in \mathcal{C}^\infty(\mathbb{R}^d)$, satisfying additional decay properties together with its derivatives, is contained in Weinstein [53]. There the evolution e^{itH} was written as a composition of a metaplectic operator with a pseudodifferential operator having symbol in particular subclasses of Hörmander classes. We generalize widely the latter result by considering rough potentials with symbols in S^s_w and showing that e^{itH} is the product of a metaplectic operator and of a pseudodifferential operator (with symbol in S^s_w) for every $t \in \mathbb{R}$, that is, as defined below, a generalized metaplectic operator. The class of the generalized metaplectic operators enters the class of the Fourier integral operators introduced and studied in [6].

First, we recall the classical metaplectic operators. Let $\mathcal{A}$ be a symplectic matrix on $\mathbb{R}^{2d}$ (we write $\mathcal{A} \in Sp(d, \mathbb{R})$), i.e., $\mathcal{A}$ is a $2d \times 2d$ invertible matrix such that $\mathcal{A}^T J \mathcal{A} = J$, where

$$J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix} \tag{13}$$

is related to the standard symplectic form on $\mathbb{R}^{2d}$

$$\omega(x, y) = {}^t x J y, \qquad x, y \in \mathbb{R}^{2d}. \tag{14}$$

Then, the metaplectic operator $\mu(\mathcal{A})$ may be defined by the intertwining relation

$$\pi(\mathcal{A}z) = c_{\mathcal{A}}\, \mu(\mathcal{A})\pi(z)\mu(\mathcal{A})^{-1} \quad \forall z \in \mathbb{R}^{2d}, \tag{15}$$

with a phase factor $c_{\mathcal{A}} \in \mathbb{C}$, $|c_{\mathcal{A}}| = 1$ (actually this only defines a projective representation of $Sp(d, \mathbb{R})$; one then needs supplementary efforts to construct, using the corresponding cocyle, a true representation of the double cover of $Sp(d)$. A detailed construction is given in [15]).

The kernel or so-called Gabor matrix of the metaplectic operator with respect to the set of the time–frequency shifts $\pi(z)$ satisfies the following estimate. If $\mathcal{A} \in \mathrm{Sp}(d, \mathbb{R})$ and $g \in \mathcal{S}(\mathbb{R}^d)$, then for every $N \geq 0$ there exists a $C_N > 0$ such that

$$|\langle \mu(\mathcal{A})\pi(z)g, \pi(w)g\rangle| \leq C_N \langle w - \mathcal{A}z\rangle^{-N}, \qquad w, z \in \mathbb{R}^{2d}. \tag{16}$$

The Gabor matrix is the point of departure in the definition of the generalized metaplectic operators.

Definition 1.1 Given $\mathcal{A} \in Sp(d, \mathbb{R})$, $g \in \mathcal{S}(\mathbb{R}^d)$, and $s \geq 0$, we say that a linear operator $T : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$ is a generalized metaplectic operator, in short $T \in FIO(\mathcal{A}, s)$, if the Gabor matrix of T satisfies the decay condition

$$|\langle T\pi(z)g, \pi(w)g\rangle| \le C\langle w - \mathcal{A}z\rangle^{-s}, \qquad w, z \in \mathbb{R}^{2d}. \tag{17}$$

The union

$$FIO(Sp(d,\mathbb{R}), s) = \bigcup_{\mathcal{A}\in Sp(d,\mathbb{R})} FIO(\mathcal{A}, s)$$

is then called the class of *generalized metaplectic operators*. A generalized metaplectic operator is then proved to be the composition of a metaplectic operator with a pseudodifferential operator having symbol in the class S^s_w, cf. Theorem 3.3 below.

The main result, that is Theorem 5.1 in the sequel, shows that the propagator of the perturbed problem (8), (9) is a generalized metaplectic operator.

The last problem which arises in the study of the evolution e^{itH} is related to propagation of singularities.

How the evolution e^{itH} propagates the singularities of the initial datum u_0?

To answer this question, we employ a new definition of wave front set, called Gabor wave front set, which is a generalization of the global wave front set introduced by Hörmander in 1991 [25] and redefined by using time–frequency analysis in [42]. See also [12]. The definition of the classical, the global and the Gabor wave front set, together with a comparison with related results in the literature, is detailed in the last section.

The contents of the next sections are the following. In Sect. 2 we recall the main time–frequency analysis tools and properties of pseudodifferential operators useful for our results. In Sect. 3 we survey the main properties of generalized metaplectic operators. Sections 4 and 5 contain the study of the unperturbed and perturbed Schrödinger equation, respectively. In particular, in Sect. 5 it is stated and proved the main result of this paper (Theorem 5.1). Finally, to give a whole treatment of this topic, in Sect. 6 we recall the definition of the Gabor wave front set and review results of propagation of singularities of the evolution e^{itH}, showing some important examples.

2 Preliminaries and time–frequency analysis tools

We refer the reader to [20] for an introduction to time–frequency concepts. We write $xy = x \cdot y$ for the scalar product on $\mathbb{R}^d$ and $|t|^2 = t \cdot t$ for $t, x, y \in \mathbb{R}^d$. The Schwartz class is denoted by $\mathcal{S}(\mathbb{R}^d)$, the space of tempered distributions by $\mathcal{S}'(\mathbb{R}^d)$. The brackets $\langle f, g\rangle$ denote the extension to $\mathcal{S}'(\mathbb{R}^d) \times \mathcal{S}(\mathbb{R}^d)$ of the inner product $\langle f, g\rangle = \int f(t)\overline{g(t)}dt$ on $L^2(\mathbb{R}^d)$. The Fourier transform is given by $\hat{f}(\eta) = \mathcal{F}f(\eta) = \int f(t)e^{-2\pi i t\eta}dt$. We write $A \asymp B$ for the equivalence $c^{-1}B \le A \le cB$.

2.1 Modulation spaces

Consider a distribution $f \in \mathcal{S}'(\mathbb{R}^d)$ and a Schwartz function $g \in \mathcal{S}(\mathbb{R}^d)\setminus\{0\}$ (the so-called *window*). The STFT of f with respect to g is defined by (6). The STFT is well-defined whenever the bracket $\langle\cdot,\cdot\rangle$ makes sense for dual pairs of function or (ultra-)distribution spaces, in particular for $f \in \mathcal{S}'(\mathbb{R}^d)$ and $g \in \mathcal{S}(\mathbb{R}^d)$, or for $f, g \in L^2(\mathbb{R}^d)$.

Weighted modulation spaces measure the decay of the STFT on the time–frequency (or phase space) plane and were defined by Feichtinger in the 80's [17].

Let us first introduce the weight functions. A weight function v on $\mathbb{R}^{2d}$ is submultiplicative if $v(z_1 + z_2) \le v(z_1)v(z_2)$, for all $z_1, z_2 \in \mathbb{R}^{2d}$. We shall work with the weight functions

$$v_s(z) = \langle z\rangle^s = (1 + |z|^2)^{\frac{s}{2}}, \quad s \in \mathbb{R}, \tag{18}$$

which are submultiplicative for $s \ge 0$.

If $\mathcal{A} \in \mathrm{GL}(d, \mathbb{R})$, the class of real $d \times d$ invertible matrices, then $|\mathcal{A}z|$ defines an equivalent norm on $\mathbb{R}^{2d}$, hence for every $s \in \mathbb{R}$, there exist $C_1, C_2 > 0$ such that

$$C_1 v_s(z) \le v_s(\mathcal{A}z) \le C_2 v_s(z), \quad \forall z \in \mathbb{R}^{2d}. \tag{19}$$

For $s \ge 0$, we denote by $\mathcal{M}_{v_s}(\mathbb{R}^{2d})$ the space of v_s-moderate weights on $\mathbb{R}^{2d}$; these are measurable positive functions m satisfying $m(z + \zeta) \le C v_s(z) m(\zeta)$ for every $z, \zeta \in \mathbb{R}^{2d}$.

Definition 2.1 Given $g \in \mathcal{S}(\mathbb{R}^d)$, $s \ge 0$, a weight function $m \in \mathcal{M}_{v_s}(\mathbb{R}^{2d})$, and $1 \le p, q \le \infty$, the *modulation space* $M_m^{p,q}(\mathbb{R}^d)$ consists of all tempered distributions $f \in \mathcal{S}'(\mathbb{R}^d)$ such that $V_g f \in L_m^{p,q}(\mathbb{R}^{2d})$ (weighted mixed-norm spaces). The norm on $M_m^{p,q}(\mathbb{R}^d)$ is

$$\|f\|_{M_m^{p,q}} = \|V_g f\|_{L_m^{p,q}} = \left(\int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} |V_g f(x, \eta)|^p m(x, \eta)^p \, dx \right)^{q/p} d\eta \right)^{1/q} \tag{20}$$

(with obvious modifications for $p = \infty$ or $q = \infty$).

When $p = q$, we simply write $M_m^p(\mathbb{R}^d)$ instead of $M_m^{p,p}(\mathbb{R}^d)$. The spaces $M_m^{p,q}(\mathbb{R}^d)$ are Banach spaces, and every nonzero $g \in M_{v_s}^1(\mathbb{R}^d)$ yields an equivalent norm in (20). Thus $M_m^{p,q}(\mathbb{R}^d)$ is independent of the choice of $g \in M_{v_s}^1(\mathbb{R}^d)$.

In the sequel we shall use the following inversion formula for the STFT (see [20, Proposition 11.3.2]): assume $g \in M_v^1(\mathbb{R}^d) \setminus \{0\}$, $f \in M_m^{p,q}(\mathbb{R}^d)$, then

$$f = \frac{1}{\|g\|_2^2} \int_{\mathbb{R}^{2d}} V_g f(z) \pi(z) g \, dz\,, \tag{21}$$

and the equality holds in $M_m^{p,q}(\mathbb{R}^d)$.

The adjoint operator of V_g, defined by

$$V_g^* F(t) = \int_{\mathbb{R}^{2d}} F(z) \pi(z) g dz\,,$$

maps the Banach space $L_m^{p,q}(\mathbb{R}^{2d})$ into $M_m^{p,q}(\mathbb{R}^d)$. In particular, if $F = V_g f$ the inversion formula (21) becomes

$$\mathrm{Id}_{M_m^{p,q}} = \frac{1}{\|g\|_2^2} V_g^* V_g. \tag{22}$$

2.2 Metaplectic and pseudodifferential operators

Consider $g \in \mathcal{S}(\mathbb{R}^d)\backslash\{0\}$ with $\|g\|_2 = 1$. Then, using the inversion formula (21), any linear continuous operator $T : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$ admits the following time–frequency representation:

$$V_g(Tf)(w) = \int_{\mathbb{R}^{2d}} k(w,z) V_g f(z)\, dz. \tag{23}$$

where we call the kernel

$$k(w,z) := \langle T\pi(z)g, \pi(w)g\rangle, \quad w, z \in \mathbb{R}^{2d} \tag{24}$$

the continuous Gabor matrix of the operator T. The name is related to the discretization of T by means of Gabor frames. More precisely, the collection of time–frequency shifts $\mathcal{G}(g,\Lambda) = \{\pi(\lambda)g : \lambda \in \Lambda\}$ for a non-zero $g \in \mathcal{S}(\mathbb{R}^d)$ (or more generally $g \in L^2(\mathbb{R}^d)$) is called a Gabor frame, if there exist constants $A, B > 0$ such that

$$A\|f\|_2^2 \le \sum_{\lambda\in\Lambda} |\langle f, \pi(\lambda)g\rangle|^2 \le B\|f\|_2^2 \qquad \forall f \in L^2(\mathbb{R}^d). \tag{25}$$

This implies the expansion with unconditional convergence in $L^2(\mathbb{R}^d)$:

$$f = \sum_{\lambda\in\Lambda} \langle f, \pi(\lambda)\gamma\rangle \pi(\lambda)g \qquad \forall f \in L^2(\mathbb{R}^d) \tag{26}$$

where γ is a dual window of g. Using (26) the following Gabor decomposition of the operator T is obtained:

$$Tf(x) = \sum_{\mu\in\Lambda}\sum_{\lambda\in\Lambda} \underbrace{\langle T\pi(\lambda)g, \pi(\mu)g\rangle}_{T_{\mu\lambda}} c_\lambda \pi(\mu)\gamma,$$

where $c_\lambda = \langle f, \pi(\lambda)\gamma\rangle$ are the Gabor coefficients of f with respect to the dual Gabor frame $\mathcal{G}(\gamma,\Lambda)$ and the infinite matrix $\{T_{\mu\lambda}\}_{\mu,\lambda\in\Lambda}$ is called the *Gabor matrix* of T. For simplicity, from now on we shall present the theory only from a continuous point of view, but the discrete counterpart by Gabor frames works as well, and this is indeed the starting point for further numerical implementations.

Metaplectic operators Given a symplectic matrix $\mathcal{A} \in Sp(d,\mathbb{R})$, the corresponding metaplectic operator $\mu(\mathcal{A})$ can be defined by the intertwining relation (15) (see also Sect. 4).

For matrices $\mathcal{A} \in Sp(d, \mathbb{R})$ in special form, the corresponding metaplectic operators can be computed explicitly. Precisely, For $f \in L^2(\mathbb{R}^d)$, we have

$$\mu\left(\begin{pmatrix} A & 0 \\ 0 & {}^tA^{-1} \end{pmatrix}\right) f(x) = (\det A)^{-1/2} f(A^{-1}x) \tag{27}$$

$$\mu\left(\begin{pmatrix} I & 0 \\ C & I \end{pmatrix}\right) f(x) = \pm e^{-i\pi Cx\cdot x} f(x) \tag{28}$$

$$\mu(J) = i^{d/2}\mathcal{F}^{-1}, \tag{29}$$

where $\mathcal{F}$ denotes the Fourier transform.

The Gabor matrix of a metaplectic operator $\mu(\mathcal{A})$ is concentrated along the graph of the symplectic phase-space transformation $\mathcal{A}$ and decays super polynomially outside, as expressed in the first part of the following version of [7, Lemma 2.2]. The second part gives a technical information used later (the proof is analogous to the one of [7, Lemma 2.2]).

Lemma 2.2 (i) *Fix $g \in \mathcal{S}(\mathbb{R}^d)$ and $\mathcal{A} \in Sp(d, \mathbb{R})$, then, for all $N \geq 0$,*

$$|\langle \mu(\mathcal{A})\pi(z)g, \pi(w)g\rangle| \leq C_N \langle w - \mathcal{A}z\rangle^{-N}. \tag{30}$$

(ii) *If $\sigma \in M^\infty_{1\otimes v_s}$ and $\mathcal{A} \in Sp(d, \mathbb{R})$, then $\sigma \circ \mathcal{A} \in M^\infty_{1\otimes v_s}$ and*

$$\|\sigma \circ \mathcal{A}^{-1}\|_{M^\infty_{1\otimes v_s}} \leq \|(\mathcal{A}^T)^{-1}\|^s \, \|V_{\Phi\circ\mathcal{A}}\Phi\|_{L^1_{v_s}} \|\sigma\|_{M^\infty_{1\otimes v_s}}, \tag{31}$$

where $\Phi \in \mathcal{S}(\mathbb{R}^{2d})$ is the window used to compute the norms of σ and $\sigma \circ \mathcal{A}^{-1}$.

In particular, using (23) for $T = \mu(\mathcal{A})$ and the estimate (30), we can write for every $N \geq 0$

$$|V_g(\mu(\mathcal{A})f)(w)| \leq C_N \int_{\mathbb{R}^{2d}} \langle w - \mathcal{A}z\rangle^{-N} |V_g f(z)|\, dz.$$

Consider now a weight $m \in \mathcal{M}_{v_s}$, $s \geq 0$. Then the v_s-moderateness yields

$$|V_g(\mu(\mathcal{A})f)(w)| m(w) \leq C_N \int_{\mathbb{R}^{2d}} \langle w - \mathcal{A}z\rangle^{s-N} m(\mathcal{A}z) |V_g f(z)|\, dz$$

and choosing N such that $s - N < -2d$ by Young's inequality we obtain the following boundedness result:

Theorem 2.3 *Consider $m \in \mathcal{M}_{v_s}$, $s \geq 0$ and $\mathcal{A} \in Sp(d, \mathbb{R})$. Then the metaplectic operator $\mu(\mathcal{A})$ is bounded from $M^p_{m\circ\mathcal{A}}(\mathbb{R}^d)$ into $M^p_m(\mathbb{R}^d)$, $1 \leq p \leq \infty$, with the norm estimate*

$$\|\mu(\mathcal{A})f\|_{M^p_m} \leq C_s \|f\|_{M^p_{m\circ\mathcal{A}}}. \tag{32}$$

The continuity property of a metaplectic operator $\mu(\mathcal{A})$ on $M^{p,q}(\mathbb{R}^d)$, with $p \neq q$, fails in general. Indeed, an example is provided by the multiplication operator defined in (28), which is bounded on $M^{p,q}(\mathbb{R}^d)$ if and only if $p = q$, as proved in [9, Proposition 7.1].

Pseudodifferential operators These operators can be described by the off-diagonal decay of their corresponding Gabor matrices, if their symbols are chosen in suitable modulations spaces. This is the main insight of the papers [19,21]. Namely, we have:

Proposition 2.4 ([19]) *Fix $g \in \mathcal{S}(\mathbb{R}^d)$, consider $\sigma \in \mathcal{S}'(\mathbb{R}^{2d})$ and $s \in \mathbb{R}$.*

(i) *The symbol σ is in $M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$ if and only if there exists a function $H \in L^1_{v_s}(\mathbb{R}^{2d})$ such that*
$$|\langle \sigma^w \pi(z)g, \pi(w)g\rangle| \leq H(w-z) \qquad \forall w, z \in \mathbb{R}^{2d}\,. \tag{33}$$
The function H can be chosen as
$$H(z) = \sup_{u\in\mathbb{R}^{2d}} |V_\Phi\sigma(u, j(z))|, \tag{34}$$
where $j(z) = (z_2, -z_1)$ for $z = (z_1, z_2) \in \mathbb{R}^{2d}$ and the window function $\Phi = W(g, g)$ is the Wigner distribution of g.

(ii) *We have $\sigma \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$ if and only if*
$$|\langle \sigma^w \pi(z)g, \pi(w)g\rangle| \leq C\langle w-z\rangle^{-s} \qquad \forall w, z \in \mathbb{R}^{2d}, \tag{35}$$
where the constant C in (35) satisfies
$$C \asymp \|\sigma\|_{M^{\infty}_{1\otimes v_s}}. \tag{36}$$

In the context of Definition 1.1 the class of pseudodifferential operators with a symbol in $M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$ is just $FIO(\mathrm{Id}, s)$.

The previous characterization is the key idea to show that the preceding pseudodifferential operators give rise to a sub-algebra of $\mathcal{B}(L^2(\mathbb{R}^d))$ (the algebra of linear bounded operators on $L^2(\mathbb{R}^d)$) which is inverse-closed (or enjoys the so-called Wiener property), as contained in the following results [19,21,46].

Theorem 2.5 *Assume that $\sigma \in M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$ (resp. $\sigma \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$, with $s > 2d$). Then:*

(i) *Boundedness: σ^w is bounded on every modulation space $M^{p,q}_m(\mathbb{R}^d)$ for $1 \leq p, q \leq \infty$ and every v_s-moderate weight m.*

(ii) *Algebra property: If $\sigma_1, \sigma_2 \in M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$ (resp. $\sigma \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$), then $\sigma_1^w\sigma_2^w = \tau^w$ with a symbol $\tau \in M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$ (resp. $\sigma \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$).*

(iii) *Wiener property: If σ^w is invertible on $L^2(\mathbb{R}^d)$, then $(\sigma^w)^{-1} = \tau^w$ with a symbol $\tau \in M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$ (resp. $\sigma \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$).*

The algebra property represents one of the main ingredients in the study of the properties of the Schrödinger propagator e^{itH} developed in Sect. 5. In particular, the kernel of the composition of n pseudodifferential operators σ_j^w, with $\sigma_j \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$, $j = 1, \dots, n$, and $s > 2d$, satisfies

$$|\langle \sigma_1^w \sigma_2^w \dots \sigma_n^w \pi(z)g, \pi(w)g\rangle| \leq C_0 C_1 \dots C_n \langle w - z\rangle^{-s} \quad w, z \in \mathbb{R}^{2d}, \tag{37}$$

where

$$C_j \asymp \|\sigma_j\|_{M^{\infty}_{1\otimes v_s}} \tag{38}$$

and $C_0 > 0$ depends only on s. The proof is straightforward: in fact, the characterization of Proposition 2.4 says that $\sigma_j \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$ if and only if $|\langle \sigma_j^w \pi(z)g, \pi(w)g\rangle| \leq C_j \langle w - z\rangle^{-s}$ and the result follows from induction and the fact that, for $s > 2d$, the weights v_s are subconvolutive: $v_s^{-1} * v_s^{-1} \leq C_0\, v_s^{-1}$ (cf. [20, Lemma 11.1.1]).

3 Properties of the class $FIO(\mathcal{A}, s)$

Generalized metaplectic operators solve evolution equations of the form (8), (9), when the perturbation is a pseudodifferential operator with symbol in the classes S^s_w. They were introduced and studied in [6], as classes of Fourier integral operators (FIOs) associated with linear symplectic transformations of the phase-space. We observe that this work studies also FIOs associated to more general symplectomorphisms.

As already mentioned, the crucial property of the generalized metaplectic operators we shall need in the study of Schrödinger equations is the algebra property of the class $FIO(\mathcal{A}, s)$. However, for sake of completeness, we recall the main properties of this class, obtained in [6], and also other properties peculiar of the weighted versions of the Sjöstrand class, i.e., the modulation spaces $M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$, cf. [7].

First of all, the definition of the class $FIO(\mathcal{A}, s)$ is independent of the window function $g \in \mathcal{S}(\mathbb{R}^d)\setminus\{0\}$ chosen in the Definition 1.1. The class $FIO(\mathcal{A}, s)$ is non-empty: every classical metaplectic operator $\mu(\mathcal{A})$ satisfies (16) for every $s \geq 0$ and so $\mu(\mathcal{A}) \in FIO(\mathcal{A}, s)$ for every $s \geq 0$.

Using the estimate of the Gabor matrix for a generalized metaplectic operator in (16) and repeating similar arguments as for the classical metaplectic operators $\mu(\mathcal{A})$ in the previous section, we obtain the following boundedness results for the class $FIO(\mathcal{A}, s)$:

Theorem 3.1 *Fix $\mathcal{A} \in Sp(d, \mathbb{R})$, $s > 2d$, $m \in \mathcal{M}_{v_s}$ and $T \in FIO(\mathcal{A}, s)$. Then T extends to a bounded operator from $M^p_{m\circ\mathcal{A}}(\mathbb{R}^d)$ to $M^p_m(\mathbb{R}^d)$, $1 \leq p \leq \infty$.*

In particular, since the weights v_s and $v_s \circ \mathcal{A}$ are equivalent for every $s \in \mathbb{R}$ and $\mathcal{A} \in Sp(d, \mathbb{R})$, the generalized metaplectic operator T in Theorem 3.1 is bounded on $M^p_{v_s}(\mathbb{R}^d)$ and on $M^p_{1/v_s}(\mathbb{R}^d)$. The previous theorem for $p = 2$ and $m \equiv 1$ says that the classes $FIO(\mathcal{A}, s)$ are subclasses of $\mathcal{B}(L^2(\mathbb{R}^d))$. The next results show that their union $FIO(Sp(d, \mathbb{R}), s)$ is indeed an algebra in $\mathcal{B}(L^2(\mathbb{R}^d))$ which enjoys the property of inverse-closedness:

Theorem 3.2 *We have:*

(i) *If* $T^{(i)} \in FIO(\mathcal{A}_i, s_i)$, $\mathcal{A}_i \in Sp(d, \mathbb{R})$, *with* $s_i > 2d$, $i = 1, 2$; *then* $T^{(1)}T^{(2)} \in FIO(\mathcal{A}_1 \circ \mathcal{A}_2, s)$ *with* $s = \min(s_1, s_2)$. *Consequently, the class* $FIO(Sp(d, \mathbb{R}), s)$ *is an algebra with respect to the composition of operators.*
(ii) *If* $T \in FIO(\mathcal{A}, s)$, $s > 2d$, *and* T *is invertible on* $L^2(\mathbb{R}^d)$, *then* $T^{-1} \in FIO(\mathcal{A}^{-1}, s)$. *Consequently, the algebra* $FIO(Sp(d, \mathbb{R}), s)$ *is inverse-closed in* $\mathcal{B}(L^2(\mathbb{R}^d))$.

Finally, the operators in the classes $FIO(\mathcal{A}, s)$ are not *abstract ghosts* since they can be explicitly written as a simple composition of a classical metaplectic operator and a pseudodifferential operator, as expressed in [6, Theorem 5.4], recalled below.

Theorem 3.3 *Fix* $s > 2d$ *and* $\mathcal{A} \in Sp(d, \mathbb{R})$. *A linear continuous operator* $T : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$ *is in* $FIO(\mathcal{A}, s)$ *if and only if there exist symbols* $\sigma_1, \sigma_2 \in M^\infty_{1\otimes v_s}(\mathbb{R}^{2d})$, *such that*

$$T = \sigma_1^w(x, D)\mu(\mathcal{A}) \quad \textit{and} \quad T = \mu(\mathcal{A})\sigma_2^w(x, D). \tag{39}$$

The symbols σ_1 *and* σ_2 *are related by*

$$\sigma_2 = \sigma_1 \circ \mathcal{A}. \tag{40}$$

The characterization (39) works also for other τ-forms of pseudodifferential operators $a_\tau(x, D)$, $\tau \in [0, 1]$, where the τ-quantization of a symbol $a(x, \xi)$ on the phase-space is formally defined by

$$a \mapsto a_\tau(x, D)f = \iint_{\mathbb{R}^{2d}} e^{2\pi i(x-y)\xi} a(\tau x + (1-\tau)y, \xi) f(y)dy\, d\xi$$

($\tau = 1/2$ is the Weyl quatization whereas $\tau = 1$ is the Kohn–Nirenberg correspondence). Instead (40) is peculiar of the Weyl correspondence and is a consequence of the symplectic invariance property of the Weyl calculus (e.g. [26, Theorem 18.5.9]):

$$\mu(A)^{-1}\sigma^w \mu(\mathcal{A}) = \mu(\mathcal{A})(\sigma \circ \mathcal{A})^w.$$

For $T \in FIO(\mathcal{A}, s)$ with $\mathcal{A} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in Sp(d, \mathbb{R})$ satisfying the additional condition $\det A \neq 0$ we have the following characterization, that can be proved by using the same arguments as those in the result [7, Theorem 5.1] [related to symbols in the classes $M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$]. We leave the details to the interested reader.

Theorem 3.4 $T \in FIO(\mathcal{A}, s)$ *if and only if* T *has the following integral representation*

$$Tf(x) = \int_{\mathbb{R}^d} e^{2\pi i \Phi(x,\xi)} \sigma(x, \xi) \hat{f}(\xi) d\xi \tag{41}$$

with the phase $\Phi(x, \xi) = \frac{1}{2} xCA^{-1}x + \xi A^{-1}x - \frac{1}{2}\xi A^{-1}B\xi$ *and a symbol* $\sigma \in M^\infty_{1\otimes v_s}(\mathbb{R}^{2d})$.

An operator T in the form (41) is called a type I Fourier integral operator, with phase Φ and symbol σ. If we drop the condition $\det A \neq 0$ the operator T is no more a FIO of type I, but certainly can be characterized by other suitable integral representations. Integral representations for classical metaplectic operators were studied by Morsche and Oonincx in [38]. Our object of further investigation will be to study the compositions of the integral representations in [38] with pseudodifferential operators and derive an integral expression for any $T \in FIO(\mathcal{A}, s)$.

4 Metaplectic operators as solutions of the unperturbed problem

We first give a brief review concerning the solution of

$$\begin{cases} i\dfrac{\partial u}{\partial t} + a^w u = 0 \\ u(0,x) = u_0(x), \end{cases} \tag{42}$$

when the symbol $a(x,\xi)$ is a quadratic form on the phase space. Writing $u(t,\cdot) = M_t u(0,\cdot)$, we obtain the following equation for the solution operator M_t:

$$\begin{cases} i\dfrac{dM_t}{dt} + a^w M_t = 0 \\ M_0 = I. \end{cases} \tag{43}$$

The properties of the operator M_t are well-known an can be found in different textbooks. We refer to [15,18,22,48] and the references therein. Moreover, we address to Voros [49, Section 4.6] (see also [53, Section 3]) for a short survey of the subject, from the viewpoint of group theory and geometrical quantization.

In short, suppose we are given a real-valued homogeneous second order polynomial $a(x,\xi)$, say

$$a(x,\xi) = -\frac{1}{2}{}^t(x,\xi)J\mathbb{A}(x,\xi) = \frac{1}{2}\xi\cdot B\xi + \xi\cdot Ax - \frac{1}{2}x\cdot Cx,$$

with

$$\mathbb{A} = \begin{pmatrix} A & B \\ C & -{}^tA \end{pmatrix} \tag{44}$$

in the symplectic algebra $\mathfrak{sp}(d,\mathbb{R})$, therefore B, C are symmetric.

Its Weyl quantization is defined as

$$a^w = -\frac{1}{8\pi^2}\sum_{j,k=1}^{d} B_{j,k}\frac{\partial^2}{\partial x_j\partial x_k} - \frac{i}{2\pi}\sum_{j,k=1}^{d} A_{j,k}x_j\frac{\partial}{\partial x_k} - \frac{i}{4\pi}\mathrm{Tr}(A) - \frac{1}{2}\sum_{j,k=1}^{d} C_{j,k}x_jx_k.$$

Then the Schrödinger equation (43) has a unique solution $M_t = \mu(\mathcal{A}_t)$, $\mathcal{A}_t = e^{t\mathbb{A}} \in Sp(d,\mathbb{R})$ [always with an ambiguity by a factor, because we are considering here the simplified version of the metaplectic representation as a map $\mu : Sp(d,\mathbb{R}) \to U(L^2(\mathbb{R}^d))$; see the remark soon after (15)].

Hence, the solution to the Cauchy problem (42), can be written as

$$u = e^{ita^w} u_0 = \mu(\mathcal{A}_t) u_0$$

with $\mathcal{A}_t = e^{t\mathbb{A}} \in Sp(d,\mathbb{R})$.

The previous theory has further extensions. First, we note that the Schrödinger representation ρ of the Heisenberg group $\mathbb{H}^d$ and μ fit together to give rise to the *extended metaplectic representation* μ_e (see [4,14] and references therein). We briefly review its construction.

The Heisenberg group $\mathbb{H}^d$ is the group obtained by defining on $\mathbb{R}^{2d+1}$ the product

$$(z,t)\cdot(z',t') = \left(z+z', t+t'+\frac{1}{2}\omega(z,z')\right), \quad z,z' \in \mathbb{R}^{2d},\ t,t' \in \mathbb{R}$$

where ω stands for the standard symplectic form in $\mathbb{R}^{2d}$ given in (14). The Schrödinger representation of the group $\mathbb{H}^d$ on $L^2(\mathbb{R}^d)$ is then defined by

$$\begin{aligned}\rho(x,\xi,t)f(y) &= e^{2\pi i t} e^{-\pi i x\xi} e^{2\pi i \xi y} f(y-x)\\ &= e^{2\pi i t} e^{-\pi i x\xi} M_\xi T_x f(y) = e^{2\pi i t} e^{-\pi i x\xi} \pi(z) f(y),\end{aligned}$$

where $z=(x,\xi)$. The representations ρ and μ can be combined and give rise to the extended metaplectic representation μ_e of the group $G = \mathbb{H}^d \rtimes Sp(d,\mathbb{R})$, the semidirect product of $\mathbb{H}^d$ and $Sp(d,\mathbb{R})$. The group law on G is

$$((z,t),A)\cdot\big((z',t'),A'\big) = \big((z,t)\cdot(Az',t'),AA'\big) \tag{45}$$

and the extended metaplectic representation μ_e of G is

$$\mu_e\left((z,t),A\right) = \rho(z,t)\circ\mu(A). \tag{46}$$

The role of the center of the Heisenberg group is only a product by a phase factor, and if we omit it, the "true" group under consideration is $\mathbb{R}^{2d} \rtimes Sp(d,\mathbb{R})$, which we denote again by G. Thus G acts naturally by affine transformations on phase space, namely

$$g\cdot(x,\xi) = ((q,p),A)\cdot(x,\xi) = A^t(x,\xi) + {}^t(q,p). \tag{47}$$

and its Lie algebra is isomorphic to the Lie algebra $\mathcal{P}_2$ of real-valued polynomials of degree ≤ 2. Indeed, the map which takes the infinitesimal (extended) metaplectic operator ia^w, with ($a \in \mathcal{P}_2$) to the hamiltonian vector field

$$\sum_{j=1}^{d}\left(\frac{\partial a}{\partial x_j}\frac{\partial}{\partial \xi_j} - \frac{\partial a}{\partial \xi_j}\frac{\partial}{\partial x_j}\right)$$

is an isomorphism between the algebra of infinitesimal (extended) metaplectic operators and the Lie algebra spanned by the constant and linear symplectic vector fields.

Another generalization is related to time-dependent symbols a_t. Suppose we are given a continuous curve ia_t^w, $a_t \in \mathcal{P}_2$, of infinitesimal (extended) metaplectic operators. Then, the theory above, written for the case of a time–independent operator ia^w) still works and the Schrödinger equation (42) (with symbol a replaced by a_t) has solution than can be uniquely represented (up to a phase factor) by the extended metaplectic operator

$$u = e^{ita_t^w} u_0 = \mu_e(g_t) u_0$$

where $g_t \in G$ is a continuous curve on G. This more general case was studied by Weinstein [53, Section 3] and is also object of our further investigations. We refer also to [15] for more details.

5 Perturbed Schrödinger equations

We now consider the Cauchy problem in (8), where the hamiltonian a^w, Weyl quantization of a real-valued homogeneous quadratic polynomial as discussed in the previous section, is perturbed by adding a pseudodifferential operator σ^w with a symbol $\sigma \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$, $s > 2d$. Results concerning the quantization a^w of a more general real-valued polynomial of degree ≤ 2 and a potential $V(t, x)$ which is only a multiplication operator are also mentioned in the end of this section. Our main result is as follows.

Theorem 5.1 *Consider the Cauchy problem* (8) *with* $H = a^w + \sigma^w$ *and* a^w *and* σ^w *as above. Then,*

(i) *The evolution operator* e^{itH} *is a generalized metaplectic operator for every* $t \in \mathbb{R}$. *Specifically, we have*

$$e^{itH} = \mu(\mathcal{A}_t) b^w_{1,t} = b^w_{2,t} \mu(\mathcal{A}_t), \quad t \in \mathbb{R} \tag{48}$$

for some symbols $b_{1,t}, b_{2,t} \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$ *and where* $\mu(\mathcal{A}_t) = e^{ita^w}$ *is the solution to* (43).

(ii) *Consider* $m \in \mathcal{M}_{v_s}$, $1 \leq p \leq \infty$. *Then* e^{itH} *extends to a bounded operator from* $M^p_{m\circ\mathcal{A}_t}(\mathbb{R}^d)$ *to* $M^p_m(\mathbb{R}^d)$. *In particular, if* $u_0 \in M^p_{v_s}$, *then* $u(t, \cdot) = e^{itH} u_0 \in M^p_{v_s}$, *for all* $t \in \mathbb{R}$.

Proof The pattern of the proof follows [7, Theorem 4.1], where symbols in the classes $M^{\infty,1}_{1\otimes v_s}(\mathbb{R}^{2d})$ were considered. The main ingredient is the theory about bounded perturbation of operator (semi)groups (see, e.g. the textbooks [41] and [16]) and is quite standard. Indeed, this is the model already employed in some of the papers that inspired our work, namely Zelditch [56] and Weinstein [53]. In what follows we shall explain the main ideas of this proof.

Since $\sigma \in M^{\infty}_{1\otimes s}(\mathbb{R}^{2d}) \subset M^{\infty,1}(\mathbb{R}^{2d})$, for $s > 2d$, the Weyl operator σ^w is bounded on $L^2(\mathbb{R}^d)$ (see [46] and Theorem 2.5 before) and more generally on every modulation space $M^p_m(\mathbb{R}^d)$ with weight m being v_s-moderate (see [19] and Theorem 2.5 before). Using the boundedness result for classical metaplectic operators in (32) we observe that the solution of the unperturbed problem $\mu(\mathcal{A}_t) = e^{ita^w}$ is a one-parameter group strongly continuous on $L^2(\mathbb{R}^d)$ and on every $M^p_m(\mathbb{R}^d)$ with $m \asymp m \circ \mathcal{A}$ for every $\mathcal{A} \in Sp(d, \mathbb{R})$. Hence also the evolution e^{itH} generates a one-parameter group strongly continuous on $M^p_m(\mathbb{R}^d)$ as above, thanks to the standard theory (see [16, Ch. 3, Cor. 1.7]). This immediately gives the boundedness $\|e^{itH}u_0\|_{M^p_{v_s}} \leq C\|u_0\|_{M^p_{v_s}}$, for all $s, t \in \mathbb{R}$, that is the second part of Theorem 5.1, (ii); whereas the continuity for a more general weight $m \in \mathcal{M}_{v_s}$ follows by Theorem 3.1, once we have proved that e^{itH} is a generalized metaplectic operator. We focus on this claim. The two main ingredients that give the result are represented by the algebra property of generalized metaplectic operators contained in Theorem 3.2, (i), and the characterization of pseudodifferential operators in Proposition 2.4, (ii). Namely, if $e^{itH} = \mu(\mathcal{A}_t)P(t)$, we need to show that for every $t \in \mathbb{R}$ the operator $P(t)$ is a pseudodifferential operator with symbol in $M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$. Writing

$$B(t) = \mu(\mathcal{A}_{-t})\sigma^w \mu(\mathcal{A}_t) \in FIO(\mathcal{A}_{-t} \circ Id \circ \mathcal{A}_t, s) = FIO(Id, s),$$

(hence $B(t)$ is a pseudodifferential operator with symbol in $M^{\infty}_{1\otimes v_s}$) the operator $P(t)$ can be written using the following *Dyson-Phillips expansion*

$$P(t) = \mathrm{Id} + \sum_{n=1}^{\infty}(-i)^n \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} B(t_1)B(t_2)\dots B(t_n)\, dt_1 \dots dt_n := \sum_{n=0}^{\infty} P_n(t)\,. \tag{49}$$

We study the Gabor matrix of $P(t)$, working on a kernel level, as done in the pioneering work of Zelditch [56] whereas we notice that Weinstein [53] uses the Weyl calculus of pseudodifferential operators and studies a similar Dyson expansion on a symbol level.

First, using (37) we have

$$\left|\left\langle \prod_{j=1}^{n} B(t_j)\pi(z)g, \pi(w)g \right\rangle\right| \leq C C_{t_1} C_{t_2} \dots C_{t_n} \langle w - z\rangle^{-s}$$

with $C_{t_j} \asymp \|\sigma \circ \mathcal{A}_{t_j}^{-1}\|_{M^{\infty}_{1\otimes v_s}}$, $j = 1, \dots n$. Using Lemma 2.2

$$\sup_{0\leq r\leq t} \|\sigma \circ \mathcal{A}_r^{-1}\|_{M^{\infty}_{1\otimes v_s}} \leq \|\sigma\|_{M^{\infty}_{1\otimes v_s}} \sup_{0\leq r\leq t} \|\mathcal{A}_r\|^s \,\|V_{\Phi\circ\mathcal{A}_r}\Phi\|_{L^1_{v_s}} \leq M(t)\|\sigma\|_{M^{\infty}_{1\otimes v_s}},$$

where $M(t) = \sup_{0\leq r\leq t} \|\mathcal{A}_r\|^s \,\|V_{\Phi\circ\mathcal{A}_r}\Phi\|_{L^1_{v_s}}$ is easily proved to be finite. The Gabor matrix of $P_n(t)$ can then by controlled by

$$|\langle P_n(t)\pi(z)g, \pi(w)g\rangle| \leq C\frac{t^n}{n!} M(t)^n \|\sigma\|^n_{M^{\infty}_{1\otimes v_s}} \langle w - z\rangle^{-s},$$

and, consequently, the Gabor matrix of $P(t)$ satisfies

$$|\langle P(t)\pi(z)g, \pi(w)g\rangle| \le \sum_{n=0}^{\infty} |\langle P_n(t)\pi(z)g, \pi(w)g\rangle| \langle w-z\rangle^{-s}$$
$$\le C \sum_{n=0}^{\infty} \frac{t^n M(t)^n \|\sigma\|^n_{M^{\infty}_{1\otimes v_s}}}{n!} \langle w-z\rangle^{-s}$$
$$= C(t)\langle z-w\rangle^{-s},$$

for a new function $C(t) > 0$. This gives by Proposition 2.4, (ii), that $P(t) = b^w_{1,t}$ for a symbol $b_{1,t}$ in $M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$. Finally, the characterization of generalized metaplectic operators in Theorem 3.3 gives also the second equality in (48):

$$e^{itH} = b^w_{2,t}\mu(\mathcal{A}_t)$$

for some $b_{2,t} \in M^{\infty}_{1\otimes v_s}(\mathbb{R}^{2d})$, and this ends the proof. □

We now compare these issues with other results in the literature. First, in the framework of time–frequency analysis, we mention the pioneering work [1] on boundedness on modulation spaces for Fourier multipliers: as special example we find the free particle evolution operator $e^{it\Delta}$. The study of PDEs and in particular of nonlinear Schrödinger equations in modulation spaces has been widely developed by B. Wang and collaborators in many papers, see e.g., [43,50,51] and the recent textbook [52]. Inspired by these new nonlinear topics we would like to use the previous techniques for a Cauchy problem (8) where the operator H contains a nonlinearity, this is our future project.

Estimates on modulation spaces for Schrödinger evolution operators e^{itH} were also performed in the works [31–34], as detailed in the Introduction.

A result similar to Theorem 5.1, were the linear affine transformation $\mathcal{A}_t$ is replaced by a more general symplectomorphism χ_t and the solution e^{itH} is no more a generalized metaplectic operator but a Fourier integral operator in the classes $FIO(\chi_t, s)$, is provided in [12, Theorem 4.1]). There the Hamiltonian $a^w(x, D)$ is a pseudodifferential operator where the symbol $a(z)$, $z = (x, \xi)$, is real-valued positively homogeneous of degree 2, i.e. $a(\lambda z) = \lambda^2 a(z)$ for $\lambda > 0$, with $a \in \mathcal{C}^{\infty}(\mathbb{R}^{2d}\setminus 0)$. Indeed, the singularity at the origin of $a(z)$ can be admitted as well, by absorbing it in a non-smooth potential. In this way, the pseudodifferential operator $a^w(x, D)$ can be modified such that its symbol is in the Shubin classes [44] (see also [24]) and the symbolic calculus can be applied.

Finally, we spend some additional words about two papers that we often mentioned in the preceding pages, namely the work of Zelditch [56] and its generalization by Weinstein [53]. The former studies propagation of singularities for evolution operators e^{itH} where $H = \Delta - V$ and V is a multiplication by a potential function $V(x)$ which differs only slightly from a positive-definite quadratic function (so H is very similar to the harmonic oscillator). A local representation of the propagator e^{itH} using metaplectic operators is obtained and the main result says that the singularities of the solution $u(t,\cdot) = e^{itH}u_0$ behave as in the case of the harmonic oscillator. The latter paper generalizes the former one by considering $H = a_t^w + V_t$, where the time–dependent hamiltonian a_t^w is the Weyl quantization of a real-valued polynomial $a(x,\xi)$ of degree ≤ 2 and the time–dependent potential $V_t(x)$ is a smooth function in $(t,x) \in \mathbb{R} \times \mathbb{R}^d$ which belongs to particular subclasses of $S^0_{0,0}$. A local representation of e^{itH} as product of a metaplectic and a pseudodifferential operator having symbol in these subclasses is obtained and propagation of singularities are studied.

6 Propagation of singularities

To have a complete understanding of the subject, we present related results concerning the propagation of singularities, obtained in [12]. There, a new definition of wave front set is given, extending the so-called global wave front set introduced by Hörmander in 1991 [25] and which is different from the classical one, already studied in [26, Chap. 8], which suits well in the study of certain classes of evolution operators of hyperbolic type.

First, we recall the classical Hörmander wave front set in [26, Chap. 8]. Given $x_0 \in \mathbb{R}^d$, we define by φ_{x_0} a test function in $\mathcal{C}_0^\infty(\mathbb{R}^d)$ such that $0 \leq \varphi_{x_0}(x) \leq 1$ for every $x \in \mathbb{R}^d$ and $\varphi_{x_0}(x) = 1$ for x in a neighborhood of x_0. Given $\xi_0 \in \mathbb{R}^d \backslash \{0\}$ we define by ψ_{ξ_0} a function in $\mathcal{C}^\infty(\mathbb{R}^d)$, supported in a conic open set $\Gamma \subset \mathbb{R}^d \backslash \{0\}$ containing ξ_0, such that $\psi_{\xi_0}(\xi) = 1$ for $\xi \in \Gamma'$, $|\xi| \geq A$ for a conic open set Γ' such that $\xi_0 \in \Gamma' \subset \Gamma$ and $\psi_{\xi_0}(\xi) = 0$ for $|\xi| < R$ for some $0 < R < A$. We define the classical Hörmander wave front set $WF_\psi(u)$ of a distribution $u \in \mathcal{S}'(\mathbb{R}^d)$ (or $u \in \mathcal{D}'(\mathbb{R}^d)$), as follows: for $(x_0,\xi_0) \in \mathbb{R}^d \times \mathbb{R}^d \backslash \{0\}$, $(x_0,\xi_0) \notin WF_\psi(u)$ if there exist φ_{x_0} and ψ_{ξ_0} such that $\psi_{\xi_0}(D)(\varphi_{x_0}u) \in \mathcal{S}(\mathbb{R}^d)$. Here $\psi_{\xi_0}(D)$ is the Fourier multiplier with symbol ψ_{ξ_0}, that is

$$\psi_{\xi_0}(D)(\varphi_{x_0}u)(x) = \int_{\mathbb{R}^d} e^{2\pi i x\xi}\psi_{\xi_0}(\xi)\widehat{\varphi_{x_0}u}(\xi)\, d\xi.$$

Hence the functions φ_{x_0} and ψ_{ξ_0} represent the cut-off in time and in frequency, respectively. For hyperbolic equations of the type

$$i\frac{\partial u}{\partial t} + a^w(t,x,D)u = 0$$

with $u(0,x) = u_0$, and where $a(t,x,\xi)$ is a real-valued hamiltonian, homogeneous of the first order in ξ, we have for the solution $u(t,x)$:

$$WF_\psi(u(t)) = \chi_t(WF_\psi(u_0))$$

where χ_t is the symplectomorphism defined by the Hamiltonian $a(t,x,\xi)$. We want a similar result for the evolution of the Schrödinger equation (8). To reach this goal, we introduce a wave front set that does the job. This is a generalization of the global Hörmander wave front set $WF_G(f)$, that we recall in what follows. Namely, we use an equivalent definition via STFT introduced (and proved to be equivalent) in [42]. Consider $u \in \mathcal{S}'(\mathbb{R}^d)$, $z_0 \in \mathbb{R}^{2d}\setminus\{0\}$ and fix $g \in \mathcal{S}(\mathbb{R}^d)\setminus\{0\}$. Then $z_0 \notin WF_G(u)$ if there exists an open conic set $\Gamma_{z_0} \subset \mathbb{R}^{2d}$ containing z_0 such that for every $r > 0$

$$|V_g u(z)| \leq C_r \langle z \rangle^{-r}, \quad z \in \Gamma_{z_0} \tag{50}$$

for a suitable $C_r > 0$. Then $WF_G(u)$ is a conic closed subset of $\mathbb{R}^{2d} \setminus \{0\}$ and its definition does not depend on the choice of the nonzero window function g in $\mathcal{S}(\mathbb{R}^d)$. Finally, we define the Gabor wave front set $WF_G^{p,r}(u)$ under our consideration as follows [12].

Definition 6.1 Let $g \in \mathcal{S}(\mathbb{R}^d)$, $g \neq 0$, $r > 0$. For $u \in M^p_{v_{-r}}(\mathbb{R}^d)$, $z_0 \in \mathbb{R}^{2d}$, $z_0 \neq 0$, we say that $z_0 \notin WF_G^{p,r}(u)$ if there exists an open conic neighborhood $\Gamma_{z_0} \subset \mathbb{R}^{2d}$ containing z_0 such that for a suitable constant $C > 0$

$$\int_{\Gamma_{z_0}} |V_g u(z)|^p \langle z \rangle^{pr} \, dz < \infty \tag{51}$$

(with obvious changes for $p = \infty$).

Then $WF_G^{p,r}(u)$ is well-defined as conic closed subset of $\mathbb{R}^{2d}\setminus\{0\}$. Furthermore, the definitions of $WF_G^{p,r}(f)$ does not depend on the choice of the window g. We have the following characterizations:

$$u \in M^p_{v_r}(\mathbb{R}^d) \Leftrightarrow WF_G^{p,r}(u) = \emptyset$$

and, similarly,

$$u \in \mathcal{S}(\mathbb{R}^d) \Leftrightarrow WF_G(f) = \emptyset.$$

The propagation of singularities for the evolution e^{itH} of our equation (8) are proved in [12] and summarized as follows.

Theorem 6.2 *Consider* $\sigma \in M^\infty_{1\otimes v_s}$, $s > 2d$, $1 \leq p \leq \infty$. *Then*

$$e^{itH} : M^p_{v_r}(\mathbb{R}^d) \to M^p_{v_r}(\mathbb{R}^d) \tag{52}$$

continuously, for $|r| < s - 2d$. *Moreover, for* $u_0 \in M^p_{v_{-r}}(\mathbb{R}^d)$,

$$WF_G^{p,r}(e^{itH}u_0) = \mathcal{A}_t(WF_G^{p,r}(u_0)), \tag{53}$$

provided $0 < 2r < s - 2d$.

Observe the more restrictive assumption on r for (53), with respect to that for (52).

Using (11) and (53), we may recapture the known results for the propagation in the case of a smooth potentials, i.e. $\sigma \in S^0_{0,0}$. Then the estimate (17) is satisfied for every s and from Theorem 6.2 we recapture for $u_0 \in \mathcal{S}'(\mathbb{R}^d)$

$$WF_G(e^{itH}u_0) = \mathcal{A}_t(WF_G(u_0)). \tag{54}$$

This identity is contained in many preceding results. Although it is impossible to do justice to the vast literature in this connection, let us mention the pioneering work of Hörmander [25] 1991, who defined the wave front set in (50) as well as its analytic version, and proved (54) in the case of the metaplectic operators. For subsequent results providing (54) and its analytic-Gevrey version for general smooth symbols, let us refer to [23,27,28,35–37,39,40,55]. The wave front sets introduced there under different names actually coincide with those of Hörmander 1991, cf. [42,45], and [3]. Finally, for sake of completeness, let us recall the propagation of singularities for a pseudodifferential operators in the framework of the global and the Gabor wave front set. Observe the difference in the symbol classes and in the domain of the distribution u.

Proposition 6.3 *Let $\sigma \in M^\infty_{1\otimes v_s}(\mathbb{R}^{2d})$, $s > 2d$ and $0 < 2r < s - 2d$. Then, for every $u \in M^p_{v_{-r}}(\mathbb{R}^d)$ we have*

$$WF_G^{p,r}(\sigma(x,D)u) \subset WF_G^{p,r}(u). \tag{55}$$

If $\sigma \in S^0_{0,0}$, then for every $u \in \mathcal{S}'(\mathbb{R}^d)$,

$$WF_G(\sigma(x,D)u) \subset WF_G(u). \tag{56}$$

From the previous results it follows that the study of the propagation of singularities of the evolution e^{itH} should be conducted as follows: if the perturbation σ^w in (9) is the quantization of a smooth potential $\sigma \in S^0_{0,0}$ we use the global wave front set $WF_G(u)$, otherwise, if the symbol is rough and $\sigma \in M^\infty_{1\otimes v_s}(\mathbb{R}^{2d})$, for some $s > 2d$, then we use the Gabor wave front set $WF_G^{p,r}(u)$, with the limitation $0 < 2r < s - 2d$. We end up this section with two examples, the first is the harmonic oscillator and the second example is a perturbation of it with a rough potential. In order to compute the wave front set $WF_G(u)$ we need the following preliminary results.

Proposition 6.4 *We have:*

(i) *Let ξ_0 be fixed in $\mathbb{R}^d$. Then*

$$WF_G(e^{2\pi i x\xi_0}) = \{z = (x,\xi), x \neq 0, \xi = 0\}$$

independently of ξ_0.

(ii) *Let $c \in \mathbb{R}$, $c \neq 0$, be fixed. Then*

$$WF_G(e^{\pi i c|x|^2}) = \{z = (x,\xi),\ x \neq 0,\ \xi = cx\}.$$

Example 1 **The harmonic oscillator**.

Consider the Cauchy problem

$$\begin{cases} i\partial_t u + \frac{1}{4\pi}\Delta u - \pi|x|^2 u = 0 \\ u(0,x) = u_0(x). \end{cases} \tag{57}$$

The solution is

$$u(t,x) = (\cos t)^{-d/2} \int_{\mathbb{R}^d} e^{2\pi i[\frac{1}{\cos t}x\xi - \frac{\tan t}{2}(x^2+\xi^2)]}\hat{u_0}(\xi)\,d\xi, \quad t \neq \frac{\pi}{2} + k\pi, \ k \in \mathbb{Z}. \tag{58}$$

The Gabor matrix with Gaussian window $g(x) = e^{-\pi|x|^2}$ can be explicitly computed as

$$|k(w,z)| = 2^{-\frac{d}{2}} e^{-\frac{\pi}{2}|z-\mathcal{A}_t(w)|^2}, \tag{59}$$

where

$$\mathcal{A}_t{}^t(y,\xi) = \begin{pmatrix} (\cos t)I & (-\sin t)I \\ (\sin t)I & (\cos t)I \end{pmatrix} \begin{pmatrix} y \\ \xi \end{pmatrix} \tag{60}$$

with I being the identity matrix. Observe that the expression (59) is meaningful for every $t \in \mathbb{R}$. Let us address to [10, Section 6.2] for applications to numerical experiments.

We may test (54) on the initial datum $u_0(x) = 1$, giving for $t < \pi/2$,

$$u(t,x) = (\cos t)^{-d/2} e^{-\pi i \tan t|x|^2}.$$

From Proposition 6.4, (i) and (ii), we have coherently with (60)

$$\begin{aligned} WF_G\,(u(t,x)) &= \{(x,\xi),\ x = (\cos t)y,\ \xi = (\sin t)y,\ y \neq 0\} \\ &= \mathcal{A}_t(WF_G\,(1)) = \mathcal{A}_t(\{(y,\eta),\ y \neq 0, \eta = 0\}). \end{aligned}$$

Example 2 **Perturbed harmonic oscillator**.
Consider the perturbed harmonic oscillator in dimension $d = 1$

$$\begin{cases} i\frac{\partial u}{\partial t} + \frac{1}{4\pi}\frac{\partial^2 u}{\partial x^2} - \pi x^2 u + |\sin x|^\mu u = 0 \\ u(0,x) = u_0(x) \end{cases} \tag{61}$$

with $\mu > 1$, $x \in \mathbb{R}$. So in this case $\sigma^w = |\sin x|^\mu$ is a multiplication operator. By [12, Corollary 2.4] we have $\sigma \in M^\infty_{1\otimes v_{\mu+1}}(\mathbb{R}^2)$. From Theorem 6.2 we have that the Cauchy problem is well-posed for $u_0 \in M^p_{v_r}(\mathbb{R})$, $|r| < \mu - 2$ and the propagation of $WF_G^{p,r}\,(u(t,\cdot))$ for $t \in \mathbb{R}$ takes place as in Example 1, for $0 < r < \mu/2 - 1$.

Similar examples are easily obtained for the free particle (1), by using (4) and (5), which we proposed as motivation of our time–frequency approach.

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