ESI **The Erwin Schrödinger International Institute for Mathematical Physics** Boltzmanngasse 9 A-1090 Wien, Austria

Semi-Classical Propagation of Wavepackets for the Phase Space Schrödinger Equation; Interpretation in Terms of the Feichtinger Algebra

Maurice A de Gosson

Vienna, Preprint ESI 1951 (2007) September 21, 2007

Supported by the Austrian Federal Ministry of Education, Science and Culture
Available via http://www.esi.ac.at

Semi-Classical Propagation of Wavepackets for the Phase Space Schrödinger Equation; Interpretation in Terms of the Feichtinger Algebra

Maurice A de Gosson*
Universität Wien,
Mathematische Fakultät, NuHAG,
Nordbergstrasse 15, A-1090 Wien
and
International Erwin Schrödinger Institute
for Mathematical Physics
Boltzmanngasse 9, A-1090 Wien

September 26, 2007

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.

Introduction

An excellent method for constructing approximate solutions of the Schrödinger equation

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

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

*Email: maurice.de.gosson@univie.ac.at , maurice.degosson@gmail.com

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 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 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

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

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 article).

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

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

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 $L^1(\mathbb{R}^{2n})$ regularity of the solutions of this equation; we will see that, perhaps somewhat surprisingly, this is is equivalent to the regularity of the solutions of the usual configuration space Schrödinger equation in a particular "modulation pace", namely the *Feichtinger algebra* $M^1(\mathbb{R}^n)$ of Gabor analysis [12].

The paper is structured as follows:

- In Section 1 we recall the basics of the rigorous theory of the Schrödinger equation in phase space, following the approach used 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", which are closely related to the short-time Fourier transform used in time-frequency and Gabor analysis.

- In Section 2 we describe in detail the nearby-orbit method and complement it with some effective calculations. We then construct a semi-classical propagator for the Schrödinger equation in phase space; we thereafter briefly discuss the range of validity of the method; the main observation is that the accuracy of the configuration space and phase space approximations are the same.

- Finally, in Section 3 we show that the previous results are best understood in terms of a certain modulation space, which plays a crucial role in Gabor analysis. 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. We are actually going to prove that the best adapted functional space is the Feichtinger algebra defined in [3, 4] in the mid eighties.

Notation

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

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

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:

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

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 $L^2(\mathbb{R}^n)$ by

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

(hence $(\psi|\phi) = \langle\phi|\psi\rangle)$ and the inner product on $L^2(\mathbb{R}^{2n})$ 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

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

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

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

1 Weyl calculus in phase space

In this Section we briefly review the phase space calculus developed in de Gosson [7, 9].

1.1 The windowed wavepacket transform

1.1.1 Definition of $\mathcal{U}_\phi$

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

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

where

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

is the Wigner–Moyal transform of the pair (ψ, ϕ); explicitly

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

thus $\mathcal{U}_\phi\psi$ is essentially the "short-time Fourier transform" from time-frequency analysis. For every window $\phi \in \mathcal{S}(\mathbb{R}^n)$ the mapping $\mathcal{U}_\phi$ is a linear isometry of $L^2(\mathbb{R}^n)$ on a closed subspace $\mathcal{H}_\phi$ of $L^2(\mathbb{R}^n)$ It follows that we have

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

and hence each of the linear mappings $\mathcal{U}_\phi$ is an isometry of $L^2(\mathbb{R}^n_x)$ onto a *closed* subspace $\mathcal{H}_\phi$ of $L^2(\mathbb{R}^{2n}_z)$ (the square integrable functions on phase space). It follows that $\mathcal{U}_\phi^*\mathcal{U}_\phi$ is the identity operator on $L^2(\mathbb{R}^n)$ and that $P_\phi = \mathcal{U}_\phi\mathcal{U}_\phi^*$ is the orthogonal projection onto the Hilbert space $\mathcal{H}_\phi$. For all ϕ we have $\mathcal{H}_\phi \neq L^2(\mathbb{R}^n)$.

For practical calculations it is often advantageous to choose for ϕ the standard coherent state $\phi^\hbar(x) = (\pi\hbar)^{-n/4}e^{-|x|^2/2\hbar}$. In this case $\mathcal{U}_\phi$ is related to the so-called *Bargmann transform* $B\psi(z)$ (see [21]); in units where $\hbar = 1/2\pi$ we have

$$B\psi(x+ip) = 2^{-n}e^{-\pi|z|^2/2}W(\psi,\phi^\hbar)(\tfrac{1}{2}x, -\tfrac{1}{2}p),$$

hence (still in these units)

$$\mathcal{U}_{\phi^\hbar}\psi(z) = e^{\pi|z|^2/2}B\psi(x-ip). \tag{7}$$

Another reason for the choice $\phi = \phi^\hbar$ is that the range $\mathcal{H}_{\phi^\hbar}$ of $\mathcal{U}_{\phi^\hbar}$ is particularly simple to characterize:

Proposition 1 *Let $\Psi \in L^2(\mathbb{R}^{2n})$. We have $\Psi \in \mathcal{H}_{\phi^\hbar}$ if and only if Ψ satisfies the "anti Cauchy–Riemann conditions"*

$$(\tfrac{\partial}{\partial x_j} + i\tfrac{\partial}{\partial p_j})\left[e^{\frac{1}{2\hbar}z^2}\Psi(z)\right] = 0$$

That is, $\Psi \in \mathcal{H}_{\phi^\hbar}$ if and only $\Psi(z) = a(\overline{z})e^{-\frac{1}{2\hbar}z^2}$ for some analytic function a.

Proof. This follows from the relation (7) between the Bargmann transform $\mathcal{U}_{\phi^\hbar}$; also see Theorem 3 in [8]. ∎

1.1.2 The metaplectic group $\mathrm{Mp}_{\mathbf{ph}}(n)$

The metaplectic group $\mathrm{Mp}(n)$ is a faithful unitary representation of $\mathrm{Sp}_2(n)$, the double cover of the symplectic group $\mathrm{Sp}(n)$. There are several different ways to describe the elements of $\mathrm{Mp}(n)$ (see for instance Leray [19], Wallach [24], de Gosson [9], and the references therein). For our purposes the most adequate is to use the notion of generating function for free symplectic matrices. The metaplectic group is generated by the generalized Fourier transforms $\widehat{S}_{\mathcal{A},m}$ associated to a quadratic form

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

with $P = P^T$, $Q = Q$", $\det L \neq 0$ by the formula

$$\widehat{S}_{\mathcal{A},m}\psi(x) = \left(\tfrac{1}{2\pi i\hbar}\right)^{n/2} i^m \sqrt{|\det L|} \int e^{\frac{i}{\hbar}\mathcal{A}(x,x')}\psi(x')\mathrm{d}^n x'; \tag{8}$$

here m corresponds to a choice of the argument of $\det L$ modulo 2π. One proves in fact (Leray [19], de Gosson [9]) that every $\widehat{S} \in \mathrm{Mp}(n)$ can be written (non-uniquely) as the product of two operators of the type (8): $\widehat{S} = \widehat{S}_{\mathcal{A},m}\widehat{S}_{\mathcal{A}',m'}$ and (de Gosson [5]) that the integer

$$m(\widehat{S}) = m + m' - \mathrm{Inert}(P' + Q) \tag{9}$$

is independent modulo 4 of the factorization $\widehat{S}_{\mathcal{A},m}\widehat{S}_{\mathcal{A}',m'}$ of $\widehat{S}$; the class modulo 4 of $m(\widehat{S})$ is the *Maslov index of the metaplectic operator* $\widehat{S}$ (for details and proofs see de Gosson [5, 9]). 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

$$\widehat{S}\widehat{T}(z_0) = \widehat{T}(Sz_0)\widehat{S} \quad , \quad W(\widehat{S}\psi, \widehat{S}\phi)(z) = W(\psi,\phi)(S^{-1}z) \tag{10}$$

hold for all $\widehat{S} \in \mathrm{Mp}(n)$ and $z_0 \in \mathbb{R}^{2n}$ (see for instance [9, 20]); the first formula (10) is the analogue, at the operator level, of the trivial formula $ST(z_0) = T(Sz_0)S$, where $T(z_0)$ is the translation operator $z \longmapsto z + z_0$

Let us apply the phase-space formalism described above to metaplectic operators. Weyl symbols $(a_{\mathcal{A},m})_\sigma$ of the generators $\widehat{S}_{\mathcal{A},m}$ of $\mathrm{Mp}(n)$ and then to extend the formula

$$\widehat{S}_{\mathcal{A},m}\psi(x) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int (a_{\mathcal{A},m})_\sigma(z_0)\widehat{T}(z_0)\psi(x)\mathrm{d}^{2n}z_0 \tag{11}$$

by setting

$$(\widehat{S}_{\mathcal{A},m})_{\mathrm{ph}}\Psi(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int (a_{\mathcal{A},m})_\sigma(z_0)\widehat{T}_{\mathrm{ph}}(z_0)\Psi(z)\mathrm{d}^{2n}z_0. \tag{12}$$

In [6] (also see [9, 11]) we have shown that if $\pi^{\mathrm{Mp}}(\widehat{S}_{\mathcal{A},m})$ does not have any eigenvalue equal to one, then its Weyl symbol is given by

$$(a_{\mathcal{A},m})_\sigma(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n i^{\nu_{\mathcal{A},m}} |\det(S-I)|^{-1/2} e^{\frac{i}{2\hbar}M_S z^2} \tag{13}$$

where M_S is the *symplectic Cayley transform* of S: it is the symmetric matrix

$$M_S = \frac{1}{2}J(S+I)(S-I)^{-1}; \qquad \text{(cayley)}$$

the exponent $\nu_{\mathcal{A},m}$ of i in formula (13) corresponds to a choice of argument for $\det(S-I)$; it is the *Conley-Zehnder index* (modulo 4) of $\widehat{S}_{\mathcal{A},m}$ and is explicitly related to $\mathcal{A}$ and m by the formula

$$\nu_{\mathcal{A},m} = m - \operatorname{Inert} \mathcal{A}''_{xx} \mod 4 \tag{14}$$

where $\operatorname{Inert} \mathcal{A}''_{xx}$ is the number of negative eigenvalues of the Hessian matrix (for a detailed study of the Conley–Zehnder index see de Gosson [6, 9, 11]).

The operators $\widehat{S}_{\mathrm{ph}}$ are in one-to-one correspondence with the metaplectic operators $\widehat{S}$ and thus generate a group which we denote by $\mathrm{Mp}_{\mathrm{ph}}(n)$; that group is of course isomorphic to $\mathrm{Mp}(n)$. The following equivalent formulae are easily deduced (see [6, 9]):

$$\widehat{S}_{\mathrm{ph}} = \left(\tfrac{1}{2\pi\hbar}\right)^n i^{\nu(S)} \sqrt{|\det(S-I)|} \int \widehat{T}_{\mathrm{ph}}(Sz)\widehat{T}_{\mathrm{ph}}(-z)\mathrm{d}^{2n}z \tag{15}$$

and

$$\widehat{S}_{\mathrm{ph}} = \left(\tfrac{1}{2\pi\hbar}\right)^n i^{\nu(S)} \sqrt{|\det(S-I)|} \int e^{-\frac{i}{2\hbar}\sigma(Sz,z)}\widehat{T}_{\mathrm{ph}}((S-I)z)\mathrm{d}^{2n}z. \tag{16}$$

Notice that 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 $S \in Sp(n)$ extends to the phase-space Weyl operators $\widehat{A}_{\mathrm{ph}}$: we have

$$\widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z_0)\widehat{S}_{\mathrm{ph}}^{-1} = \widehat{T}_{\mathrm{ph}}(Sz) \ \ , \ \ \widehat{A\circ S}_{\mathrm{ph}} = \widehat{S}_{\mathrm{ph}}^{-1}\widehat{A}_{\mathrm{ph}}\widehat{S}_{\mathrm{ph}}. \tag{17}$$

The following metaplectic covariance formulae, which follow from the definitions, are also useful:

$$\widehat{S}_{\mathrm{ph}}\mathcal{U}_\phi\psi = \mathcal{U}_\phi\widehat{S}\psi \ , \ \widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z_0) = \widehat{T}_{\mathrm{ph}}(Sz_0)\widehat{S}_{\mathrm{ph}} \ . \tag{18}$$

1.1.3 Phase space Schrödinger equation

The consideration of Schrödinger equations in phase space is rather recent; their introduction and systematic study 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 $\widehat{T}_{\rm ph}(z_0)$ the operator $\mathcal{S}'(\mathbb{R}^{2n}) \longrightarrow \mathcal{S}'(\mathbb{R}^{2n})$ defined by

$$\widehat{T}_{\rm ph}(z_0)\Psi(z) = e^{-\frac{i}{2\hbar}\sigma(z,z_0)}\Psi(z-z_0); \tag{19}$$

these operators are unitary when restricted to $L^2(\mathbb{R}^{2n})$ and lead to an irreducible representation of the Heisenberg group. They satisfy the product formula

$$\widehat{T}_{\rm ph}(z_0+z_1) = e^{-\frac{i}{2\hbar}\sigma(z_0,z_1)}\widehat{T}_{\rm ph}(z_0)\widehat{T}_{\rm ph}(z_1) \tag{20}$$

and hence they verify the same commutation relations

$$\widehat{T}_{\rm ph}(z_0)\widehat{T}_{\rm ph}(z_1) = e^{\frac{i}{2\hbar}\sigma(z_0,z_1)}\widehat{T}_{\rm ph}(z_1)\widehat{T}_{\rm ph}(z_0) \tag{21}$$

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

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

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

we have

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

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

$$\widehat{A}_{\rm ph}\Psi(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int a_\sigma(z)\widehat{T}_{\rm ph}(z_0)\Psi(z)\mathrm{d}^{2n}z. \tag{22}$$

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

The following results are key to the passage to phase-space Schrödinger equations:

Proposition 2 *For every $\phi \in \mathcal{S}(\mathbb{R}^n)$ we have the following intertwining relations:*

$$\widehat{T}_{ph}(z_0)\mathcal{U}_\phi = \mathcal{U}_\phi\widehat{T}(z_0)\ ,\ \widehat{A}_{ph}\mathcal{U}_\phi = \mathcal{U}_\phi\widehat{A}. \tag{23}$$

Proof. The first formula (23) is obtained by a direct calculation; the second formula (23) immediately follows from using definition (22). (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:

$$\mathcal{U}_\phi(x_j\psi) = \left(\tfrac{1}{2}x_j + i\hbar\tfrac{\partial}{\partial p_j}\right)\mathcal{U}_\phi\psi, \tag{24}$$

$$\mathcal{U}_\phi(-i\hbar\tfrac{\partial}{\partial x_j}\psi) = \left(\tfrac{1}{2}p_j - i\hbar\tfrac{\partial}{\partial x_j}\right)\mathcal{U}_\phi\psi; \tag{25}$$

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

$$\widehat{X}_{\mathrm{ph}} = \tfrac{1}{2}x + i\hbar\tfrac{\partial}{\partial p} \quad , \quad \widehat{P}_{\mathrm{ph}} = \tfrac{1}{2}p - i\hbar\tfrac{\partial}{\partial x}$$

formulae (24), (25) justify the notation

$$\widehat{A}_{\mathrm{ph}} = A(\widehat{X}_{\mathrm{ph}}, \widehat{P}_{\mathrm{ph}}).$$

One has the following result linking the solutions of the ordinary Schrödinger equation (1) to the corresponding phase space Schrödinger equations:

Proposition 3 *Let ψ be a solution of the configuration space Schrödinger equation*

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

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

$$i\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}_{ph}\Psi \quad , \quad \Psi(\cdot, t_0) = \mathcal{U}_\phi\psi_0 \tag{26}$$

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

Proof. This follows from formulae (23) and the discussion above (see [7, 8] for details). ■

Notice that the phase-space Schrödinger equations may have solutions that are not in the range of the transform $\mathcal{U}_\phi$. Also, to one solution of the standard Schrödinger equation one can in general associate infinitely many solutions of (26) by choosing different windows ϕ.

2 The Nearby Orbit Method

Let us begin by reviewing the method in the usual situation of the configuration space Schrödinger equation.

2.1 Description of the method

2.1.1 Schrödinger equation in configuration space

Let H be the Weyl symbol of the operator $\widehat{H}$ (it is the classical Hamiltonian), we denote by (f_{t,t_0}) 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

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

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 4 *Let H be a quadratic Hamiltonian: $H_M(z,t) = \frac{1}{2}M(t)z^2$ for 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 $\psi_0 \in \mathcal{S}(\mathbb{R}^n)$ set $\psi(x,t) = \widehat{S}_{t,t_0}\psi_0(x)$. The function ψ is the solution of the Cauchy problem*

$$i\hbar\frac{\mathrm{d}\psi}{\mathrm{d}t} = \widehat{H_M}\psi \quad , \quad \psi(\cdot,t_0) = \psi_0 \tag{27}$$

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

For a detailed proof see [9] and the references therein; the fact that $\widehat{S}_{t,t_0}$ is the exact propagator highlights the well-known property that the classical dynamics entirely and unambiguously determines the quantum evolution as far as quadratic Hamiltonians are concerned (*cf.* Ehrenfest's theorem).

Consider the Schrödinger's equation

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

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

$$\psi^{(0)}(x,t) = U^{(0)}_{t,t_0}(z_0)\psi_0 = e^{\frac{i}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\widehat{T}(z_0)^{-1}\psi_0; \tag{28}$$

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

$$\gamma(t,t_0;z_0) = \int_{t_0}^{t}\left(\tfrac{1}{2}\sigma(z_{t'},\dot{z}_{t'}) - H(z_{t'},t')\right)\mathrm{d}t' \tag{29}$$

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

Remark 5 *The function $\psi^{(0)}(x,t)$ defined by (28) is the exact solution of the Schrödinger equation obtained by replacing H by its truncated Taylor series*

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

around z_t; notice that H_{z_0} is time-dependent even if H is not.

Remark 6 *Beware! The semi-classical "propagator" $U^{(0)}_{t,t_0}(z_0)$ is* not *a linear operator.*

2.1.2 The case of coherent states

An interesting case is when the initial function ψ_0 is a *coherent state*. The standard coherent state (already mentioned in §1.1.1) is the function

$$\phi^\hbar(x) = \left(\tfrac{1}{\pi\hbar}\right)^{n/4} e^{-\frac{1}{2\hbar}|x|^2}; \tag{30}$$

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

$$\phi^\hbar_{z_0}(x) = \widehat{T}(z_0)\phi_\hbar = e^{\frac{i}{\hbar}(p_0\cdot x - \frac{1}{2}p_0\cdot x_0)}\phi^\hbar(x-x_0). \tag{31}$$

Coherent states are normalized: $||\phi^\hbar_{z_0}|| = 1$, and we have

$$W\phi^\hbar(z) = \left(\tfrac{1}{\pi\hbar}\right)^n e^{-\frac{1}{\hbar}|z|^2}. \tag{32}$$

Remark 7 *The functions $\phi^\hbar$ and $\phi^\hbar_{z_0}$ are often also denoted by $|0\rangle$ and $|z_0\rangle$, respectively, in the quantum-mechanical literature.*

If we use coherent states as initial wavefunctions, formula (28) becomes particularly simple:

Proposition 8 *The approximate solution to Schrödinger's equation*

$$i\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi \quad , \quad \psi(\cdot, t_0) = \phi^\hbar_{z_0}$$

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

$$\psi^{(0)} = e^{\frac{i}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar. \tag{33}$$

Proof. Formula (33) is of course an immediate consequence of formula (28) and definition (31) of $\phi^\hbar_{z_0}$ since

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

■

Formula (33) shows that in the nearby orbit approximation Gaussian wavepackets are first deformed (or "squeezed") by a metaplectic operator, and then propagated along the classical trajectories. The "squeezing" actually preserves the Gaussian character of the initial wavepacket. 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

$$\phi^\hbar_M(x) = \left(\tfrac{\det \operatorname{Im} M}{(\pi\hbar)^n}\right)^{1/4} e^{\frac{i}{2\hbar}Mx^2} \tag{34}$$

and

$$\phi^\hbar_{M,z_0}(x) = \widehat{T}(z_0)\phi^\hbar_M(x) \tag{35}$$

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 takes a coherent state into another coherent state: if $\widehat{S} \in \mathrm{Mp}(n)$ has projection $S = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ on $\mathrm{Sp}(n)$ then

$$\widehat{S}\phi^\hbar_{M,z_0} = \phi^\hbar_{\alpha(S)M,Sz_0} \quad , \quad \alpha(S)M = (C + DM)(A + BM)^{-1} \tag{36}$$

where $\alpha(S)M \in \Sigma_n^+$. This result allows us to rewrite formula (33) in the very concise form

$$\psi^{(0)} = e^{\frac{i}{\hbar}\gamma(t,t_0;z_0)}\phi^{\hbar}_{M_t,z_t} \quad , \quad M_t = S_{t,t_0}(z_0)(iI) \tag{37}$$

which shows in an explicit way the "squeezing" of the wavepacket as it moves along the classical trajectory.

2.1.3 Some estimates

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

- The mapping $(z,t) \longrightarrow H(z,t)$ is continuous for $|t-t_0| \leq T$ 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 $|\partial_z^\alpha H(z,t)| \leq C_\alpha(T)(1+|z|^2)^{\mu_\alpha}$ for$|t-t_0| \leq T$

we have the following precise result:

Proposition 9 *Assume that the Cauchy problem*

$$\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi \quad , \quad \psi(\cdot,t_0) = \phi^{\hbar}_{z_0}$$

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

$$\psi^{(N)}(x,t) = e^{\frac{i}{\hbar}\gamma(t,t_0;z_0)} \sum_{0\leq j\leq N} \hbar^{j/2} P_j(\hbar^{-1/2}(x-x_t))\phi^{\hbar}_{M_t,z_t}. \tag{38}$$

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

$$||\psi(\cdot,t) - \psi^{(N)}(\cdot,t)|| \leq C_N(z_0,T)\hbar^{(N+1)/2}|t-t_0|. \tag{39}$$

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

$$\psi^{(0)}(x,t) = e^{\frac{i}{\hbar}\gamma(t,t_0;z_0)}\phi^{\hbar}_{M_t,z_t}$$

and

$$||\psi(\cdot,t) - \psi^{(0)}(\cdot,t)|| \leq C_0(z_0,T)\hbar^{1/2}|t-t_0|. \tag{40}$$

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 9. Also see Nazaikiinskii *et al.* [21] (Ch.2, §2.1) for related results using a slightly different method.

2.2 Nearby-orbit method in phase space

2.2.1 Statement of results

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

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

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

Proposition 10 *The semi-classical propagator $U_{t,t_0}^{(0)}$ takes $\Psi_0 = \mathcal{U}_\phi\psi_0$ to the function*

$$\Psi^{(0)} = e^{\frac{i}{\hbar}\gamma(t,t_0;z_0)}\widehat{T}_{ph}(z_t)(\widehat{S}_{t,t_0}(z_0))_{ph}\widehat{T}(z_0)_{ph}^{-1}\Psi_0 \tag{41}$$

with $\Psi_0 = \mathcal{U}_\phi\psi_0$ and

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

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

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

hence, by repeated use of the intertwining formulae (18):

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

which proves (41). ∎

An immediate consequence of Proposition 10 above is:

Corollary 11 *(i) If* $\Psi_0 = \mathcal{U}_\phi \phi^\hbar_{z_0}$ *then*

$$\Psi^{(0)} = e^{\frac{i}{\hbar}\gamma(z_0,t)} \widehat{T}_{ph}(z_t) \widehat{S}_t(z_0)_{ph} \Phi^\hbar \tag{42}$$

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

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

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

Proof. (i) In view of formula (41) we have

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

Formula (42) follows since we have

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

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

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

∎

2.2.2 Validity of the method

Of course, a natural question is arising at this point:

How good are the semi-classical approximations

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

and

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

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

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

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

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

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

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

■

From the results above we deduce:

Proposition 13 *Assume that the solution Ψ of the phase-space Schrödinger equation*

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

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 9. Then, for $|t| < T$ there exists a constant $C_T \geq 0$ such that

$$|||U^{(0)}_{t,t_0}(z_0)_{ph}\Phi^\hbar_{z_0} - \Psi(\cdot,t)||| \leq C(z_0,T)|t-t_0|\sqrt{\hbar}. \tag{43}$$

Proof. It suffices to apply Lemma 12 above together with Proposition 9. ■

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

Proposition 14 *Under the same assumptions as above the function $\Psi^{(N)} = \mathcal{U}_\phi\psi^{(N)}$ where $\psi^{(N)} = U^{(N)}_{t,t_0}(z_0)\psi_0$ is of the type*

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

with $\Phi^\hbar = \mathcal{U}_\phi\phi^\hbar$ and satisfies

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

Proof. In view of formula (38) in Proposition 9 the N-th order approximation is given by

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

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

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

We have

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

In view of the intertwining formula (24) we have

$$\mathcal{U}_\phi\left[P_j(\hbar^{-1/2}(x-x_t))\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar_{z_0}\right] = \\ P_j(\hbar^{-1/2}(\widehat{X}_{\mathrm{ph}}-x_t))\mathcal{U}_\phi\left[\widehat{T}(z_t)\widehat{S}_{t,t_0}(z_0)\phi^\hbar\right]$$

and

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

hence the result, using again Lemma 12 and the estimate (39). ■

3 Regularity in Modulation Spaces

In this Section we study the regularity of semi-classical solutions in a class of functional spaces due to Feichtinger [3, 4] an to which a voluminous literature has been devoted (see Gröchenig's book [12] for complements and references).

3.1 The Feichtinger algebra $M^1(\mathbb{R}^n)$

3.1.1 The short-time Fourier transform

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

$$V_\phi\psi(z) = \int e^{-2\pi i p\cdot x'}\psi(x')\overline{\phi(x'-x)}\mathrm{d}^n x'; \tag{44}$$

it is related to the Wigner–Moyal transform by

$$W(\psi,\phi)(z) = \left(\tfrac{2}{\pi\hbar}\right)^{-n/2} e^{\frac{2i}{\hbar}p\cdot x} V_{\phi^\vee_{\sqrt{2\pi\hbar}}}\psi_{\sqrt{2\pi\hbar}}(2z/\sqrt{\hbar}) \tag{45}$$

where $\psi_{\sqrt{2\pi\hbar}}(x)=\psi(x\sqrt{2\pi\hbar})$, $\phi^{\vee}(x)=\phi(-x)$. Using formulae (5) and (45) we thus have the following simple relation between the windowed wavepacket transform $\mathcal{U}_\phi\psi$ and V_ϕ:

$$\mathcal{U}_\phi\psi(z)=e^{\frac{i}{2\hbar}p\cdot x}V_{\phi^{\vee}_{\sqrt{2\pi\hbar}}}\psi_{\sqrt{2\pi\hbar}}(z/\sqrt{2\pi\hbar}). \tag{46}$$

3.1.2 Definition of $M^1(\mathbb{R}^n)$

Let $\phi\in\mathcal{S}(\mathbb{R}^n)$. By definition, the Feichtinger algebra $M^1(\mathbb{R}^n)$ (sometimes also denoted by $S_0(\mathbb{R}^n)$) is the "modulation space" consisting of all ψ such that $V_\phi\psi\in L^1(\mathbb{R}^{2n})$; it immediately follows from formula (46) that this condition is equivalent to $\mathcal{U}_\phi\psi\in L^1(\mathbb{R}^{2n})$. A crucial (and highly non-trivial!) fact, which ensures the validity of the definition of $M^1(\mathbb{R}^n)$, is that the condition $V_\phi\psi\in L^1(\mathbb{R}^{2n})$ (resp. $\mathcal{U}_\phi\psi\in L^1(\mathbb{R}^{2n})$) does not depend on the choice of the window ϕ. In addition the formulae

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

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

Proposition 15 *A distribution $\psi\in\mathcal{S}'(\mathbb{R}^n)$ is in $M^1(\mathbb{R}^n)$ if and only if $W\psi\in L^1(\mathbb{R}^n)$.*

One moreover shows that $M^1(\mathbb{R}^n)$ is complete for the topology thus defined, hence a Banach space; it is in fact even a Banach algebra (see Remark 18 below).

We have the inclusions:

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

it follows from the (continuous) inclusions $\mathcal{S}(\mathbb{R}^n)\subset M^1(\mathbb{R}^n)\subset L^2(\mathbb{R}^n)$ that $M^1(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$. Using the theory of rigged Hilbert spaces one can show that $(M^1(\mathbb{R}^n),L^2(\mathbb{R}^n),M^1(\mathbb{R}^n)^*$ actually is a "Gelfand triple".

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

Remark 16 *More generally, it is often useful to consider the weighted modulation spaces $M^1_{v^s}(\mathbb{R}^n)$, $s\geq 0$, where $v_s(z)=(1+|z|^2)^{s/2}$; by definition $\psi\in M^1_{v^s}(\mathbb{R}^n)$ if and only if $v_s\mathcal{U}_\phi\psi\in L^1(\mathbb{R}^{2n})$ for one (and hence all) $\phi\in\mathcal{S}(\mathbb{R}^n)$.*

3.2 Application to the nearby-orbit method; a conjecture

3.2.1 An essential property of $M^1(\mathbb{R}^n)$

The Feichtinger algebra has the two following crucial properties:

Proposition 17 *Let $\psi \in M^1(\mathbb{R}^n)$. We have:*
(i) $\widehat{T}(z_0)\psi \in M^1(\mathbb{R}^n)$ for every $z_0 \in \mathbb{R}^{2n}$;
(ii) $\widehat{S}\psi \in M^1(\mathbb{R}^n)$ for every $\widehat{S} \in \mathrm{Mp}(n)$. (In particular $M^1(\mathbb{R}^n)$ is invariant under Fourier transformation)

Proof. (i) A straightforward calculation shows that we have

$$W(\widehat{T}(z_0)\psi, \phi)(z) = e^{\frac{i}{\hbar}\sigma(z,z_0)}W(\psi, \phi)(z - \tfrac{1}{2}z_0)$$

and hence

$$\begin{aligned}\mathcal{U}_\phi(\widehat{T}(z_0)\psi) &= \left(\tfrac{\pi\hbar}{2}\right)^{n/2} W(\widehat{T}(z_0)\psi, \phi)(\tfrac{1}{2}z) \\ &= \left(\tfrac{\pi\hbar}{2}\right)^{n/2} e^{\frac{i}{2\hbar}\sigma(z,z_0)}W(\psi, \phi)(\tfrac{1}{2}(z - z_0)) \\ &= \mathcal{U}_\phi\psi(z - z_0)\end{aligned}$$

where the last quality follows from the fact that $\sigma(z - z_0, z_0) = \sigma(z, z_0)$. We thus have

$$||\mathcal{U}_\phi(\widehat{T}(z_0)\psi)||_{L^1(\mathbb{R}^{2n})} = \int |\mathcal{U}_\phi\psi(z - z_0)|\mathrm{d}^{2n}z = ||\mathcal{U}_\phi\psi||_{L^1(\mathbb{R}^{2n})}$$

and hence $\widehat{T}(z_0)\psi \in M^1(\mathbb{R}^n)$. (ii) We have, using the second metaplectic covariance formula (10)

$$\begin{aligned}\mathcal{U}_\phi(\widehat{S}\psi) &= \left(\tfrac{\pi\hbar}{2}\right)^{n/2} W(\widehat{S}\psi, \phi)(\tfrac{1}{2}z) \\ &= \left(\tfrac{\pi\hbar}{2}\right)^{n/2} W(\psi, \widehat{S}^{-1}\phi)(\tfrac{1}{2}S^{-1}z) \\ &= U_{\widehat{S}^{-1}\phi}\psi(S^{-1}z).\end{aligned}$$

Since $\det S = 1$,

$$\int |U_{\widehat{S}^{-1}\phi}\psi(S^{-1}z)|\mathrm{d}^{2n}z = \int |U_{\widehat{S}^{-1}\phi}\psi(z)|\mathrm{d}^{2n}z$$

hence the integral in the right-hand side is convergent if and only if $\mathcal{U}_\phi\psi \in L^1(\mathbb{R}^{2n})$. It follows that $\mathcal{U}_\phi(\widehat{S}\psi) \in L^1(\mathbb{R}^{2n})$ hence $\widehat{S}\psi \in M^1(\mathbb{R}^n)$. ■

Remark 18 *The Feichtinger algebra is actually the* smallest *Banach space containing $\mathcal{S}(\mathbb{R}^n)$ and which is invariant under the action of the Heisenberg–Weyl operators.*

3.2.2 Application to semi-classical solutions

The properties of $M^1(\mathbb{R}^n)$ listed in Proposition 17 allow us to prove the following regularity result for the semi-classical approximations $\psi^{(0)} = U_{t,t_0}^{(0)}(z_0)\psi_0$:

Proposition 19 *The two following equivalent statements hold:*
(i) If $\psi_0 \in M^1(\mathbb{R}^n)$ then $U_{t,t_0}^{(0)}(z_0)\psi_0 \in M^1(\mathbb{R}^n)$;
(ii) $\Psi_0 \in L^1(\mathbb{R}^{2n})$ then $U_{t,t_0}^{(0)}(z_0)_{ph}\Psi_0 \in L^1(\mathbb{R}^{2n})$.

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

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

statement (i) follows by repeated use of Proposition 17. ∎

Remark 20 *A rather straightforward adaptation of the proof of Proposition 17 shows that the more general weighted spaces $M_{v^s}^1(\mathbb{R}^n)$ mentioned in Remark 16 also are closed under Heisenberg–Weyl and metaplectic operators. It follows that the conclusion of Proposition 19 remain true mutatis mutandis, replacing $M^1(\mathbb{R}^n)$ and $L^1(\mathbb{R}^{2n})$ by $M_{v^s}^1(\mathbb{R}^n)$ and $L_{v^s}^1(\mathbb{R}^{2n})$, 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 to a Schrödinger equation with quadratic Hamiltonian (this is actually an immediate consequence of Proposition 4). In fact, we conjecture

Conjecture 21 *The conclusions of Proposition 19 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.

4 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 haven't 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

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

They show that if certain analytical conditions on the potential V are satisfied the error is of order $e^{-\gamma/\hbar}$ 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; conversely it is also clear that the methods used in quantum mechanics are not always known by applied mathematicians (the Schrödinger equation is one typical example, the uncertainty principle is another). I think that a synergetic approach to both Sciences would lead to unexpected advances in many directions. I hope to come back to this fascinating interaction in a very near future.

Acknowledgement 22 *This paper was written during a stay of the author at the International Erwin Schrödinger Institute in Vienna. It is a duty and a pleasure to thank Professor Jakob Yngvason for his kind and generous invitation and hospitality. An early version of this work has also benefitted from financial support from the European Union EUCETIFA grant MEXT-CT-2004-517154.*

References

[1] D Chruscinski and K Mlodawski. Wigner function and Schrödinger equation in phase space representation. *Phys. Rev. A*,.**71** (2005), 052104-1–052104-6; Preprint, arXiv: quant-ph/ 0501163 v1, 2005.

[2] M Combescure and D Robert 1997 Semiclassical spreading of quantum wave packets and applications near unstable fixed points of the classical flow. *Asymptotic Analysis* **14** 377–404.

[3] H G Feichtinger 1991 On a new Segal algebra. *Monatsh. Math.*, 92(4): 269–289

[4] H G Feichtinger 2006 Modulation Spaces; Looking back and ahead. *Sampl. Theory Signal Image Process* **5**, 109–140.

[5] M de Gosson 1990 Maslov Indices on Mp(n). *Ann. Inst. Fourier,* Grenoble, **40**(3) 537–555.

[6] M de Gosson 2005 The Weyl Representation of Metaplectic Operators. *Lett. Math. Phys*, **72** 129–142.

[7] M de Gosson 2005 Extended Weyl Calculus and Application to the Phase-Space Schrödinger Equation. *J. Phys. A: Math. and General* **38**.

[8] M de Gosson 2005 Symplectically Covariant Schrödinger Equation in Phase Space. *J. Phys.A:Math. Gen.* **38** 9263–9287.

[9] M de Gosson 2006 Symplectic Geometry and Quantum Mechanics. *Birkhäuser, Basel,* Series Operator Algebras and Applications.

[10] M de Gosson 2006 Schrödinger Equation in Phase Space, Irreducible Representations of the Heisenberg Group, and Deformation Quantization. Resenhas **6**, no. 4, 383–395.

[11] M de Gosson and S de Gosson 2006 An extension of the Conley–Zehnder Index, a product formula and an application to the Weyl representation of metaplectic operators. *J. Math. Phys.,* **47**.

[12] K Gröchenig 2001 *Foundations of Time-Frequency Analysis.* Birkhäuser, Boston.

[13] G Hagedorn 1981 Semiclassical quantum mechanics III. *Ann. Phys.* **135**, 58–70.

[14] G Hagedorn 1985 Semiclassical quantum mechanics IV. *Ann. Inst.* H. Poincaré **42**, 363–374.

[15] G Hagedorn and A Joye 2004 Semiclassical Dynamics with Exponentially Small Error Estimates. Comm. in Math. Physics, **207**(2) 439–465.

[16] E Heller 1975 Time-dependent approach to semiclassical dynamics. *The Journal of Chemical Physics* **62**(4),1544–1555.

[17] J Isidro and M de Gosson 2007 Abelian Gerbes as a Gauge Theory of Quantum Mechanics on Phase Space. *J. Phys. A: Math. Theor.* **40** 3549–3567.

[18] J Isidro and M de Gosson. A Gauge Theory of Quantum Mechanics. *Modern Physics Letters A*, **22**(3), 191–200, 2007

[19] J Leray 1981 Lagrangian Analysis and Quantum Mechanics, a mathematical structure related to asymptotic expansions and the Maslov index. *The MIT Press*, Cambridge, Mass.

[20] R G Littlejohn 1986 The semiclassical evolution of wave packets. *Physics Reports* **138(**4–5), 193–291.

[21] V Nazaikiinskii, B-W Schulze, and B Sternin 2002 Quantization Methods in Differential Equations. Differential and Integral Equations and Their Applications, *Taylor & Francis.*

[22] G Torres-Vega and J H Frederick 1990 Quantum mechanics in phase space: New approaches to the correspondence principle. *J. Chem. Phys.* **93**(12), 8862–8874.

[23] G Torres-Vega and J H Frederick 1993 A quantum mechanical representation in phase space. *J. Chem. Phys.* **98**(4), 3103–3120.

[24] N Wallach 1977 *Lie Groups: History, Frontiers and Applications*, **5**. Symplectic Geometry and Fourier Analysis, Math Sci Press, Brookline, MA.

[25] J. Williamson. *On the algebraic problem concerning the normal forms of linear dynamical systems*, Amer. J. of Math. **58**, 141–163, 1963.