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Semi-classical propagation of wavepackets for the phase space Schrödinger equation: interpretation in terms of the Feichtinger algebra

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Abstract

The nearby orbit method is a powerful tool for constructing semi-classical solutions of Schrödinger's equation when the initial datum is a coherent state. In this paper, we first extend this method to arbitrary squeezed states and thereafter apply our results to the Schrödinger equation in phase space. This adaptation requires the phase-space Weyl calculus developed in previous work of ours. We also study the regularity of the semi-classical solutions from the point of view of the Feichtinger algebra familiar from the theory of modulation spaces.

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Introduction

An excellent method for constructing approximate solutions of the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi, \qquad \psi(\cdot, t_0) = \psi_0 \tag{1}$$

when the initial function ψ_0 is a strongly localized wavepacket is the *nearby orbit method* initiated by Heller [16] and Littlejohn [20]. It is a method of choice, because it allows a simultaneous control of the accuracy of the approximate solutions for both small time and small h (it has been extended by various authors to 'large' times as well, but the results are less complete). Its gist is the following: let H be the classical Hamiltonian), and denote by $z_t = (x_t, p_t)$ the solution to Hamilton's equations $\dot{x} = \partial_p H$, $\dot{p} = -\partial_x H$ passing through $z_0 = (x_0, p_0)$ at time $t = 0$; here x_0 and p_0 are the position and momentum expectation

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vectors at time $t = 0$. Expanding H in a Taylor series around z_t and truncating at the second order one obtains the function

$$H_{z_0}(z,t) = H(z_t) + H'(z_t)(z - z_t) + \tfrac{1}{2}H''(z_t)(z - z_t)^2.$$

Consider now the new Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \widehat{H_{z_0}}\psi, \qquad \psi(\cdot, t_0) = \psi_0. \tag{2}$$

Due to the fact that H_{z_0} is a quadratic polynomial in the position and momentum variables, this equation can be explicitly solved using metaplectic and Heisenberg operators. The corresponding solutions are then used to construct approximate solutions of the initial Schrödinger equation (1) (we will also discuss higher-order approximations in this paper).

The aim of this work is to apply the nearby-orbit method to construct semi-classical solutions of the phase space Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi = H\left(\frac{1}{2}x + \mathrm{i}\hbar\frac{\partial}{\partial p}, \frac{1}{2}p - \mathrm{i}\hbar\frac{\partial}{\partial x}\right)\Psi$$

which we have studied in some detail in our previous works [7, 8] and [9], and which is obtained by constructing a Weyl calculus in phase space. We will in addition study the $L^1\left(\mathbb{R}^{2n}_z\right)$ regularity of the solutions of this equation; we will see that, perhaps somewhat surprisingly, this is equivalent to the regularity of the solutions of the usual configuration space Schrödinger equation in a particular 'modulation pace', namely the *Feichtinger algebra* $M^1\left(\mathbb{R}^n_x\right)$ of Gabor analysis [12].

The paper is structured as follows:

- In section 1, we review the theory of the Schrödinger equation in phase space developed in our previous work [7, 8]. The basic tool is the use of a Weyl calculus in phase space obtained by using what we call 'windowed wavepacket transforms'.
- In section 2, we describe the nearby-orbit method for the solutions to Schrödinger's equation as exposed in Littlejohn [20].
- In section 3 we construct a semi-classical propagator for the Schrödinger equation in phase space; we thereafter briefly discuss the accuracy of the method.
- Finally, in section 4 we show that the previous results are best understood in terms of a certain modulation space, which plays a crucial role in Gabor analysis. We are actually going to prove that the best adapted functional space is the Feichtinger algebra [3, 4].

Notation

The position vector will be denoted by $x = (x_1, \ldots, x_n)$ and the momentum vector by $p = (p_1, \ldots, p_n)$, and we write $z = (x, p)$ for the generic phase space variable. We will use the generalized gradients

$$\partial_x = \left[\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right], \qquad \partial_p = \left[\frac{\partial}{\partial p_1}, \ldots, \frac{\partial}{\partial p_n}\right]$$

and $\partial_z = (\partial_x, \partial_p)$.

The symplectic product of $z = (x, p)$, $z' = (x', p')$ is denoted by $\sigma(z, z')$

$$\sigma(z, z') = p \cdot x' - p' \cdot x$$

where the dot $\cdot$ is the usual (Euclidean) scalar product. In matrix notation

$$\sigma(z, z') = (z')^T J z, \qquad J = \begin{bmatrix} 0_{n\times n} & I_{n\times n} \\ -I_{n\times n} & 0_{n\times n} \end{bmatrix}.$$

The corresponding symplectic group is denoted by $\mathrm{Sp}(n)$: the relation $S \in \mathrm{Sp}(n)$ means that S is a real $2n \times 2n$ matrix such that $\sigma(Sz, Sz') = \sigma(z, z')$; equivalently

$$S^T JS = SJS^T = J.$$

We denote the inner product on $L^2(\mathbb{R}^n_x)$ by

$$(\psi|\phi) = \int \psi(x)\overline{\phi(x)}\,\mathrm{d}^n x$$

and the inner product on $L^2(\mathbb{R}^{2n}_z)$ by

$$((\Psi|\Phi)) = \int \Psi(z)\overline{\Phi(z)}\,\mathrm{d}^{2n} z;$$

the associated norms are denoted by $\|\psi\|$ and $|||\Psi|||$, respectively.

The Heisenberg–Weyl operators are denoted by $\widehat{T}(z_0)$; by definition

$$\widehat{T}(z_0)\psi(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p_0\cdot x - \frac{1}{2}p_0\cdot x_0)}\psi(x - x_0)$$

for any function ψ defined on $\mathbb{R}^n_x$ and $z_0 = (x_0, p_0)$.

The usual Schwarz spaces of rapidly decreasing functions and tempered distribution are denoted by $\mathcal{S}(\mathbb{R}^n_x)$ and $\mathcal{S}'(\mathbb{R}^n_x)$, respectively.

1. Weyl calculus in phase space

1.1. The windowed wavepacket transform

To each ϕ in $\mathcal{S}(\mathbb{R}^n_x)$ such that $\|\phi\| = 1$ we associate the *wavepacket transform* $\mathcal{U}_\phi$ *with window* ϕ as being the mapping $\mathcal{S}(\mathbb{R}^n_x) \longrightarrow \mathcal{S}(\mathbb{R}^{2n}_z)$ which to ψ associates the function

$$\mathcal{U}_\phi\psi(z) = \left(\frac{\pi\hbar}{2}\right)^{n/2} W(\psi, \phi)\left(\frac{1}{2}z\right). \tag{3}$$

where

$$W(\psi, \phi)(z) = \left(\frac{1}{2\pi\hbar}\right)^n \int \mathrm{e}^{-\mathrm{i}py/\hbar}\psi\left(x + \frac{1}{2}y\right)\overline{\phi\left(x - \frac{1}{2}y\right)}\,\mathrm{d}^n y; \tag{4}$$

is the Wigner–Moyal (or: cross-Wigner) transform of the pair (ψ, ϕ); explicitly

$$\mathcal{U}_\phi\psi(z) = \left(\frac{1}{2\pi\hbar}\right)^{n/2} \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}p\cdot x}\int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\cdot x'}\psi(x')\overline{\phi(x - x')}\,\mathrm{d}^n x'. \tag{5}$$

For every window $\phi \in \mathcal{S}(\mathbb{R}^n_x)$ the mapping $\mathcal{U}_\phi$ is a linear isometry of $L^2(\mathbb{R}^n_x)$ on a closed subspace $\mathcal{H}_\phi$ of $L^2(\mathbb{R}^{2n}_z)$

$$((\mathcal{U}_\phi\psi|\mathcal{U}_\phi\psi')) = (\psi|\psi'). \tag{6}$$

It follows that $\mathcal{U}^*_\phi\mathcal{U}_\phi$ is the identity operator on $L^2(\mathbb{R}^n_x)$ and that $P_\phi = \mathcal{U}_\phi\mathcal{U}^*_\phi$ is the orthogonal projection onto the Hilbert space $\mathcal{H}_\phi \subset L^2(\mathbb{R}^{2n}_z)$.

1.2. Phase space Schrödinger equation

The consideration of Schrödinger equations in phase space seems to go back to Frederick and Torres-Vega [22, 23]; in [1] Chruscinski and Mlodawski discuss the relationship between the Schrödinger equation in phase space and the star-product of deformation quantization (this relation is also considered in de Gosson [10]).

Let us denote by $\widehat{T}_{\text{ph}}(z_0)$ the operator $\mathcal{S}(\mathbb{R}_z^{2n}) \longrightarrow \mathcal{S}(\mathbb{R}_z^{2n})$ defined by

$$\widehat{T}_{\text{ph}}(z_0)\Psi(z) = \mathrm{e}^{-\frac{\mathrm{i}}{2\hbar}\sigma(z,z_0)}\Psi(z - z_0); \tag{7}$$

the operators $\widehat{T}_{\text{ph}}(z_0)$ extend into operators $\mathcal{S}'(\mathbb{R}_z^{2n}) \longrightarrow \mathcal{S}'(\mathbb{R}_z^{2n})$ which are unitary when restricted to $L^2(\mathbb{R}_z^{2n})$. They satisfy the product formula

$$\widehat{T}_{\text{ph}}(z_0 + z_1) = \mathrm{e}^{-\frac{\mathrm{i}}{2\hbar}\sigma(z_0,z_1)}\widehat{T}_{\text{ph}}(z_0)\widehat{T}_{\text{ph}}(z_1) \tag{8}$$

and hence they verify the same commutation relations

$$\widehat{T}_{\text{ph}}(z_0)\widehat{T}_{\text{ph}}(z_1) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sigma(z_0,z_1)}\widehat{T}_{\text{ph}}(z_1)\widehat{T}_{\text{ph}}(z_0) \tag{9}$$

as the usual Heisenberg–Weyl operators $\widehat{T}(z_0)$. Also note that $\widehat{T}_{\text{ph}}(z_0)^{-1} = \widehat{T}_{\text{ph}}(-z_0)$.

Let $\widehat{A} : \mathcal{S}(\mathbb{R}_x^n) \longrightarrow \mathcal{S}'(\mathbb{R}_x^n)$ be a $\hbar$-Weyl operator with symbol a; defining the 'twisted' Weyl symbol a_σ by

$$a_\sigma(z) = \left(\frac{1}{2\pi\hbar}\right)^n \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\sigma(z,z')}a(z')\,\mathrm{d}^{2n}z'$$

we have

$$\widehat{A}\psi(x) = \left(\frac{1}{2\pi\hbar}\right)^n \int a_\sigma(z_0)\widehat{T}(z_0)\psi(x)\,\mathrm{d}^{2n}z_0.$$

We will denote by $\widehat{A}_{\text{ph}}$ the operator $\mathcal{S}(\mathbb{R}_z^{2n}) \longrightarrow \mathcal{S}'(\mathbb{R}_z^{2n})$ defined by replacing $\widehat{T}(z_0)$ by $\widehat{T}_{\text{ph}}(z_0)$ in the formula above

$$\widehat{A}_{\text{ph}}\Psi(z) = \left(\frac{1}{2\pi\hbar}\right)^n \int a_\sigma(z)\widehat{T}_{\text{ph}}(z_0)\Psi(z)\,\mathrm{d}^{2n}z. \tag{10}$$

Note that, as in ordinary Weyl calculus, $\widehat{A}_{\text{ph}}$ is a symmetric operator if and only if $\widehat{A}$ is, that is if and only if the symbol a is real.

Proposition 1. *For every $\phi \in \mathcal{S}(\mathbb{R}_x^n)$ we have the following intertwining relations:*

$$\widehat{T}_{\text{ph}}(z_0)\mathcal{U}_\phi = \mathcal{U}_\phi\widehat{T}(z_0), \qquad \widehat{A}_{\text{ph}}\mathcal{U}_\phi = \mathcal{U}_\phi\widehat{A}. \tag{11}$$

Proof. The first formula (11) is obtained by a direct calculation; the second formula (11) immediately follows from using definition (10). (See [7, 9, 11] for a detailed study of these intertwining relations.) □

It is easy to check by a direct computation that the following intertwining relations holds for the windowed wavepacket transforms:

$$\mathcal{U}_\phi(x_j\psi) = \left(\frac{1}{2}x_j + \mathrm{i}\hbar\frac{\partial}{\partial p_j}\right)\mathcal{U}_\phi\psi, \tag{12}$$

$$\mathcal{U}_\phi\left(-\mathrm{i}\hbar\frac{\partial}{\partial x_j}\psi\right) = \left(\frac{1}{2}p_j - \mathrm{i}\hbar\frac{\partial}{\partial x_j}\right)\mathcal{U}_\phi\psi; \tag{13}$$

note that these relations are independent of a particular choice of the window ϕ.

Proposition 2. *Let ψ be a solution of the configuration space Schrödinger equation*

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi, \qquad \psi(\cdot, t_0) = \psi_0$$

The function $\Psi = \mathcal{U}_\phi\psi$ is a solution of the phase space Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}_{\text{ph}}\Psi, \qquad \Psi(\cdot, t_0) = \mathcal{U}_\phi\psi_0 \tag{14}$$

where $\widehat{H}_{\text{ph}} = H(\widehat{X}_{\text{ph}}, \widehat{P}_{\text{ph}})$.

Proof. This follows from formulae (11) and the discussion above (see [7, 8] for details). □

1.3. The metaplectic group $\mathrm{Mp}_{\mathrm{ph}}(n)$

The metaplectic group $\mathrm{Mp}(n)$ is a faithful unitary representation of $\mathrm{Sp}_2(n)$, the double cover of the symplectic group $\mathrm{Sp}(n)$ (see for instance Leray [19], Wallach [24], de Gosson [9]). $\mathrm{Mp}(n)$ is generated by the generalized Fourier transforms $\widehat{S}_{\mathcal{A},m}$ associated with a quadratic form

$$\mathcal{A}(x,x') = \tfrac{1}{2}Px^2 - Lx\cdot x' + \tfrac{1}{2}Qx'^2$$

with $P = P^T$, $Q = Q^T$, $\det L \neq 0$ (and $Px^2 = x^TPx$, etc) by the formula

$$\widehat{S}_{\mathcal{A},m}\psi(x) = \left(\frac{1}{2\pi\mathrm{i}\hbar}\right)^{n/2} \mathrm{i}^m\sqrt{|\det L|}\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{A}(x,x')}\psi(x')\,\mathrm{d}^nx'; \tag{15}$$

m corresponds to a choice of the argument of $\det L$ modulo 2π. One proves that every $\widehat{S}\in\mathrm{Mp}(n)$ can be written as the product of two operators of the type (15): $\widehat{S} = \widehat{S}_{\mathcal{A},m}\widehat{S}_{\mathcal{A}',m'}$. Since $\mathrm{Mp}(n)$ is a realization of the double cover of $\mathrm{Sp}(n)$ there exists a natural projection $\pi^{\mathrm{Mp}} : \mathrm{Mp}(n) \longrightarrow \mathrm{Sp}(n)$; that projection is a 2-to-1 group epimorphism defined by the condition that $S_{\mathcal{A}} = \pi^{\mathrm{Mp}}(\widehat{S}_{\mathcal{A},m})$ *is the free symplectic matrix generated by* $\mathcal{A}$, that is $(x,p) = S_{\mathcal{A}}(x',p')$ if and only if $p = \partial_x\mathcal{A}(x,x')$ and $p' = -\partial_{x'}\mathcal{A}(x,x')$.

The following important metaplectic covariance formulae:

$$\widehat{S}\widehat{T}(z_0) = \widehat{T}(Sz_0)\widehat{S}, \qquad W(\widehat{S}\psi,\widehat{S}\phi)(z) = W(\psi,\phi)(S^{-1}z) \tag{16}$$

hold for all $\widehat{S}\in\mathrm{Mp}(n)$ and $z_0\in\mathbb{R}^{2n}_z$.

In [6] we have shown that if the projection S of $\widehat{S}\in\mathrm{Mp}(n)$ has no eigenvalue equal to one, then

$$\widehat{S}\psi(x) = \left(\frac{1}{2\pi\hbar}\right)^n \int a_\sigma(z_0)\widehat{T}(z_0)\psi(x)\,\mathrm{d}^{2n}z_0 \tag{17}$$

where the symbol a_σ is given by

$$a_\sigma(z) = \left(\frac{1}{2\pi\hbar}\right)^n \mathrm{i}^\nu|\det(S-I)|^{-1/2}\,\mathrm{e}^{\frac{\mathrm{i}}{2\hbar}M_Sz^2}; \tag{18}$$

the symmetric matrix M_S is the *symplectic Cayley transform* of S

$$M_S = \tfrac{1}{2}J(S+I)(S-I)^{-1}; \tag{19}$$

the exponent ν of i in formula (18) is the *Conley–Zehnder index* of $\widehat{S}$ (see de Gosson [6, 9, 11]). Defining

$$\widehat{S}_{\mathrm{ph}}\Psi(z) = \left(\frac{1}{2\pi\hbar}\right)^n \int a_\sigma(z_0)\widehat{T}_{\mathrm{ph}}(z_0)\Psi(z)\,\mathrm{d}^{2n}z_0, \tag{20}$$

the operators $\widehat{S}_{\mathrm{ph}}$ generate a group which we denote by $\mathrm{Mp}_{\mathrm{ph}}(n)$; that group is isomorphic to $\mathrm{Mp}(n)$. The well known 'metaplectic covariance' relation $\widehat{A\circ S} = \widehat{S}^{-1}\widehat{A}\widehat{S}$ valid for any $\widehat{S}\in\mathrm{Mp}(n)$ with projection $S\in\mathrm{Sp}(n)$ extends to the operators $\widehat{A}_{\mathrm{ph}}$: we have

$$\widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z_0)\widehat{S}_{\mathrm{ph}}^{-1} = \widehat{T}_{\mathrm{ph}}(Sz), \qquad \widehat{A\circ S}_{\mathrm{ph}} = \widehat{S}_{\mathrm{ph}}^{-1}\widehat{A}_{\mathrm{ph}}\widehat{S}_{\mathrm{ph}} \tag{21}$$

and also

$$\widehat{S}_{\mathrm{ph}}\mathcal{U}_\phi\psi = \mathcal{U}_\phi\widehat{S}\psi, \qquad \widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z_0) = \widehat{T}_{\mathrm{ph}}(Sz_0)\widehat{S}_{\mathrm{ph}}. \tag{22}$$

2. The nearby orbit method

Let us begin by reviewing the method in the usual situation of the configuration space Schrödinger equation (see Littlejohn [20] for details).

2.1. Description of the method

Let H be the Weyl symbol of the operator $\widehat{H}$ (it is the classical Hamiltonian), we denote by $\left(f_{t,t_0}\right)$ the time-dependent flow determined by H: $t \longmapsto f_{t,t_0}(z_0)$ is the solution of Hamilton's equations $\dot{z} = J\partial_z H(z,t)$ passing through the phase-space point z_0 at time $t = t_0$. We will write $z_t = (x_t, p_t) = f_{t,t_0}(z_0)$. Let H'' be the Hessian matrix of H in the variables x_j, p_k and consider the 'variational equation'

$$\frac{\mathrm{d}}{\mathrm{d}t} S_{t,t_0}(z_0) = JH''(z_t,t) S_{t,t_0}(z_0)$$

satisfied by the Jacobian matrix

$$S_{t,t_0}(z_0) = \frac{\partial(x_t,p_t)}{\partial\left(x_{t_0},p_{t_0}\right)} = \frac{\partial z_t}{\partial z_{t_0}}$$

of the canonical transformation f_{t,t_0} calculated at the point z_0. This equation determines a path $t \longmapsto S_{t,t_0}(z_0)$ of symplectic matrices passing through the identity matrix I at time $t = t_0$. This path can be lifted in a unique way to a path $t \longmapsto \widehat{S}_{t,t_0}$ in $\mathrm{Mp}(n)$ such that $\widehat{S}_{t_0,t_0}$ is the identity. we have the following fundamental property:

Proposition 3. *Let H be a quadratic Hamiltonian: $H_M(z,t) = \frac{1}{2}z^T M(t) z$ where $M(t)$ is a symmetric matrix depending smoothly on t. Denote by $S_{t,t'}$ the classical propagator: $S_{t,t'} \in \mathrm{Sp}(n)$. For given t_0 let $t \longmapsto \widehat{S}_{t,t_0}$ be the unique path in $\mathrm{Mp}(n)$ covering the symplectic path $t \longmapsto S_{t,t_0}$ and such that $\widehat{S}_{t_0,t_0} = I$. For $\psi_0 \in \mathcal{S}\left(\mathbb{R}^n_x\right)$ set $\psi(x,t) = \widehat{S}_{t,t_0}\psi_0(x)$. The function ψ is the solution of the Cauchy problem*

$$\mathrm{i}\hbar\frac{\mathrm{d}\psi}{\mathrm{d}t} = \widehat{H_M}\psi, \qquad \psi(\cdot,t_0) = \psi_0 \tag{23}$$

where $\widehat{H_M}$ is the operator with Weyl symbol H_M.

For a detailed proof see [9] and the references therein.

Consider the Schrödinger's equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi, \qquad \psi(\cdot,t_0) = \psi_0$$

where the initial wave function ψ_0 is 'concentrated' around z_0. The nearby orbit method (at order $N = 0$) consists in making the Ansatz that the approximate solution is given by the formula $\psi^{(0)}(x,t) = U^{(0)}_{t,t_0}(z_0)\psi_0$ where the propagator' $U^{(0)}_{t,t_0}(z_0)$ is defined by

$$\psi^{(0)}(x,t) = U^{(0)}_{t,t_0}(z_0)\psi_0 = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1}\psi_0; \tag{24}$$

the phase $\gamma(t,t_0;z_0)$ is here the symmetrized action

$$\gamma(t,t_0;z_0) = \int_{t_0}^{t}\left(\frac{1}{2}\sigma(z_{t'},\dot{z}_{t'}) - H(z_{t'},t')\right)\mathrm{d}t' \tag{25}$$

calculated along the Hamiltonian trajectory leading from z_0 at time t_0 to z_t at time t.

An interesting case occurs when the initial function ψ_0 is a *coherent state*. The standard coherent state is the function

$$\phi^\hbar(x) = \left(\frac{1}{\pi\hbar}\right)^{n/4}\mathrm{e}^{-\frac{1}{2\hbar}|x|^2}; \tag{26}$$

more generally one defines the standard coherent state centered at z_0 by the formula

$$\phi^\hbar_{z_0}(x) = \widehat{T}(z_0)\phi^\hbar = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p_0\cdot x - \frac{1}{2}p_0\cdot x_0)}\phi^\hbar(x - x_0). \tag{27}$$

Coherent states are normalized: $\left\|\phi^\hbar_{z_0}\right\|_{L^2} = 1$, and the Wigner transform $W\phi^\hbar = W(\phi^\hbar,\phi^\hbar)$ is given by

$$W\phi^{\hbar}(z) = \left(\frac{1}{\pi\hbar}\right)^n \mathrm{e}^{-\frac{1}{\hbar}|z|^2}. \tag{28}$$

To understand this, it is useful to generalize the notion of coherent state, by introducing the notion of 'squeezed coherent states'. These are more general (normalized) Gaussians of the type

$$\phi_M^{\hbar}(x) = \left(\frac{\det \operatorname{Im} M}{(\pi\hbar)^n}\right)^{1/4} \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}x^T Mx} \tag{29}$$

and

$$\phi_{M,z_0}^{\hbar}(x) = \widehat{T}(z_0)\phi_M^{\hbar}(x) \tag{30}$$

where M belongs to the Siegel half-space $\Sigma_n^+ = \{M : M = M^T, \operatorname{Im} M > 0\}$ (M a complex $n \times n$ matrix).

Metaplectic operators take coherent states into coherent states: if $\widehat{S} \in \mathrm{Mp}(n)$ has projection $S = \left[\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right]$ on $\mathrm{Sp}(n)$ then

$$\widehat{S}\phi_{M,z_0}^{\hbar} = \phi_{\alpha(S)M,Sz_0}^{\hbar}, \qquad \alpha(S)M = (C + DM)(A + BM)^{-1} \tag{31}$$

where $\alpha(S)M \in \Sigma_n^+$.

If we use coherent states as initial wavefunctions, formula (24) becomes particularly simple

Proposition 4. *The approximate solution to Schrödinger's equation*

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi, \qquad \psi(\cdot, t_0) = \phi_{z_0}^{\hbar}$$

in the nearby orbit method (at order $N = 0$) is given by the formula

$$\psi^{(0)} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^{\hbar} \tag{32}$$

that is, by

$$\psi^{(0)} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\phi_{M_t,z_t}^{\hbar}, \qquad M_t = \alpha(S_{t,t_0}(z_0))(\mathrm{i}I). \tag{33}$$

Proof. Formula (32) is of course an immediate consequence of formula (24) and definition (27) of $\phi_{z_0}^{\hbar}$ since we have

$$\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1}\phi_{z_0}^{\hbar} = \widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^{\hbar}.$$

Formulae (33) follow from (31). □

2.2. Accuracy of the method

Making the following (rather mild) assumptions on the Hamiltonian function H:

- The mapping $(z, t) \longrightarrow H(z, t)$ is continuous for $|t - t_0| \leqslant T$ and C^∞ in $z = (x, p)$,
- For every multi-index $\alpha \in \mathbb{N}^{2n}$ there exist $C_\alpha > 0$ and $\mu_\alpha \in \mathbb{R}$ such that $\left|\partial_z^\alpha H(z, t)\right| \leqslant C_\alpha(T)(1 + |z|^2)^{\mu_\alpha}$ for $|t - t_0| \leqslant T$,

  we have the following precise result:

Proposition 5. *Assume that the Cauchy problem*

$$\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi, \qquad \psi(\cdot, t_0) = \phi_{z_0}^{\hbar}$$

has a unique solution defined for $0 \leqslant |t - t_0| \leqslant T$*. There exist for each integer* N *polynomial functions* P_j *with degree* $\leqslant 3j$ *and a constant* $C_N(z_0, T)$ *such that the function*

$$\psi^{(N)}(x,t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)} \sum_{0 \leqslant j \leqslant N} \hbar^{j/2} P_j\left(\frac{1}{\sqrt{\hbar}}(x - x_t)\right)\phi^{\hbar}_{M_t,z_t}. \tag{34}$$

with $M_t = \alpha(S_t(z_0))(iI)$ *satisfies*

$$\|\psi(\cdot,t) - \psi^{(N)}(\cdot,t)\| \leqslant C_N(z_0,T)\hbar^{(N+1)/2}|t - t_0|. \tag{35}$$

Note that in particular, at the order $N = 0$, we have

$$\|\psi(\cdot,t) - \psi^{(0)}(\cdot,t)\| \leqslant C_0(z_0,T)\hbar^{1/2}|t - t_0| \tag{36}$$

where $\psi^{(0)}$ is given by formula (33).

The first to prove estimates of the type above (for Hamiltonians H of the type 'kinetic energy plus potential') was Hagedorn in his pioneering work [13, 14]; his results were extended by Combescure and Robert [2] to arbitrary Hamiltonians satisfying the properties listed before the statement of proposition 5. Also see Nazaikiinskii *et al* [21] (chapter 2, section 2.1) for related results using a slightly different method.

3. Nearby-orbit method in phase space

3.1. The main results

We want to find similar expressions for approximate solutions of the Schrödinger equation in phase space

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = H_{\mathrm{ph}}\Psi, \qquad \Psi(\cdot,t_0) = \Psi_0.$$

The following result gives an explicit formula for the semi-classical propagator in phase space:

Proposition 6. *The semi-classical propagator* $U^{(0)}_{t,t_0}$ *takes* $\Psi_0 = \mathcal{U}_\phi\psi_0$ *to the function*

$$\Psi^{(0)} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}_{\mathrm{ph}}(z_t)\big(\widehat{S}_{t,t_0}(z_0)\big)_{\mathrm{ph}}\widehat{T}(z_0)^{-1}_{\mathrm{ph}}\Psi_0 \tag{37}$$

with

$$\gamma(t,t_0;z_0) = \int_0^t \left(\frac{1}{2}\sigma(z_{t'},\dot{z}_{t'}) - H(z_{t'},t')\right)\mathrm{d}t'.$$

Proof. Set $\psi^{(0)} = U^{(0)}_{t,t_0}(z_0)\psi_0$; by definition of $U^{(0)}_{t,t_0}(z_0)$ we have

$$\psi^{(0)} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(z_0,t)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1}\psi_0$$

hence, by repeated use of the intertwining formulae (22):

$$\begin{aligned}
\mathcal{U}_\phi\psi &= \mathcal{U}_\phi\big[\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1}\psi_0\big]\\
&= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\big[\mathcal{U}_\phi(\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1})\psi_0\big]\\
&= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}_{\mathrm{ph}}(z_t)\big[\mathcal{U}_\phi(\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1})\psi_0\big]\\
&= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}_{\mathrm{ph}}(z_t)\widehat{S}_{t,t_0}(z_0)_{\mathrm{ph}}[\mathcal{U}_\phi(\widehat{T}(z_0)^{-1}\psi_0)]\\
&= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}_{\mathrm{ph}}(z_t)\widehat{S}_{t,t_0}(z_0)_{\mathrm{ph}}\widehat{T}(z_0)^{-1}_{\mathrm{ph}}\mathcal{U}_\phi\psi_0
\end{aligned}$$

which proves (37). □

An immediate consequence of proposition 6 above is

Corollary 7. *(i) If* $\Psi_0 = \mathcal{U}_\phi \phi^\hbar_{z_0}$ *then*

$$\Psi^{(0)} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(z_0,t)} \widehat{T}_{\mathrm{ph}}(z_t)\widehat{S}_t(z_0)_{\mathrm{ph}}\Phi^\hbar \tag{38}$$

where $\Phi^\hbar = \mathcal{U}_\phi \phi^\hbar$.

(ii) When $\phi = \phi^\hbar$ *the function* $\Phi^\hbar$ *is the Gaussian*

$$\Phi^\hbar = \left(\frac{1}{2\pi\hbar}\right)^{n/2} \mathrm{e}^{-\frac{\mathrm{i}}{2\hbar}\sigma(z,z_0)}\,\mathrm{e}^{-\frac{1}{4\hbar}|z-z_0|^2}.$$

Proof. (i) In view of formula (37) we have

$$\mathcal{U}_\phi\psi = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}_{\mathrm{ph}}(z_t)\widehat{S}_{t,t_0}(z_0)_{\mathrm{ph}}\widehat{T}(z_0)^{-1}_{\mathrm{ph}}\mathcal{U}_\phi\phi^\hbar_{z_0}.$$

Formula (38) follows since we have

$$\widehat{T}(z_0)^{-1}_{\mathrm{ph}}\mathcal{U}_\phi\phi^\hbar_{z_0} = \mathcal{U}_\phi\big(\widehat{T}(z_0)^{-1}\phi^\hbar_{z_0}\big) = \mathcal{U}_\phi\phi^\hbar = \Phi^\hbar.$$

(ii) We have $\mathcal{U}_{\phi^\hbar}\phi^\hbar_{z_0} = \widehat{T}_{\mathrm{ph}}(z_0)\mathcal{U}_{\phi^\hbar}\phi^\hbar$ and $W\phi^\hbar(z) = (\pi\hbar)^{-n}\,\mathrm{e}^{-|z|^2/\hbar}$ hence

$$\mathcal{U}_{\phi^\hbar}\phi^\hbar_{z_0} = \left(\frac{1}{2\pi\hbar}\right)^{n/2} \mathrm{e}^{-\frac{\mathrm{i}}{2\hbar}\sigma(z,z_0)}\,\mathrm{e}^{-\frac{1}{4\hbar}|z-z_0|^2}$$

□

3.2. Accuracy of our results

Of course, a natural question is arising at this point

How good are the semi-classical approximations

$$U^{(0)}_{t,t_0}(z_0)\psi_0(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1}\psi_0(x)$$

and

$$U^{(0)}_{t,t_0}(z_0)_{\mathrm{ph}} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(z_0,t)}\widehat{T}_{\mathrm{ph}}(z_t)(\widehat{S}_t(z_0))_{\mathrm{ph}}\widehat{T}(z_0)^{-1}_{\mathrm{ph}}\Psi_0(x)?$$

The main observation is that the study of accuracy of the nearby-orbit methods for the configuration space Schrödinger equation and of its phase space variant are *equivalent*.

Lemma 8. *Let* $\Psi_0 = \mathcal{U}_\phi\psi_0$. *We have*

$$\big|\big|\big|U^{(N)}_{t,t_0}(z_0)_{\mathrm{ph}}\Psi_0 - \Psi(\cdot,t)\big|\big|\big| = \big\|U^{(N)}_{t,t_0}(z_0)\psi_0 - \psi(\cdot,t)\big\|.$$

Proof. The solution Ψ is given by $\Psi(\cdot,t) = \mathcal{U}_\phi(\psi(\cdot,t))$ where ψ is the solution of the usual Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi, \qquad \psi(\cdot,t_0) = \psi_0;$$

since $\mathcal{U}_\phi$ is a linear isometry we have

$$\big|\big|\big|U^{(N)}_{t,t_0}(z_0)_{\mathrm{ph}}\Psi_0 - \Psi(\cdot,t)\big|\big|\big| = \big\|U^{(N)}_{t,t_0}(z_0)\psi_0 - \psi(\cdot,t)\big\|.$$

□

From the results above we deduce

Proposition 9. *Assume that the solution* Ψ *of the phase-space Schrödinger equation*

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}_{\mathrm{ph}}\Psi, \qquad \Psi(\cdot,t_0) = \Phi^\hbar_{z_0}$$

with $\Phi^\hbar_{z_0} = \mathcal{U}_\phi\phi^\hbar_{z_0}$ *is unique. Suppose that H satisfies the conditions listed before the statement of proposition 5. Then, for* $|t-t_0| < T$ *there exists a constant* $C_T \geqslant 0$ *such that*

$$\big|\big|\big|U^{(0)}_{t,t_0}(z_0)_{\mathrm{ph}}\Phi^\hbar_{z_0} - \Psi(\cdot,t)\big|\big|\big| \leqslant C(z_0,T)|t-t_0|\sqrt{\hbar}. \tag{39}$$

Proof. It suffices to apply lemma 8 above together with proposition 5. □

This result can be generalized to the higher-order approximations $\Psi^{(N)} = U_{t,t_0}^{(N)}(z_0)_{\mathrm{ph}}\Psi_0$ without difficulty:

Proposition 10. *Under the same assumptions as above the function* $\Psi^{(N)} = \mathcal{U}_\phi\psi^{(N)}$ *where* $\psi^{(N)} = U_{t,t_0}^{(N)}(z_0)\psi_0$ *is of the type*

$$\Psi^{(N)}(z,t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)} \sum_{0\leqslant j\leqslant N} \hbar^{j/2} P_j\left(\frac{1}{\sqrt{\hbar}}(\widehat{X}_{\mathrm{ph}} - x_t)\right) \widehat{T}_{\mathrm{ph}}(z_t)\widehat{S}_{t,t_0}(z_0)_{\mathrm{ph}}\Phi^\hbar$$

with $\Phi^\hbar = \mathcal{U}_\phi\phi^\hbar$, $\widehat{X}_{\mathrm{ph}} = \frac{1}{2}x + \mathrm{i}\hbar\frac{\partial}{\partial p}$, *and it satisfies*

$$|||\Psi^{(N)}(\cdot,t) - \Psi(\cdot,t)||| \leqslant C_N(z_0,T)\hbar^{(N+1)/2}|t-t_0|.$$

Proof. In view of formula (34) in proposition 5 the Nth order approximation is given by

$$\psi^{(N)}(x,t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)} \sum_{0\leqslant j\leqslant N} \hbar^{j/2} P_j\left(\frac{1}{\sqrt{\hbar}}(x - x_t)\right) \phi^\hbar_{M_t,z_t},$$

where the P_j are polynomials with degree $\leqslant 3j$ and $M_t = \alpha(\widehat{S}_{t,t_0}(z_0))(\mathrm{i}I)$; this formula is just a concise form of

$$\psi^{(N)}(x,t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)} \sum_{0\leqslant j\leqslant N} \hbar^{j/2} P_j\left(\frac{1}{\sqrt{\hbar}}(x - x_t)\right) \widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar.$$

We have

$$\mathcal{U}_\phi\psi^{(N)}(z,t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)} \sum_{0\leqslant j\leqslant N} \hbar^{j/2}\mathcal{U}_\phi\left[P_j\left(\frac{1}{\sqrt{\hbar}}(x - x_t)\right) \widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar\right](z,t).$$

In view of the intertwining formula (12) we have

$$\mathcal{U}_\phi\left[P_j\left(\frac{1}{\sqrt{\hbar}}(x - x_t)\right) \widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar_{z_0}\right] = P_j\left(\frac{1}{\sqrt{\hbar}}(\widehat{X}_{\mathrm{ph}} - x_t)\right)\mathcal{U}_\phi[\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar]$$

and

$$\mathcal{U}_\phi[\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar] = \widehat{T}_{\mathrm{ph}}(z_t)\widehat{S}_{t,t_0}(z_0)_{\mathrm{ph}}\Phi^\hbar$$

hence the result, using again lemma 8 and the estimate (35). □

4. Regularity in modulation spaces

The idea of studying functional regularity of the semi-classical solutions of Schrödinger equations is not new; for instance in [21] there are interesting results in terms of a class of Sobolev spaces. In this section we study the regularity of semi-classical solutions in Feichtinger's algebra [3, 4] (see Gröchenig's book [12] for complements and references).

4.1. The Feichtinger algebra $M^1(\mathbb{R}^n_x)$

The short-time Fourier transform V_ϕ with window $\phi \in \mathcal{S}(\mathbb{R}^n_x)$ is defined by

$$V_\phi\psi(z) = \int \mathrm{e}^{-2\pi \mathrm{i} p\cdot x'}\psi(x')\overline{\phi(x'-x)}\mathrm{d}^n x'; \tag{40}$$

it is related to the Wigner–Moyal transform by

$$W(\psi,\phi)(z) = \left(\frac{2}{\pi\hbar}\right)^{n/2} \mathrm{e}^{\frac{2\mathrm{i}}{\hbar}p\cdot x} V_{\phi^\vee_{\sqrt{2\pi\hbar}}}\psi_{\sqrt{2\pi\hbar}}(2z/\sqrt{2\pi\hbar}) \tag{41}$$

where $\psi_{\sqrt{2\pi\hbar}}(x) = \psi(x\sqrt{2\pi\hbar})$, $\phi^\vee(x) = \phi(-x)$. Using formulae (5) and (41) we thus have the following simple relation between the windowed wavepacket transform $\mathcal{U}_\phi\psi$ and V_ϕ:

$$\mathcal{U}_\phi\psi(z) = \left(\frac{1}{\pi\hbar}\right)^{n/2} \mathrm{e}^{\frac{2i}{\hbar}p\cdot x} V_{\phi^\vee_{\sqrt{2\pi\hbar}}}\psi_{\sqrt{2\pi\hbar}}(z/\sqrt{2\pi\hbar}). \tag{42}$$

Let $\phi \in \mathcal{S}(\mathbb{R}^n_x)$. By definition, the Feichtinger algebra $M^1(\mathbb{R}^n_x)$ (sometimes also denoted by $S_0(\mathbb{R}^n_x)$) is the 'modulation space' consisting of all ψ such that $V_\phi\psi \in L^1(\mathbb{R}^{2n}_z)$; it immediately follows from formula (42) that this condition is equivalent to $\mathcal{U}_\phi\psi \in L^1(\mathbb{R}^{2n}_z)$. A crucial (and highly non-trivial!) fact, which ensures the validity of the definition of $M^1(\mathbb{R}^n_x)$, is that the condition $V_\phi\psi \in L^1(\mathbb{R}^{2n}_z)$ (respectively $\mathcal{U}_\phi\psi \in L^1(\mathbb{R}^{2n}_z)$) does not depend on the choice of the window ϕ. In addition the formulae

$$\|\psi\|_\phi = \|\mathcal{U}_\phi\psi\|_{L^1(\mathbb{R}^{2n}_z)} = \int |\mathcal{U}_\phi\psi(z)|\,\mathrm{d}^{2n}z$$

define a family of equivalent norms on $M^1(\mathbb{R}^n_x)$. One moreover has the very simple and remarkable characterization in terms of the Wigner distribution ([12], p 247):

Proposition 11. *A distribution $\psi \in \mathcal{S}'(\mathbb{R}^n_x)$ is in $M^1(\mathbb{R}^n_x)$ if and only if $W\psi \in L^1(\mathbb{R}^{2n}_z)$.*

One, moreover, shows that $M^1(\mathbb{R}^n_x)$ is complete for the topology thus defined, hence a Banach space; it is in fact even a Banach algebra (see remark 14 below).

We have the inclusions

$$\mathcal{S}(\mathbb{R}^n_x) \subset M^1(\mathbb{R}^n_x) \subset C^0(\mathbb{R}^n_x) \cap L^1(\mathbb{R}^n_x) \cap L^2(\mathbb{R}^n_x);$$

it follows, in particular, that $M^1(\mathbb{R}^n_x)$ is dense in $L^2(\mathbb{R}^n_x)$.

A typical example of a function that is in $M^1(\mathbb{R}^n_x)$ but not in $\mathcal{S}(\mathbb{R}^n_x)$ is given (in the case $n = 1$) by the 'triangle function' $\psi(x) = 1 - |x|$ if $|x| \leqslant 1$ and $\psi(x) = 0$ if $|x| \geqslant 1$.

Remark 12. More generally, it is often useful to consider the weighted modulation spaces $M^1_{v^s}(\mathbb{R}^n_x)$, $s \geqslant 0$, where $v_s(z) = (1 + |z|^2)^{s/2}$; by definition $\psi \in M^1_{v^s}(\mathbb{R}^n_x)$ if and only if $v_s\mathcal{U}_\phi\psi \in L^1(\mathbb{R}^{2n}_z)$ for one (and hence all) $\phi \in \mathcal{S}(\mathbb{R}^n_x)$.

The Feichtinger algebra has the two following crucial properties:

Proposition 13. *Let $\psi \in M^1(\mathbb{R}^n_x)$. We have*

(i) $\widehat{T}(z_0)\psi \in M^1(\mathbb{R}^n_x)$ for every $z_0 \in \mathbb{R}^{2n}_z$;

(ii) $\widehat{S}\psi \in M^1(\mathbb{R}^n_x)$ for every $\widehat{S} \in \mathrm{Mp}(n)$. (In particular $M^1(\mathbb{R}^n_x)$ is invariant under Fourier transformation).

Property (i) follows from the definition of $M^1(\mathbb{R}^n_x)$; for (ii) see [12], proposition 12.1.3.

Remark 14. The Feichtinger algebra is actually the *smallest* Banach space containing $\mathcal{S}(\mathbb{R}^n_x)$ and which is invariant under the action of the Heisenberg–Weyl operators.

4.2. Application to the nearby-orbit method; a conjecture

The properties of $M^1(\mathbb{R}^n_x)$ listed in proposition 13 allow us to prove the following regularity result for the semi-classical approximations $\psi^{(0)} = U^{(0)}_{t,t_0}(z_0)\psi_0$:

Proposition 15. *The two following equivalent statements hold:*
(i) If $\psi_0 \in M^1(\mathbb{R}^n_x)$ *then* $U^{(0)}_{t,t_0}(z_0)\psi_0 \in M^1(\mathbb{R}^n_x)$*;*
(ii) If $\Psi_0 \in L^1(\mathbb{R}^{2n}_z)$ *then* $U^{(0)}_{t,t_0}(z_0)_{\mathrm{ph}}\Psi_0 \in L^1(\mathbb{R}^{2n}_z)$*.*

Proof. That both statements are equivalent is obvious from the definition of the Feichtinger algebra. Since

$$U^{(0)}_{t,t_0}(z_0)\psi_0(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1}\psi_0(x)$$

statement (i) follows by repeated use of proposition 13. □

Remark 16. A rather straightforward adaptation of the proof of proposition 13 shows that the more general weighted spaces $M^1_{v^s}(\mathbb{R}^n_x)$ mentioned in remark 12 also are closed under Heisenberg–Weyl and metaplectic operators. It follows that the conclusion of proposition 15 remain true mutatis mutandis, replacing $M^1(\mathbb{R}^n_x)$ and $L^1(\mathbb{R}^{2n}_z)$ by $M^1_{v^s}(\mathbb{R}^n_x)$ and $L^1_{v^s}(\mathbb{R}^{2n}_z)$, respectively.

We note that the conclusions above remain true if we replace $U_{t,t_0}(z_0)$ by the exact propagator U_{t,t_0} associated with a Schrödinger equation with quadratic Hamiltonian (this is actually an immediate consequence of proposition 3). In fact, we conjecture:

Conjecture 17. *The conclusions of proposition 15 remain true for the exact propagator of Schrödinger equations with arbitrary Hamiltonians.*

We hope to be able to prove this very important regularity property in a forthcoming paper.

5. Discussion and perspectives

Needless to say, there are several problems and questions we have not discussed in this paper, and to which we will come back in forthcoming publications. There is one outstanding omission: we have not analyzed the domain of validity of the nearby-orbit method very much in detail; it is on the other hand well-known that there are problems with long times ('Ehrenfest time') when the associated classical systems exhibits a chaotic behavior; as Littlejohn already pointed out in his seminal paper [20], the nearby orbit method fails for long times near classically unstable points; in this sense the method is very dependent on results on classically chaotic Hamiltonian systems (which is hardly surprising). We mention that Hagedorn and Joye [15] have constructed exponentially precise semi-classical approximations (for small $\hbar$) of the solutions of the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi.$$

They show that if certain analytical conditions on the potential V are satisfied the error is of order $\mathrm{e}^{-\gamma/\hbar}$ for some $\gamma > 0$. It is however not quite clear how their results and methods could be applied to the phase space Schrödinger equation; this is a question which certainly deserves to be investigated.

In the last part of this paper we investigated the relation between the regularity of the solutions of Schrödinger equations in configuration and phase space using the Feichtinger algebra, and we made a conjecture. It seems that the techniques that have been developed during the last two decades by researchers in Gabor and time-frequency analysis are not so well-known, in general, by quantum physicists. I think that a synergetic approach to both sciences would lead to unexpected advances in many directions.

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