Symplectically covariant Schrödinger equation in phase space

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Abstract
A classical theorem of Stone and von Neumann states that the Schrödinger representation is, up to unitary equivalences, the only irreducible representation of the Heisenberg group on the Hilbert space of square-integrable functions on configuration space. Using the Wigner–Moyal transform, we construct an irreducible representation of the Heisenberg group on a certain Hilbert space of square-integrable functions defined on phase space. This allows us to extend the usual Weyl calculus into a phase-space calculus and leads us to a quantum mechanics in phase space, equivalent to standard quantum mechanics. We also briefly discuss the extension of metaplectic operators to phase space and the probabilistic interpretation of the solutions of the phase-space Schrödinger equation.

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1. Introduction and motivations

In a recent letter [12], we have shortly discussed and justified the Schrödinger equation in phase space

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

proposed by Torres-Vega and Frederick in [28, 29] and obtained by these authors using a generalized version of the Husimi transform. In this paper, we set out to sketch a complete theory for the related equation

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

where the variables x and p are placed on equal footing. We will see that in addition to the greater aesthetic[1] appeal of the latter equation, it has the advantage of yielding a more straightforward physical interpretation of its solutions.

This paper is reasonably self-contained; we have given rather detailed proofs since there are many technicalities which are not always immediately obvious.

1.1. General discussion

One of the pillars of non-relativistic quantum mechanics is Schrödinger's equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 \psi + V(\vec{r}, t)\psi, \tag{1}$$

where the operator on the right-hand side is obtained from the Hamiltonian function

$$H = \frac{1}{2m} \vec{p}^2 + V(\vec{r}, t)$$

by replacing the momentum vector $\vec{p}$ by the operator $-i\hbar \nabla_{\vec{r}}$ and letting the position vector $\vec{r}$ stand as it is. But how did Schrödinger arrive at this equation? He arrived at it using what the novelist Arthur Koestler called a 'sleepwalker' argument, elaborating on Hamilton's optical–mechanical analogy and taking several mathematically illegitimate steps (see [15] or [18] for a thorough discussion of Schrödinger's argument). In fact, Schrödinger's equation can be rigorously justified for quadratic or linear potentials if one uses the theory of the metaplectic group (see our discussion in [9], chapters 6 and 7), but it *cannot* be mathematically justified for arbitrary Hamiltonian functions; it can only be made *plausible* by using formal analogies: this is what is done in all texts on quantum mechanics, and Dirac's treatise ([4], pp 108–11) is of course not an exception. The gist of Schrödinger's argument, recast in modern terms, is the following: a 'matter wave' consists—as all waves do—of an amplitude and a phase. Consider now a particle with initial position vector $\vec{r}_0 = (x(0), y(0), z(0))$. That particle moves under the influence of some potential and its position vector becomes $\vec{r}(t) = (x(t), y(t), z(t))$ at time t. The change of phase of the matter wave associated with the particle is then *postulated* to be the integral

$$\Delta \Phi = \frac{1}{\hbar} \int_{\Gamma} \vec{p} \cdot d\vec{r} - H \, dt \tag{2}$$

calculated along the arc of trajectory Γ joining the initial point $\vec{r}_0$ to the final point $\vec{r}(t)$ in spacetime; $\vec{p} = (p_x, p_y, p_z)$ is the momentum vector and $H = H(\vec{r}, \vec{p}, t)$ is the Hamiltonian function. The choice (2) for $\Delta \Phi$ is dictated by the fact that it represents the variation in action when the particle moves from its initial position to its final position. Now, in most cases of interest, the initial and final *position* vectors uniquely determine the initial and final *momentum vectors* if t is sufficiently small, so that $\hbar \Delta \Phi$ can be identified with Hamilton's principal function $W(\vec{r}_0, \vec{r}, t)$ (see [7, 9]) and the latter is a solution of Hamilton–Jacobi's equation

$$\frac{\partial W}{\partial t} + H(\vec{r}, \nabla_{\vec{r}} W, t) = 0. \tag{3}$$

Schrödinger knew that the properties of the 'action form'

$$\mathcal{A} = \vec{p} \cdot d\vec{r} - H \, dt \tag{4}$$

led to this equation, and this was all he needed to describe the time evolution of the phase. We now make an essential remark: the property that $\Delta \Phi$ can be identified with Hamilton's

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[1] Admittedly, this is a subjective criterion!

principal function is intimately related to the fact that the action form $\mathcal{A}$ is a *relative integral invariant*. This means that if γ and γ' are two closed curves in the $(\vec{r}, \vec{p}, t)$ space encircling the same tube of Hamiltonian trajectories, then we have

$$\oint_{\gamma} \vec{p} \cdot \mathrm{d}\vec{r} - H \, \mathrm{d}t = \oint_{\gamma'} \vec{p} \cdot \mathrm{d}\vec{r} - H \, \mathrm{d}t$$

(this formula is a consequence of Stoke's theorem and generalizes to an arbitrary number of dimensions; see for instance [1, 9]).

1.2. Other possible Schrödinger equations

We now make the following crucial observation, upon which much of this paper relies: the action form $\mathcal{A}$ is not the only relative integral invariant associated with the Hamiltonian H. In fact, for any real scalar λ, the differential form

$$\mathcal{A}_{\lambda} = \lambda \vec{p} \cdot \mathrm{d}\vec{r} + (\lambda - 1)\vec{r} \cdot \mathrm{d}\vec{p} - H \, \mathrm{d}t$$

also satisfies the equality

$$\oint_{\gamma} \mathcal{A}_{\lambda} = \oint_{\gamma'} \mathcal{A}_{\lambda}$$

and is hence also a relative integral invariant. This is immediately checked by noting that since γ is a closed curve we have

$$\oint_{\gamma} \vec{p} \cdot \mathrm{d}\vec{r} + \vec{r} \cdot \mathrm{d}\vec{p} = \oint_{\gamma} \mathrm{d}(\vec{p} \cdot \vec{r}) = 0$$

and hence

$$\oint_{\gamma} \lambda \vec{p} \cdot \mathrm{d}\vec{r} + (\lambda - 1)\vec{r} \cdot \mathrm{d}\vec{p} = \oint_{\gamma} \lambda \vec{p} \cdot \mathrm{d}\vec{r} + (1 - \lambda)\lambda \vec{p} \cdot \mathrm{d}\vec{r} = \oint_{\gamma} \vec{p} \cdot \mathrm{d}\vec{r}.$$

A particularly neat choice is $\lambda = 1/2$; it leads to the 'symmetrized action'

$$\mathcal{A}_{1/2} = \tfrac{1}{2}(\vec{p} \cdot \mathrm{d}\vec{r} - \vec{r} \cdot \mathrm{d}\vec{p}) - H \, \mathrm{d}t, \tag{5}$$

where the position and momentum variables now play identical roles, up to the sign.

Let us investigate the quantum-mechanical consequences of the choice $\lambda = 1/2$. We consider the very simple situation where the Hamiltonian function is linear in the position and momentum variables; more specifically, we assume that

$$H_0 = \vec{p} \cdot \vec{r}_0 - \vec{p}_0 \cdot \vec{r}.$$

The solutions of the associated equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{r}(t) = \vec{r}_0 \qquad \text{and} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\vec{p}(t) = \vec{p}_0$$

are the functions

$$\vec{r}(t) = \vec{r}(0) + \vec{r}_0 t \qquad \text{and} \qquad \vec{p}(t) = \vec{p}(0) + \vec{p}_0 t;$$

hence, the motion is just translation in phase space in the direction of the vector $(\vec{r}_0, \vec{p}_0)$. An immediate calculation shows that the standard change in phase (2), expressed in terms of the final position $\vec{r} = \vec{r}(t)$, is

$$\Delta\Phi = \Phi(\vec{r}; t) = \frac{1}{\hbar}\left(t\vec{p}_0 \cdot \vec{r} - \frac{t^2}{2}\vec{p}_0 \cdot \vec{r}_0\right); \tag{6}$$

this function, of course, trivially satisfies the Hamilton–Jacobi equation for H_0. Assuming that the initial wavefunction is $\psi_0 = \psi_0(\vec{r})$, a straightforward calculation shows that the function

$$\psi(\vec{r}, t) = \exp\left[\frac{i}{\hbar}\Phi(\vec{r}; t)\right]\psi_0(\vec{r} - t\vec{r}_0) \tag{7}$$

is a solution of the standard Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = (-i\hbar\vec{r}_0 \cdot \nabla_{\vec{r}} - \vec{p}_0 \cdot \vec{r})\psi = H_0(\vec{r}, -i\hbar\nabla_r)\psi.$$

Suppose now that instead of using definition (2) for the change in phase, we use instead the modified action associated with $\mathcal{A}_{1/2}$. Then,

$$\Delta\Phi_{1/2} = \frac{1}{\hbar}\int_\Gamma \frac{1}{2}(\vec{p} \cdot d\vec{r} - \vec{r} \cdot d\vec{p}) - H\,dt; \tag{8}$$

integrating and replacing $\vec{r}(0)$ with $\vec{r} - \vec{r}_0 t$ and $\vec{p}(0)$ with $\vec{p} - \vec{p}_0 t$, this leads to the expression

$$\Phi_{1/2}(\vec{r}, \vec{p}; t) = \frac{t}{2}(\vec{p} \cdot \vec{r}_0 - \vec{p}_0 \cdot \vec{r}),$$

which, in addition to time, depends on both $\vec{r}$ and $\vec{p}$; it is thus defined on *phase space*, and not on configuration space as was the case for (6). The function $\Phi_{1/2}(\vec{r}, \vec{p}; t)$ does not verify the ordinary Hamilton–Jacobi equation (3); it however verifies its symmetrized variant

$$\frac{\partial\Phi_{1/2}}{\partial t} + H_0\left(\frac{1}{2}\vec{r} + \nabla_{\vec{p}}\Phi_{1/2}, \frac{1}{2}\vec{p} - \nabla_{\vec{r}}\Phi_{1/2}\right) = 0 \tag{9}$$

as is checked by a straightforward calculation. This property opens the gates to *quantum mechanics in phase space*: assume again that we have an initial wavefunction $\psi_0 = \psi_0(\vec{r})$ and set

$$\Psi(\vec{r}, \vec{p}, t) = \exp\left[\frac{i}{\hbar}\Phi_{1/2}(\vec{r}; t)\right]\psi_0(\vec{r} - t\vec{r}_0). \tag{10}$$

Using (9), one finds that

$$i\hbar\frac{\partial\Psi}{\partial t} = \widehat{H_0}\left(\frac{1}{2}\vec{r} + i\hbar\nabla_{\vec{p}}, \frac{1}{2}\vec{p} - i\hbar\nabla_{\vec{r}}\right)\Psi; \tag{11}$$

there is in fact no reason to assume that the initial wavefunction depends only on $\vec{r}$. Choosing $\Psi_0 = \Psi_0(\vec{r}, \vec{p})$, the same argument shows that the function

$$\Psi(\vec{r}, \vec{p}, t) = \exp\left[\frac{i}{\hbar}\Phi_{1/2}(\vec{r}; t)\right]\Psi_0(\vec{r} - t\vec{r}_0, \vec{p} - t\vec{p}_0) \tag{12}$$

is a solution of (11) with initial condition Ψ_0. Observe that the operator $\widehat{H_0}$ in the 'phase-space Schrödinger equation' (11) is obtained from the Hamiltonian function H_0 using the phase-space quantization rule

$$x \longrightarrow \widehat{X} = \frac{1}{2}x + i\hbar\frac{\partial}{\partial p_x}, \qquad p_x \longrightarrow \widehat{P}_x = \frac{1}{2}p_x - i\hbar\frac{\partial}{\partial x}$$

and similar rules for the y, z variables. The operators $\widehat{X}, \widehat{P}_x$, etc obey the usual canonical commutation relations

$$[\widehat{X}, \widehat{P}_x] = -i\hbar, \qquad [\widehat{Y}, \widehat{P}_y] = -i\hbar, \qquad [\widehat{Z}, \widehat{P}_z] = -i\hbar$$

and this suggests that these quantization rules could be consistent with the existence of an irreducible representation of the Heisenberg group in phase space. This will be proved in section 3, where we will explicitly construct this representation.

Equation (11) corresponds, as we have seen, to the choice $\lambda = 1/2$ for the integral invariant $\mathcal{A}_\lambda$; any other choice is *per se* equally good. For instance, $\lambda = 1$ corresponds

to the standard Schrödinger equation; if we took $\lambda = 0$, we would obtain the phase-space Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H_0(\vec{r} + i\hbar \nabla_{\vec{p}}, -i\hbar \nabla_r)\Psi \tag{13}$$

considered by Torres-Vega and Frederick [28, 29] and discussed in [12].

The aesthetic appeal of the Schrödinger equation in phase space in the form (11) is indisputable, because it reinstates in quantum mechanics the symmetry of classical mechanics in its Hamiltonian formulation

$$\frac{d\vec{r}}{dt} = \nabla_{\vec{p}} H, \qquad \frac{d\vec{p}}{dt} = -\nabla_{\vec{r}} H; \tag{14}$$

in both (1) and (14), the variables x and p are placed, up to a change of sign, on the same footing.

1.3. Notations

We will work with systems having N degrees of freedom; we denote the position vector of such a system by $x = (x_1, \ldots, x_N)$ and its momentum vector by $p = (p_1, \ldots, p_N)$. We will also use the collective notation $z = (x, p)$ for the generic phase-space variable. Configuration space is denoted by $\mathbb{R}_x^N$ and phase space by $\mathbb{R}_z^{2N}$. The generalized gradients in x and p are written as follows:

$$\frac{\partial}{\partial x} = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_N}\right), \qquad \frac{\partial}{\partial p} = \left(\frac{\partial}{\partial p_1}, \ldots, \frac{\partial}{\partial p_N}\right).$$

For reasons of notational economy, we will write Mu^2 instead of $Mu \cdot u$, where M is a matrix and u is a vector.

We denote by $z \wedge z'$ the symplectic product of $z = (x, p)$, $z' = (x', p')$:

$$z \wedge z' = p \cdot x' - p' \cdot x,$$

where the dot is the usual (Euclidean) scalar product. In matrix notation,

$$z \wedge z' = (z')^T J z, \qquad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

where J is the standard symplectic matrix (0 and I are the $N \times N$ zero and identity matrices). We denote by $Sp(N)$ the symplectic group of the (x, p) phase space: it consists of all real $2N \times 2N$ matrices S such that $Sz \wedge Sz' = z \wedge z'$; equivalently,

$$S^T J S = S J S^T = J.$$

We denote by $(\cdot, \cdot)$ the L^2-norm of functions on configuration $\mathbb{R}_x^N$ and by $((\cdot, \cdot))$ that of functions on phase space $\mathbb{R}_z^{2N}$. The corresponding norms are denoted by $\|\cdot\|$ and $\|\|\cdot\|\|$, respectively.

$\mathcal{S}(\mathbb{R}^m)$ is the Schwartz space of rapidly decreasing functions on $\mathbb{R}^m$ and we denote by F the unitary Fourier transform defined on $L^2(\mathbb{R}_x^N)$ by

$$F\psi(p) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \int e^{-\frac{i}{\hbar} p \cdot x} \psi(x) \, d^N x. \tag{15}$$

2. The Wigner wavepacket transform

In the following, ϕ will be a rapidly decreasing function normalized to unity:

$$\phi \in \mathcal{S}(\mathbb{R}_x^N), \qquad \|\phi\|_{L^2(\mathbb{R}_x^N)}^2 = 1. \tag{16}$$

2.1. Definition and relation with the Wigner–Moyal transform

We associate with ϕ the integral operator $U_\phi : L^2(\mathbb{R}_x^N) \longrightarrow L^2(\mathbb{R}_z^{2N})$ defined by

$$U_\phi \psi(z) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} e^{\frac{i}{2\hbar} p \cdot x} \int e^{-\frac{i}{\hbar} p \cdot x'} \psi(x') \phi(x - x') \, d^N x' \tag{17}$$

and we call U_ϕ the 'Wigner wavepacket transform' associated with ϕ. This terminology is justified by the fact that the operator U_ϕ is easily expressed in terms of the Wigner–Moyal transform

$$W(\psi, \overline{\phi})(x, p) = \left(\frac{1}{2\pi\hbar}\right)^N \int_{\mathbb{R}^N} e^{-\frac{i}{\hbar} p \cdot y} \psi\left(x + \frac{1}{2} y\right) \overline{\phi}\left(x - \frac{1}{2} y\right) d^N y \tag{18}$$

of the pair $(\psi, \overline{\phi})$ (see [6, 16]). In fact, performing the change of variable $x' = \frac{1}{2}(x + y)$ in (17) we get

$$U_\phi \psi(z) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} 2^{-N} \int e^{-\frac{i}{2\hbar} p \cdot y} \psi\left(\frac{1}{2}(x + y)\right) \phi\left(\frac{1}{2}(x - y)\right) d^N y,$$

that is

$$U_\phi \psi(z) = \left(\frac{\pi\hbar}{2}\right)^{N/2} W(\psi, \overline{\phi})\left(\frac{1}{2} z\right). \tag{19}$$

Remark 1. A standard—but by no means mandatory—choice is to take for ϕ the real Gaussian

$$\phi_\hbar(x) = \left(\frac{1}{\pi\hbar}\right)^{N/4} \exp\left(-\frac{1}{2\hbar} |x|^2\right); \tag{20}$$

the corresponding operator U_ϕ is then (up to an exponential factor) the 'coherent state representation' familiar to quantum physicists.

2.2. The fundamental property

The interest of the Wigner wavepacket transform U_ϕ comes from the fact that it is an isometry of $L^2(\mathbb{R}_x^N)$ onto a closed subspace $\mathcal{H}_\phi$ of $L^2(\mathbb{R}_z^{2N})$ and that it takes the operators x and $-i\hbar\partial/\partial x$ into the operators $x/2 + i\hbar\partial/\partial p$ and $p/2 - i\hbar\partial/\partial x$.

Theorem 2. *The Wigner wavepacket transform U_ϕ has the following properties. (i) U_ϕ is an isometry: the Parseval formula*

$$((U_\phi \psi, U_\phi \psi')) = (\psi, \psi') \tag{21}$$

holds for all $\psi, \psi' \in \mathcal{S}(\mathbb{R}_x^N)$. In particular, $U_\phi^* U_\phi = I$ on $L^2(\mathbb{R}_x^N)$. (ii) The range $\mathcal{H}_\phi$ of U_ϕ is closed in $L^2(\mathbb{R}_z^{2N})$ (and is hence a Hilbert space), and the operator $P_\phi = U_\phi U_\phi^*$ is the orthogonal projection in $L^2(\mathbb{R}_z^{2N})$ onto $\mathcal{H}_\phi$. (iii) The following intertwining relations:

$$\left(\frac{x}{2} + i\hbar\frac{\partial}{\partial p}\right) U_\phi \psi = U_\phi(x\psi), \qquad \left(\frac{p}{2} - i\hbar\frac{\partial}{\partial x}\right) U_\phi \psi = U_\phi\left(-i\hbar\frac{\partial}{\partial x}\psi\right) \tag{22}$$

hold for $\psi \in \mathcal{S}(\mathbb{R}_x^N)$.

Proof. (i) Formula (21) is an immediate consequence of the property

$$((W(\psi, \phi), W(\psi', \phi'))) = \left(\frac{1}{2\pi\hbar}\right)^N (\psi, \psi')\overline{(\phi, \phi')} \tag{23}$$

of the Wigner–Moyal transform (see, e.g. [6], p 56; beware of the fact that Folland uses normalizations different from ours). In fact, taking $\phi = \phi'$ we have

$$((U_\phi \psi, U_\phi \psi')) = \left(\frac{\pi \hbar}{2}\right)^N \int W(\psi, \overline{\phi}) \left(\frac{1}{2} z\right) \overline{W(\psi', \overline{\phi})} \left(\frac{1}{2} z\right) \mathrm{d}^{2N} z$$
$$= (2\pi \hbar)^N ((W(\psi, \overline{\phi}), W(\psi', \overline{\phi})))$$
$$= (\psi, \psi')(\phi, \phi),$$

which is formula (21) since ϕ is normalized. To prove (ii), we note that $P_\phi^* = P_\phi$ and

$$P_\phi^2 = U_\phi (U_\phi^* U_\phi) U_\phi^* = U_\phi^* U_\phi = P_\phi;$$

hence, P_ϕ is indeed an orthogonal projection. Let us show that its range is $\mathcal{H}_\phi$; the closedness of $\mathcal{H}_\phi$ will follow since the range of a projection in a Hilbert space always is closed. Since $U_\phi^* U_\phi = I$ on $L^2(\mathbb{R}_x^N)$, we have $U_\phi^* U_\phi \psi = \psi$ for every ψ in $L^2(\mathbb{R}_x^N)$ and hence the range of U_ϕ^* is $L^2(\mathbb{R}_x^N)$. It follows that the range of U_ϕ is that of $U_\phi U_\phi^* = P_\phi$ and we are done. (iii) The verification of formulae (22) is purely computational, using differentiations and partial integrations; it is therefore left to the reader. $\qquad\square$

The intertwining formulae (22) show that the Wigner wavepacket transform takes the usual quantization rules $x \longrightarrow x$, $x \longrightarrow -\mathrm{i}\hbar \frac{\partial}{\partial x}$ leading to the standard Schrödinger equation to the phase-space quantization rules

$$x \longrightarrow \frac{1}{2} x + \mathrm{i}\hbar \frac{\partial}{\partial p}, \qquad p \longrightarrow \frac{1}{2} p - \mathrm{i}\hbar \frac{\partial}{\partial x};$$

observe that these rules are independent of the choice of ϕ and that these rules are thus a common features of all the transforms U_ϕ.

2.3. The range of U_ϕ

One should be aware of the fact that the Hilbert space $\mathcal{H}_\phi$ is smaller than $L^2(\mathbb{R}_z^{2N})$. This is intuitively clear since functions in $L^2(\mathbb{R}_z^{2N})$ depend on twice as many variables as those in $L^2(\mathbb{R}_x^N)$ of which $\mathcal{H}_\phi$ is an isometric copy. Let us discuss this in some detail.

Theorem 3. *(i) The range of the Wigner wavepacket transform $U_{\phi_\hbar}$ associated with the Gaussian (20) consists of the functions $\Psi \in L^2(\mathbb{R}_z^{2N})$ for which the conditions*

$$\left(\frac{\partial}{\partial x_j} - \mathrm{i}\frac{\partial}{\partial p_j}\right) \left[\exp\left(\frac{1}{2\hbar}|z|^2\right) \Psi(z)\right] = 0 \qquad \text{for} \quad 1 \leqslant j \leqslant N \qquad (24)$$

hold. (ii) For every ϕ, the range of the Wigner wavepacket transform U_ϕ is isometric to $\mathcal{H}_{\phi_\hbar}$.

Proof. (i) We have $U_{\phi_\hbar} = \mathrm{e}^{-\frac{\mathrm{i}}{2\hbar} p \cdot x} V_{\phi_\hbar}$, where the operator $V_{\phi_\hbar}$ is defined by

$$V_\phi \psi(z) = \left(\frac{1}{2\pi \hbar}\right)^{N/2} \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} p \cdot x'} \phi(x - x') \psi(x') \, \mathrm{d}^N x'.$$

It is shown in [22] that the range of $V_{\phi_\hbar}$ consists of all $\Psi \in L^2(\mathbb{R}_z^{2N})$ such that

$$\left(\frac{\partial}{\partial x_j} - \mathrm{i}\frac{\partial}{\partial p_j}\right) \left[\exp\left(\frac{1}{2\hbar}|p|^2\right) \Psi(z)\right] = 0 \qquad \text{for} \quad 1 \leqslant j \leqslant N.$$

That the range of $U_{\phi_\hbar}$ is characterized by (24) follows by an immediate calculation that is left to the reader. (ii) If U_{ϕ_1} and U_{ϕ_2} are two Wigner wavepacket transforms corresponding to the choices ϕ_1, ϕ_2, then $U_{\phi_2} U_{\phi_1}^*$ is an isometry of $\mathcal{H}_{\phi_1}$ onto $\mathcal{H}_{\phi_2}$. $\qquad\square$

The above result leads us to address the following more precise question: given $\Psi \in L^2(\mathbb{R}_z^{2N})$, can we find ϕ and ψ in $L^2(\mathbb{R}_x^N)$ such that $\Psi = U_\phi \psi$? We are going to see that the answer is *no*. Intuitively speaking, the reason is the following: if Ψ is too 'concentrated' in phase space, it cannot correspond via the inverse transform $U_\phi^{-1} = U_\phi^*$ to a solution of the standard Schrödinger equation, because the uncertainty principle would be violated. Let us make this precise when the function Ψ is a Gaussian. We first make the following obvious remark: in view of condition (24), every Gaussian

$$\Psi_0(z) = \lambda \exp\left(\frac{1}{2\hbar}|z|^2\right), \qquad \lambda \in \mathbb{C}$$

is in the range of $U_{\phi_\hbar}$. It turns out that not only does this particular Gaussian belong to the range of every Wigner wavepacket transform U_ϕ, but so does also the compose $\Psi_0 \circ S$ for every $S \in Sp(N)$.

Theorem 4. *Let G be a real positive-definite $2N \times 2N$ matrix: $G = G^T > 0$. Let $\Psi_G \in L^2(\mathbb{R}_z^{2N})$ be the Gaussian*

$$\Psi_G(z) = \exp\left(-\frac{1}{2\hbar}Gz^2\right). \tag{25}$$

(i) There exist $\psi, \phi \in \mathcal{S}(\mathbb{R}_x^N)$ such that $U_\phi \psi = \Psi_G$ if and only if $G \in Sp(N)$, in which case we have

$$\phi = \alpha\phi_\hbar, \qquad \psi = 2^{N/2}\overline{\alpha}\,(\pi\hbar)^{N/4}\,\phi_\hbar,$$

where $\phi_\hbar$ is the Gaussian (20) and α is an arbitrary complex constant with modulus 1. (ii) Equivalently, $|\Psi_G|^2$ must be the Wigner transform $W\psi$ of a Gaussian state

$$\psi(x) = c\,(\det X)^{1/4}\,(\pi\hbar)^{3N/4}\exp\left[-\frac{1}{2\hbar}(X + iY)x^2\right], \tag{26}$$

with $|c| = 1$, X and Y real and symmetric, and $X > 0$.

Proof. In view of relation (19) between U_ϕ and the Wigner–Moyal transform, (19) is equivalent to

$$W(\psi, \overline{\phi})(z) = \left(\frac{2}{\pi\hbar}\right)^{N/2}\exp\left(-\frac{2}{\hbar}Gz^2\right).$$

In view of Williamson's symplectic diagonalization theorem [30], there exists $S \in Sp(N)$ such that $G = S^T D S$, where D is the diagonal matrix

$$D = \begin{bmatrix} \Lambda & 0 \\ 0 & \Lambda \end{bmatrix}, \qquad \Lambda = \mathrm{diag}[\lambda_1, \ldots, \lambda_N],$$

the numbers $\pm i\lambda_1, \ldots, \lambda_N, \lambda_j > 0$, being the eigenvalues of JG^{-1}; it follows that

$$W(\psi, \overline{\phi})(S^{-1}z) = \left(\frac{2}{\pi\hbar}\right)^{N/2}\exp\left(-\frac{2}{\hbar}Dz^2\right).$$

In view of the metaplectic covariance property of the Wigner–Moyal transform (see (47) in section 4), there exists a unitary operator $\widehat{S} : \mathcal{S}(\mathbb{R}_x^N) \longrightarrow \mathcal{S}(\mathbb{R}_x^N)$ such that

$$W(\psi, \overline{\phi})(S^{-1}z) = W(\widehat{S}\psi, \widehat{S}\overline{\phi})(z);$$

hence, there is no restriction to assume $S = I$ and

$$W(\psi, \overline{\phi})(z) = \left(\frac{2}{\pi\hbar}\right)^{N/2}\exp\left(-\frac{2}{\hbar}Dz^2\right).$$

By definition (18) of the Wigner–Moyal transform, this is the same thing as

$$\left(\frac{1}{2\pi\hbar}\right)^{N/2}\int e^{-\frac{i}{\hbar}p\cdot y}\,\psi\left(x+\frac{1}{2}y\right)\phi\left(x-\frac{1}{2}y\right)d^N y = 2^N\exp\left(-\frac{2}{\hbar}Dz^2\right),$$

that is, in view of the Fourier inversion formula,

$$\psi\left(x+\frac{1}{2}y\right)\phi\left(x-\frac{1}{2}y\right) = 2^N\left(\frac{1}{2\pi\hbar}\right)^{N/2}\int e^{-\frac{i}{\hbar}p\cdot y}\,e^{-\frac{2}{\hbar}Dz^2}\,d^N p$$

$$= \left(\frac{2}{\pi\hbar}\right)^{N/2}e^{-\frac{1}{\hbar}\Lambda x^2}\int e^{\frac{i}{\hbar}p\cdot y}\,e^{-\frac{1}{\hbar}\Lambda p^2}\,d^N p.$$

Setting $Q = 2\Lambda$ in the generalized Fresnel formula

$$\left(\frac{1}{2\pi\hbar}\right)^{N/2}\int e^{-\frac{i}{\hbar}p\cdot y}\,e^{-\frac{1}{2\hbar}Qp^2}\,d^N p = (\det Q)^{-1/2}\,e^{-\frac{1}{2\hbar}Q^{-1}y^2}$$

valid for all $Q > 0$, we thus have

$$\psi\left(x+\frac{1}{2}y\right)\phi\left(x-\frac{1}{2}y\right) = 2^{N/2}(\det\Lambda)^{-1/2}\exp\left[-\frac{1}{\hbar}\left(\Lambda x^2 + \frac{1}{4}\Lambda y^2\right)\right].$$

Setting $u = x + \frac{1}{2}y$ and $v = x - \frac{1}{2}y$, this is

$$\psi(u)\phi(v) = 2^{N/2}(\det\Lambda)^{-1/2}\exp\left[-\frac{1}{4\hbar}((\Lambda+\Lambda^{-1})(u^2+v^2)+2(\Lambda-\Lambda^{-1})u\cdot v)\right]$$

and this is only possible if there are no terms $u\cdot v$. This condition requires that $\Lambda = \Lambda^{-1}$; since Λ is positive definite, we must have $\Lambda = I$ and hence $\Delta = I$. It follows that

$$\psi(u)\phi(v) = 2^{N/2}\exp\left[-\frac{1}{2\hbar}(u^2+v^2)\right],$$

so that

$$\psi(x)\phi(0) = \psi(0)\phi(x) = 2^{N/2}\exp\left(-\frac{1}{2\hbar}x^2\right).$$

It follows that both ψ and ϕ are Gaussians of the type

$$\psi(x) = \psi(0)\exp\left(-\frac{1}{2\hbar}x^2\right),\qquad \phi(x) = \phi(0)\exp\left(-\frac{1}{2\hbar}x^2\right);$$

since ϕ is normalized this requires that $\phi = \alpha\phi_\hbar$ with $|\alpha| = 1$ and hence

$$\phi(0) = \alpha\left(\frac{1}{\pi\hbar}\right)^{N/4}.$$

Since we have $\psi(0)\phi(0) = 2^{N/2}$, we must have

$$\psi(0) = \overline{\alpha}2^{N/2}(\pi\hbar)^{N/4},$$

which concludes the proof of part (i) of the theorem. To prove (ii), recall from [16] that the Wigner transform of the Gaussian (26) is given by the formula

$$W\psi(z) = \exp\left(-\frac{1}{\hbar}Gz^2\right),$$

where

$$G = \begin{bmatrix} X+YX^{-1}Y & YX^{-1} \\ X^{-1}Y & X^{-1} \end{bmatrix}.$$

It is immediate to verify that $G \in Sp(N)$ and that G is symmetric positive definite. One proves [11] that, conversely, every such G can be put in the above form, and which ends the proof of (ii) since the datum of $W\psi$ determines ψ up to a complex factor with modulus 1. □

3. Phase-space Weyl calculus

Let $\mathbf{H}_N$ be the $(2N+1)$-dimensional Heisenberg group; it is (see, e.g. [6, 24]) the set of all vectors

$$(z,t) = (x_1, \ldots, x_N; p_1, \ldots, p_N; t)$$

equipped with the multiplicative law

$$(z,t)(z',t') = \left(z + z', t + t' + \tfrac{1}{2} z \wedge z'\right).$$

3.1. The Schrödinger representation

The Schrödinger representation of $\mathbf{H}_N$ is, by definition, the mapping $\widehat{T}_{\mathrm{Sch}}$ which to every (z_0, t_0) in $\mathbf{H}_N$ associates the unitary operator $\widehat{T}_{\mathrm{Sch}}(z_0, t_0)$ on $L^2(\mathbb{R}_x^N)$ defined by

$$\widehat{T}_{\mathrm{Sch}}(z_0, t_0)\psi(x) = \exp\left[\frac{\mathrm{i}}{\hbar}\left(-t_0 + p_0 \cdot x - \frac{1}{2} p_0 \cdot x_0\right)\right]\psi(x - x_0). \qquad (27)$$

A classical theorem due to Stone and von Neumann (see, for instance, [6, 24] for a proof) states that the Schrödinger representation is irreducible (that is, no closed subspace of $L^2(\mathbb{R}_x^N)$ other than $\{0\}$ and $L^2(\mathbb{R}_x^N)$ is invariant by $\widehat{T}_{\mathrm{Sch}}$) and that every irreducible unitary representation of $\mathbf{H}_N$ is unitarily equivalent to $\widehat{T}_{\mathrm{Sch}}$: if $\widehat{T}$ is another irreducible representation of $\mathbf{H}_N$ on some Hilbert space $\mathcal{H}$, then there exists a unitary operator U from $L^2(\mathbb{R}_x^N)$ to $\mathcal{H}$ which is bijective, and such that the following intertwining formula holds:

$$[U \circ \widehat{T}_{\mathrm{Sch}}](z,t) = [\widehat{T} \circ U](z,t) \qquad \text{for all} \quad (z,t) \quad \text{in} \quad \mathbf{H}_N.$$

Conversely, if U is a unitary operator for which this formula holds, then $\widehat{T}$ must be irreducible. We emphasize—heavily!—that in the above statement it is nowhere assumed that $\mathcal{H}$ must be $L^2(\mathbb{R}_x^N)$; it can *a priori* be any Hilbert space, and in particular it can be (and will be!) any of the spaces $\mathcal{H}_\phi$ defined in theorem 2. We will come back to this point in a while, but let us first recall how one passes from the Heisenberg group to the Weyl pseudo-differential calculus. In Weyl calculus, one associates with a 'symbol' $A = A(x, p)$ an operator $\widehat{A}$ on $\mathcal{S}(\mathbb{R}_x^N)$ by the formula

$$\widehat{A}\psi(x) = \left(\frac{1}{2\pi\hbar}\right)^N \iint \mathrm{e}^{\frac{\mathrm{i}}{\hbar} p \cdot (x-y)} A\left(\frac{1}{2}(x+y), p\right)\psi(y)\, \mathrm{d}^N y\, \mathrm{d}^N p. \qquad (28)$$

This formula makes perfectly sense if, for instance, $A \in \mathcal{S}(\mathbb{R}_z^{2N})$ and one easily verifies that the 'Weyl correspondence' $A \overset{\mathrm{Weyl}}{\longleftrightarrow} \widehat{A}$ leads to the standard quantization rules

$$x \overset{\mathrm{Weyl}}{\longleftrightarrow} \widehat{X} = x, \qquad p \overset{\mathrm{Weyl}}{\longleftrightarrow} \widehat{P} = -\mathrm{i}\hbar\frac{\partial}{\partial x}. \qquad (29)$$

For more general symbols, the double integral must be interpreted in some particular way. For instance, if A belongs to the standard symbol class $S_{\rho,\delta}^m(\mathbb{R}_z^{2N})$ with $0 \leqslant \delta < \rho \leqslant 1$ that is, if for every compact $K \subset \mathbb{R}_x^N$ and all multi-indices $\alpha, \beta \in \mathbb{N}^N$ there exists $C_{K,\alpha,\beta}$ such that

$$\left|\partial_p^\alpha \partial_x^\beta A(x, p)\right| \leqslant C_{K,\alpha,\beta}(1 + |p|)^{m-\rho|\alpha|+\delta|\beta|},$$

then (28) should be viewed as an 'oscillatory integral'. There are however other possible ways to interpret this formula and make it rigorous; we refer to [5, 6, 31] for detailed discussions. (In particular, it is shown in [31] that $\widehat{A}$ is a Hilbert–Schmidt operator if and only if $A \in L^2(\mathbb{R}_x^N)$.)

3.2. Heisenberg–Weyl operators

There is another very useful way of writing Weyl operators and this will lead us to Weyl calculus in phase space. Setting $t_0 = 0$ in formula (27), one obtains the so-called Heisenberg–Weyl operators $\widehat{T}_{\mathrm{Sch}}(z_0)$

$$\widehat{T}_{\mathrm{Sch}}(z_0)\psi(x) = \exp\left[\frac{\mathrm{i}}{\hbar}\left(p_0 \cdot x - \frac{1}{2}p_0 \cdot x_0\right)\right]\psi(x - x_0). \tag{30}$$

It is easy to show, using Fourier analysis, that we can write operator (28) in the form

$$\widehat{A}\psi(x) = \left(\frac{1}{2\pi\hbar}\right)^N \int (\mathcal{F}_\sigma A)(z_0)\widehat{T}_{\mathrm{Sch}}(z_0)\psi(x)\,\mathrm{d}^{2N}z_0, \tag{31}$$

provided that $\mathcal{F}_\sigma A$, the 'symplectic Fourier transform' of A, exists. The latter is defined in analogy with the ordinary Fourier transform on $\mathbb{R}_z^{2N}$ by

$$\mathcal{F}_\sigma A(z) = \left(\frac{1}{2\pi\hbar}\right)^N \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}z\wedge z'}A(z')\,\mathrm{d}^{2N}z'. \tag{32}$$

The conditions of existence of $\mathcal{F}_\sigma A$ are actually the same as for the usual Fourier transform on $L^2(\mathbb{R}_z^{2N})$ to which it reduces replacing z by $-Jz$. Note that $\mathcal{F}_\sigma$ is an involution: $\mathcal{F}_\sigma^2 = I$.

Remark 5. It is often convenient to write formula (31) more economically as

$$\widehat{A} = \left(\frac{1}{2\pi\hbar}\right)^N \int (\mathcal{F}_\sigma A)(z)\widehat{T}_{\mathrm{Sch}}(z)\,\mathrm{d}^{2N}z, \tag{33}$$

where the right-hand side is interpreted as a 'Bochner integral', i.e. an integral with value in a Banach space.

3.3. Extension to phase space

We now observe that when a Weyl operator is written in the form (31) or (33), it literally begs to be extended to phase space! In fact, we can make the Heisenberg–Weyl operators act on functions Ψ in $L^2(\mathbb{R}_z^{2N})$ by replacing definition (30) by its obvious extension

$$\widehat{T}_{\mathrm{Sch}}(z_0)\Psi(z) = \exp\left[\frac{\mathrm{i}}{\hbar}\left(p_0 \cdot x - \frac{1}{2}p_0 \cdot x_0\right)\right]\Psi(z - z_0)$$

and thereafter define the action of $\widehat{A}$ on $\Psi \in \mathcal{S}(\mathbb{R}_z^{2N})$ by the formula

$$\widehat{A}\Psi(z) = \left(\frac{1}{2\pi\hbar}\right)^N \int (\mathcal{F}_\sigma A)(z_0)\widehat{T}_{\mathrm{Sch}}(z_0)\Psi(z)\,\mathrm{d}^{2N}z_0.$$

This (perfectly honest) choice would lead, using the method we will outline in section 5, to the Torres–Vega equation

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

(see [28, 29]) which we discussed in [12]. Since we prefer, for reasons of symplectic covariance, a more symmetric phase-space Schrödinger equation in which x and p are placed on equal footing, we will replace $\widehat{T}_{\mathrm{Sch}}(z_0)$ with the operator $\widehat{T}_{\mathrm{ph}}(z_0)$ given by

$$\widehat{T}_{\mathrm{ph}}(z_0)\Psi(z) = \exp\left(-\frac{\mathrm{i}}{2\hbar}z\wedge z_0\right)\Psi(z - z_0) \tag{34}$$

(the subscript 'ph' standing for phase space) and then define the phase-space Weyl operator associated with A by the formula

$$\widehat{A}_{\text{ph}}\Psi(z) = \left(\frac{1}{2\pi\hbar}\right)^{N} \int (\mathcal{F}_{\sigma}A)(z_0)\widehat{T}_{\text{ph}}(z_0)\Psi(z)\, \mathrm{d}^{2N}z_0. \tag{35}$$

This operator $\widehat{A}_{\text{ph}}$ acts continuously on $\mathcal{S}(\mathbb{R}_z^{2N})$ provided that A is a *bona fide* symbol and can hence be extended to $L^2(\mathbb{R}_z^{2N})$ by continuity. In accordance with the convention in remark 5, we will often write for short

$$\widehat{A}_{\text{ph}} = \left(\frac{1}{2\pi\hbar}\right)^{N} \int (\mathcal{F}_{\sigma}A)(z)\widehat{T}_{\text{ph}}(z)\, \mathrm{d}^{2N}z, \tag{36}$$

where the right-hand side is again viewed as a Bochner integral.

Observe that the operators $\widehat{T}_{\text{ph}}$ satisfy the same commutation relation as the usual Weyl–Heisenberg operators:

$$\widehat{T}_{\text{ph}}(z_1)\widehat{T}_{\text{ph}}(z_0) = \exp\left(-\frac{\mathrm{i}}{\hbar}z_0 \wedge z_1\right)\widehat{T}_{\text{ph}}(z_0)\widehat{T}_{\text{ph}}(z_1) \tag{37}$$

and we have

$$\widehat{T}_{\text{ph}}(z_0)\widehat{T}_{\text{ph}}(z_1) = \exp\left(\frac{\mathrm{i}}{2\hbar}z_0 \wedge z_1\right)\widehat{T}_{\text{ph}}(z_0 + z_1). \tag{38}$$

These properties suggest that we define the phase-space representation $\widehat{T}_{\text{ph}}$ of $\mathbf{H}_N$ in analogy with (27) by setting for $\Psi \in L^2(\mathbb{R}_z^{2N})$

$$\widehat{T}_{\text{ph}}(z_0, t_0)\Psi(z) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}t_0}\widehat{T}_{\text{ph}}(tz_0)\Psi(z). \tag{39}$$

Clearly, $\widehat{T}_{\text{ph}}(z_0, t_0)$ is a unitary operator in $L^2(\mathbb{R}_z^{2N})$; moreover, a straightforward calculation shows that

$$\widehat{T}_{\text{ph}}(z_0, t_0)\widehat{T}_{\text{ph}}(z_1, t_1) = \widehat{T}_{\text{ph}}\left(z_0 + z_1, t_0 + t_1 + \tfrac{1}{2}z_0 \wedge z_1\right). \tag{40}$$

Hence, $\widehat{T}_{\text{ph}}$ is indeed a representation of the Heisenberg group in $L^2(\mathbb{R}_z^{2N})$. We claim that the following diagram is commutative for every Wigner wavepacket transform U_ϕ:

$$
\begin{array}{ccc}
L^2(\mathbb{R}_x^N) & \xrightarrow{U_\phi} & L^2(\mathbb{R}_z^{2N}) \\
\widehat{T}_{\text{Sch}}\downarrow & & \downarrow \widehat{T}_{\text{ph}} \\
L^2(\mathbb{R}_x^N) & \xrightarrow{U_\phi} & L^2(\mathbb{R}_z^{2N}).
\end{array}
$$

More precisely

Theorem 6. *Let U_ϕ be an arbitrary Wigner wavepacket transform. (i) We have*

$$\widehat{T}_{\text{ph}}(z_0, t_0)U_\phi = U_\phi\widehat{T}_{\text{Sch}}(z_0, t_0); \tag{41}$$

hence, the representation $\widehat{T}_{\text{ph}}$ is unitarily equivalent to the Schrödinger representation and thus an irreducible representation of $\mathbf{H}_N$ on each of the Hilbert spaces $\mathcal{H}_\phi$. (ii) The following intertwining formula holds for every operator $\widehat{A}_{\text{ph}}$:

$$\widehat{A}_{\text{ph}}U_\phi = U_\phi\widehat{A}_{\text{Sch}}. \tag{42}$$

Proof. Proof of (i). It suffices to prove formula (41) for $t_0 = 0$, that is

$$\widehat{T}_{\text{ph}}(z_0)U_\phi = U_\phi\widehat{T}_{\text{Sch}}(z_0). \tag{43}$$

Let us write the operator U_ϕ in the form $U_\phi = \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}p\cdot x}W_\phi$, where the operator W_ϕ is thus defined by

$$W_\phi\psi(z) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\cdot x'}\phi(x - x')\psi(x')\, \mathrm{d}^N x'. \tag{44}$$

We have, by definition of $\widehat{T}_{\mathrm{ph}}(z_0)$,

$$\widehat{T}_{\mathrm{ph}}(z_0)U_\phi\psi(z) = \exp\left[-\frac{\mathrm{i}}{2\hbar}(z \wedge z_0) + (p - p_0) \cdot (x - x_0)\right] W_\phi\psi(z - z_0)$$

$$= \exp\left[\frac{\mathrm{i}}{2\hbar}(-2p \cdot x_0 + p_0 \cdot x_0 + p \cdot x)\right] W_\phi\psi(z - z_0)$$

and, by definition of $W_\phi\psi$,

$$W_\phi\psi(z - z_0) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(p - p_0)\cdot x'} \overline{\phi}(x - x' - x_0)\psi(x')\,\mathrm{d}^N x'$$

$$= \left(\frac{1}{2\pi\hbar}\right)^{N/2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p - p_0)\cdot x_0} \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(p - p_0)\cdot x''} \overline{\phi}(x - x'')\psi(x'')\,\mathrm{d}^N x'',$$

where we have set $x'' = x' + x_0$. The overall exponential in $\widehat{T}_{\mathrm{ph}}(z_0)U_\phi\psi(z)$ is thus

$$u_1 = \exp\left[\frac{\mathrm{i}}{2\hbar}(-p_0 \cdot x_0 + p \cdot x - 2p \cdot x'' + 2p_0 \cdot x'')\right].$$

Similarly,

$$U_\phi(\widehat{T}_{\mathrm{Sch}}(z_0)\psi)(z) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}p\cdot x}$$

$$\times \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\cdot x''} \overline{\phi}(x - x'')\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p_0\cdot x'' - \frac{1}{2}p_0\cdot x_0)}\psi(x'' - x_0)\,\mathrm{d}^N x'',$$

yielding the overall exponential

$$u_2 = \exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{1}{2}p \cdot x - p \cdot x'' + p_0 \cdot x'' - \frac{1}{2}p_0 \cdot x_0\right)\right] = u_1,$$

which proves (43). The irreducibility statement follows from Stone–von Neumann's theorem. Let us prove formula (42). In view of formula (43), we have

$$\widehat{A}_{\mathrm{ph}}U_\phi\psi = \left(\frac{1}{2\pi\hbar}\right)^N \int (\mathcal{F}_\sigma A)(z_0)\widehat{T}_{\mathrm{ph}}(z_0)(U_\phi\psi)(z)\,\mathrm{d}^{2N}z_0$$

$$= \left(\frac{1}{2\pi\hbar}\right)^N \int (\mathcal{F}_\sigma A)(z_0)U_\phi(\widehat{T}_{\mathrm{Sch}}(z_0)\psi)(z)\,\mathrm{d}^{2N}z_0$$

$$= \left(\frac{1}{2\pi\hbar}\right)^N U_\phi\left(\int (\mathcal{F}_\sigma A)(z_0)(\widehat{T}_{\mathrm{Sch}}(z_0)\psi)(z)\,\mathrm{d}^{2N}z_0\right)$$

$$= U_\phi(\widehat{A}_{\mathrm{Sch}}\psi)(z)$$

(the passage from the second equality to the third is legitimated by the fact that U_ϕ is both linear and continuous). $\qquad\square$

4. Metaplectic covariance

Since $Sp(N)$ is the symmetry group for the usual CCR (canonical commutation relations)

$$[\widehat{X}_j, \widehat{P}_k] = \mathrm{i}\hbar\delta_{jk}$$

(for $\widehat{X}_j = x_j$, $\widehat{P}_k = -\mathrm{i}\hbar\partial/\partial x_k$), the uniqueness of these relations implies that for each S in $Sp(N)$ there must be some associated unitary operator linking them to quantization. These operators are the metaplectic operators.

4.1. Metaplectic operators

Let us recall how the metaplectic operators are defined (for details and proofs see, for instance, [6, 8, 9, 16]). Assume that S is a free symplectic matrix, that is $S \in Sp(N)$ and

$$S = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \qquad \text{with} \quad \det B \neq 0.$$

To every such S, one associates the operators $\pm \widehat{S}_{W,m}$ defined by the formula

$$\widehat{S}_{W,m} \psi(x) = \left(\frac{1}{2\pi i\hbar}\right)^{N/2} \frac{i^m}{\sqrt{|\det B|}} \int e^{\frac{i}{\hbar} W(x,x')} \psi(x') \, d^N x'; \tag{45}$$

here W is Hamilton's characteristic function familiar from classical mechanics (see, for instance, [7, 9]):

$$W(x, x') = \tfrac{1}{2} D B^{-1} x^2 - B^{-1} x \cdot x' + \tfrac{1}{2} B^{-1} A x'^2 \tag{46}$$

and m is an integer ('Maslov index') corresponding to a choice of $\arg \det B$. The operators $\widehat{S}_{W,m}$ are a sort of generalized Fourier transform, and it is not difficult to check that they are unitary. In addition, the inverse of $\widehat{S}_{W,m}$ is given by

$$\widehat{S}_{W,m}^{-1} = \widehat{S}_{W^*,m^*}, \qquad W^*(x, x') = -W(x', x), \qquad m^* = N - m;$$

hence, $\widehat{S}_{W,m}$ generate a group: this group is the metaplectic group $Mp(N)$ (see [9] for a complete discussion of the properties of $Mp(N)$ and of the associated Maslov indices). If we choose for S the standard symplectic matrix

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

the quadratic form (46) reduces to $W(x, x') = -x \cdot x'$; choosing $\arg \det B = \arg \det I = 0$, the corresponding metaplectic operator is

$$\widehat{J} \psi(x) = \left(\frac{1}{2\pi i\hbar}\right)^{N/2} \int e^{-\frac{i}{\hbar} x \cdot x'} \psi(x') \, d^N x' = i^{-N/2} F \psi(x'),$$

where F thus is the usual unitary Fourier transform (15).

The Wigner–Moyal transform enjoys the following metaplectic covariance property: for every $\widehat{S} \in Mp(N)$ with projection $S \in Sp(N)$ we have

$$W(\widehat{S}\psi, \widehat{S}\phi) = W(\psi, \phi) \circ S^{-1}. \tag{47}$$

Since the Wigner wavepacket transform is defined in terms of $W(\psi, \phi)$ by formula (19), it follows that

$$\begin{aligned} U_\phi(\widehat{S}\psi) &= \left(\frac{\pi\hbar}{2}\right)^{N/2} W(\widehat{S}\psi, \overline{\phi}) \left(\tfrac{1}{2} z\right) \\ &= \left(\frac{\pi\hbar}{2}\right)^{N/2} W(\widehat{S}\psi, \widehat{S}(\widehat{S}^{-1}\overline{\phi})) \left(\tfrac{1}{2} z\right) \\ &= \left(\frac{\pi\hbar}{2}\right)^{N/2} W(\psi, \widehat{S}^{-1}\overline{\phi}) \left(\tfrac{1}{2} S^{-1}(z)\right) \end{aligned}$$

and hence

$$U_\phi(\widehat{S}\psi) = \left(U_{\phi_{\widehat{S}}}\psi\right) \circ S^{-1}, \qquad \phi_{\widehat{S}} = \overline{\widehat{S}^{-1}\overline{\phi}}. \tag{48}$$

4.2. Metaplectic group and Weyl calculus

In [13] we have shown, following an idea of Mehlig and Wilkinson [17], that the metaplectic group is generated by operators of the type

$$\widehat{S}\psi(x) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \frac{i^{\nu(S)}}{\sqrt{|\det(S-I)|}} \int e^{\frac{i}{2\hbar}M_S z_0^2} \widehat{T}_{\text{Sch}}(z_0)\psi(x)\, d^{2N}z_0, \qquad (49)$$

where $\det(S-I) \neq 0$, M_S is the symplectic Cayley transform of S:

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

and $\nu(S)$ is the Conley–Zehnder index (modulo 4) of a path joining the identity to I in $Sp(N)$ (see, for instance, [21] for a discussion of this index). For instance, if $\widehat{S} = \widehat{S}_{W,m}$, then

$$\widehat{S}_{W,m}\psi(x) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \frac{i^{m-\text{Inert}\, W_{xx}}}{\sqrt{|\det(S-I)|}} \int e^{\frac{i}{2\hbar}M_S z_0^2} \widehat{T}_{\text{Sch}}(z_0)\psi(x)\, d^{2N}z_0, \quad (50)$$

where Inert W_{xx} is the number of negative eigenvalues of the Hessian matrix of W. Formulae (49) and (50) are thus the Weyl representations of the metaplectic operators $\widehat{S}$ and $\widehat{S}_{W,m}$. They allow us to define phase-space metaplectic operators $\widehat{S}_{\text{ph}}$ in the following way: if $\det(S-I) \neq 0$, we set

$$\widehat{S}_{\text{ph}}\Psi(z) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \frac{i^{\nu(S)}}{\sqrt{|\det(S-I)|}} \int e^{\frac{i}{2\hbar}M_S z_0^2} \widehat{T}_{\text{ph}}(z_0)\Psi(z)\, d^{2N}z_0; \qquad (51)$$

the operators $\widehat{S}_{\text{ph}}$ are in one-to-one correspondence with the metaplectic operators $\widehat{S}$ and thus generate a group which we denote by $Mp_{\text{ph}}(N)$ (the 'phase-space metaplectic group'). In following lemma, we give alternative descriptions of the operators (49) in terms of the operators $\widehat{T}_{\text{ph}}$.

Lemma 7. *Let $\widehat{S}_{\text{ph}} \in Mp_{\text{ph}}(N)$ have projection $S \in Mp(N)$ such that $\det(S-I) \neq 0$. We have*

$$\widehat{S}_{\text{ph}} = \left(\frac{1}{2\pi}\right)^N i^{\nu(S)}\sqrt{|\det(S-I)|} \int e^{-\frac{i}{2}Sz\wedge z}\widehat{T}_{\text{ph}}((S-I)z)\, d^{2N}z \qquad (52)$$

and

$$\widehat{S}_{\text{ph}} = \left(\frac{1}{2\pi}\right)^N i^{\nu(S)}\sqrt{|\det(S-I)|} \int \widehat{T}_{\text{ph}}(Sz)\widehat{T}_{\text{ph}}(-z)\, d^{2N}z. \qquad (53)$$

Proof. It is *mutatis mutandis* the proof of lemma 1 in [13]: we have

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

hence, in view of the antisymmetry of J,

$$M_S z \cdot z = J(S-I)^{-1}z \cdot z = (S-I)^{-1}z \wedge z.$$

Performing the change of variables $z \longmapsto (S-I)z$, we can rewrite the integral on the right-hand side of (50) as

$$\int e^{\frac{i}{2}\langle M_S z, z\rangle}\widehat{T}(z)\, d^{2N}z = \sqrt{|\det(S-I)|} \int e^{\frac{i}{2}z\wedge(S-I)z}\widehat{T}_{\text{ph}}((S-I)z)\, d^{2N}z$$

$$= \sqrt{|\det(S-I)|} \int e^{-\frac{i}{2}Sz\wedge z}\widehat{T}_{\text{ph}}((S-I)z)\, d^{2N}z,$$

hence (52). Taking into account formula (38) for the product of two metaplectic operators $\widehat{T}_{\mathrm{ph}}(z_0)$ and $\widehat{T}_{\mathrm{ph}}(z_1)$, we get

$$\widehat{T}((S-I)z) = \mathrm{e}^{\frac{\mathrm{i}}{2}\sigma Sz \wedge z}\, \widehat{T}_{\mathrm{ph}}(Sz)\widehat{T}_{\mathrm{ph}}(-z)$$

and formula (53) follows. $\qquad\square$

This result will allows us to show in a simple way that the well-known 'metaplectic covariance' relation

$$\widehat{A \circ S}_{\mathrm{Sch}} = \widehat{S}^{-1}\widehat{A}_{\mathrm{Sch}}\widehat{S} \tag{54}$$

valid for any $\widehat{S} \in Mp(N)$ with projection $S \in Sp(N)$ extends to the phase-space Weyl operators $\widehat{A}_{\mathrm{ph}}$ provided one replaces $Mp(N)$ with $Mp_{\mathrm{ph}}(N)$.

Theorem 8. *Let S be a symplectic matrix and $\widehat{S}_{\mathrm{ph}}$ any of the two operators in $Mp_{\mathrm{ph}}(N)$ associated with S. The following phase-space metaplectic covariance formulae hold:*

$$\widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z_0)\widehat{S}_{\mathrm{ph}}^{-1} = \widehat{T}_{\mathrm{ph}}(Sz), \qquad \widehat{A \circ S}_{\mathrm{ph}} = \widehat{S}_{\mathrm{ph}}^{-1}\widehat{A}_{\mathrm{ph}}\widehat{S}_{\mathrm{ph}}. \tag{55}$$

Proof. To prove the first formula in (55), it is sufficient to assume that $\det(S - I) \neq 0$ and that $\widehat{S}_{\mathrm{ph}}$ is thus given by formula (51), since such operators generate $Mp_{\mathrm{ph}}(N)$. Let us thus prove that

$$\widehat{T}_{\mathrm{ph}}(Sz_0)\widehat{S}_{\mathrm{ph}} = \widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z_0) \qquad \text{if} \quad \det(S - I) \neq 0. \tag{56}$$

Using formula (53) in lemma 7 and setting

$$C_S = \left(\frac{1}{2\pi}\right)^N \mathrm{i}^{\nu(S)}\sqrt{|\det(S-I)|},$$

we have

$$\widehat{T}_{\mathrm{ph}}(Sz_0)\widehat{S}_{\mathrm{ph}} = C_S \int \widehat{T}_{\mathrm{ph}}(Sz_0)\widehat{T}_{\mathrm{ph}}(Sz)\widehat{T}_{\mathrm{ph}}(-z)\,\mathrm{d}^{2N}z$$

and

$$\widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z_0) = C_S \int \widehat{T}_{\mathrm{ph}}(Sz)\widehat{T}_{\mathrm{ph}}(-z)\widehat{T}_{\mathrm{ph}}(z_0)\,\mathrm{d}^{2N}z.$$

Setting

$$A(z_0) = \int \widehat{T}_{\mathrm{ph}}(Sz_0)\widehat{T}_{\mathrm{ph}}(Sz)\widehat{T}_{\mathrm{ph}}(-z)\,\mathrm{d}^{2N}z$$

and

$$B(z_0) = \int \widehat{T}_{\mathrm{ph}}(Sz)\widehat{T}_{\mathrm{ph}}(-z)\widehat{T}_{\mathrm{ph}}(z_0)\,\mathrm{d}^{2N}z,$$

we have, by repeated use of (38),

$$A(z_0) = \int \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}\Phi_1(z,z_0)}\widehat{T}_{\mathrm{ph}}(Sz_0 + (S-I)z)\,\mathrm{d}^{2N}z,$$

$$B(z_0) = \int \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}\Phi_2(z,z_0)}\widehat{T}_{\mathrm{ph}}(z_0 + (S-I)z)\,\mathrm{d}^{2N}z,$$

where the phases Φ_1 and Φ_2 are given by

$$\Phi_1(z, z_0) = z_0 \wedge z - S(z + z_0) \wedge z,$$
$$\Phi_2(z, z_0) = -Sz \wedge z + (S-I)z \wedge z_0.$$

Performing the change of variables $z' = z + z_0$ in the integral defining $A(z_0)$, we get

$$A(z_0) = \int e^{\frac{i}{2\hbar}\Phi_1(z'-z_0,z_0)}\widehat{T}_{ph}(z_0 + (S-I)z')\,d^{2N}z'$$

and

$$\begin{aligned}\Phi_1(z'-z_0,z_0) &= z_0 \wedge (z'-z_0) - Sz' \wedge (z'-z_0)\\ &= (S-I)z' \wedge z_0 - Sz' \wedge z'\\ &= \Phi_2(z',z_0),\end{aligned}$$

hence (56). The second formula in (55) easily follows from the first: noting that the symplectic Fourier transform (32) satisfies

$$\begin{aligned}\mathcal{F}_\sigma[A \circ S](z) &= \left(\frac{1}{2\pi\hbar}\right)^N \int e^{-\frac{i}{\hbar}z_0 \wedge z'} A(Sz')\,d^{2N}z'\\ &= \left(\frac{1}{2\pi\hbar}\right)^N \int e^{-\frac{i}{\hbar}Sz_0 \wedge z'} A(z')\,d^{2N}z'\\ &= \mathcal{F}_\sigma A(Sz),\end{aligned}$$

we have

$$\begin{aligned}\widehat{A \circ S}_{ph} &= \left(\frac{1}{2\pi\hbar}\right)^N \int \mathcal{F}_\sigma A(Sz)\widehat{T}_{ph}(z)\,d^{2N}z\\ &= \left(\frac{1}{2\pi\hbar}\right)^N \int \mathcal{F}_\sigma A(z)\widehat{T}_{ph}(S^{-1}z)\,d^{2N}z\\ &= \left(\frac{1}{2\pi\hbar}\right)^N \int \mathcal{F}_\sigma A(z)\widehat{S}_{ph}^{-1}\widehat{T}_{ph}(z)\widehat{S}_{ph}\,d^{2N}z,\end{aligned}$$

which concludes the proof. $\qquad\square$

It can be shown, adapting the proof of a classical result of Shale [25] (see [31], chapter 30, for a proof), that the metaplectic covariance formula

$$\widehat{A \circ S}_{ph} = \widehat{S}_{ph}^{-1}\widehat{A}_{ph}\widehat{S}_{ph}$$

actually characterizes the phase-space Weyl operators $\widehat{A}_{ph}$. That is, any operator satisfying this relation for all operators $\widehat{S}_{ph} \in Mp_{ph}(N)$ is necessarily of the type

$$\widehat{A}_{ph} = \left(\frac{1}{2\pi\hbar}\right)^N \int (\mathcal{F}_\sigma A)(z)\widehat{T}_{ph}(z)\,d^{2N}z.$$

For example, if H is the Hamiltonian function of the one-dimensional harmonic oscillator put in normal form

$$H = \frac{\omega}{2}(p^2 + x^2), \tag{57}$$

we get

$$\widehat{H}_{ph} = -\frac{\hbar^2\omega}{2}\nabla_z^2 - i\frac{\hbar\omega}{2}z \wedge \nabla_z + \frac{\omega}{8}|z|^2, \tag{58}$$

where ∇_z is the gradient operator in (x, p).

5. Schrödinger equation in phase space

We now have all the machinery needed to justify and study the Schrödinger equation in phase space.

5.1. The relationship between ψ and Ψ

The following consequence of theorem 6 links standard 'configuration-space' quantum mechanics to phase-space quantum mechanics via the Wigner wavepacket transform and the extended Heisenberg group studied in the previous sections. For clarity, we denote by $\widehat{A}_{\mathrm{Sch}}$ the usual Weyl operator associated by (31) with an observable A.

Corollary 9. *Let $U_\phi, \phi \in \mathcal{S}(\mathbb{R}_x^N)$, be an arbitrary Wigner wavepacket transform. (i) If $\psi = \psi(x, t)$ is a solution of the usual Schrödinger equation*

$$i\hbar \frac{\partial \psi}{\partial t} = \widehat{H}_{\mathrm{Sch}} \psi,$$

then $\Psi = (U_\phi \psi)(z, t)$ is a solution of the phase-space Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \widehat{H}_{\mathrm{ph}} \Psi. \tag{59}$$

(ii) Assume that Ψ is a solution of this equation and that $\Psi_0 = \Psi(\cdot, 0)$ belongs to the range $\mathcal{H}_\phi$ of U_ϕ. Then, $\Psi(\cdot, t) \in \mathcal{H}_\phi$ for every t for which Ψ is defined.

Proof. Since time derivatives obviously commute with U_ϕ we have, using (42),

$$i\hbar \frac{\partial \Psi}{\partial t} = U_\phi(\widehat{H}_{\mathrm{Sch}} \psi) = \widehat{H}_{\mathrm{ph}}(U_\phi \psi) = \widehat{H}_{\mathrm{ph}} \Psi,$$

hence (i). Statement (ii) follows. $\square$

The above result leads to the following interesting questions: since the solutions of the phase-space Schrödinger equation (59) exist independently of the choice of any isometry U_ϕ, what is the difference between the physical interpretations of the corresponding configuration-space wavefunctions $\psi = U_\phi^* \Psi$ and $\psi' = U_{\phi'}^* \Psi$? The answer is that there is no difference at all provided that ϕ and ϕ' are not orthogonal.

Theorem 10. *Let Ψ be a solution of the phase-space Schrödinger equation (59) with initial condition Ψ_0 and define functions ψ_1 and ψ_2 in $L(\mathbb{R}_x^N)$ by*

$$\Psi = U_{\phi_1} \psi_1 = U_{\phi_2} \psi_2.$$

We assume that $\Psi_0 \in \mathcal{H}_{\phi_1} \cap \mathcal{H}_{\phi_2}$.
(i) We have $\Psi(\cdot, t) \in \mathcal{H}_{\phi_1} \cap \mathcal{H}_{\phi_2}$ for all t.
(ii) If $(\phi_1, \phi_2) = 0$, then ψ_1 and ψ_2 are orthogonal quantum states: $(\psi_1, \psi_2) = 0$.

Proof. Property (i) follows from corollary 9(ii). Let us prove (ii). In view of formula (23), we have

$$((U_{\phi_1} \psi_1, U_{\phi_2} \psi_2)) = (\psi_1, \psi_2)\overline{(\overline{\phi_1}, \overline{\phi_2})},$$

that is $\|\Psi\|^2 = \lambda(\psi_1, \psi_2)$ with $\lambda = (\phi_1, \phi_2)$. The assertion follows. $\square$

5.2. Spectral properties

The operators $\widehat{A}_{\mathrm{ph}}$ defined by (35) enjoy the same property which makes the main appeal of ordinary Weyl operators, namely that they are self-adjoint if and only if their symbols are real.

Theorem 11. *Let $\widehat{A}_{\mathrm{ph}}$ and $\widehat{A}_{\mathrm{Sch}}$ be the operators associated with a symbol A. We assume that the symplectic Fourier transform $\mathcal{F}_\sigma A$ is defined. (i) The operator $\widehat{A}_{\mathrm{ph}}$ is self-adjoint in $L^2(\mathbb{R}_z^{2N})$ if and only if $A = \overline{A}$. (ii) Every eigenvalue of $\widehat{A}_{\mathrm{Sch}}$ is also an eigenvalue of $\widehat{A}_{\mathrm{ph}}$.*

Proof. (i) By definitions of $\widehat{A}_{\mathrm{ph}}$ and $\widehat{T}_{\mathrm{ph}}$, we have

$$\widehat{A}_{\mathrm{ph}}\Psi(z) = \left(\frac{1}{2\pi\hbar}\right)^N \int \mathcal{F}_\sigma A(z_0)\, \mathrm{e}^{-\frac{\mathrm{i}}{2\hbar}z\wedge z_0}\Psi(z-z_0)\,\mathrm{d}^{2N}z_0$$

$$= \left(\frac{1}{2\pi\hbar}\right)^N \int \mathcal{F}_\sigma A(z-z')\, \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}z\wedge z'}\Psi(z')\,\mathrm{d}^{2N}z';$$

hence, the kernel of the operator $\widehat{A}_{\mathrm{ph}}$ is

$$K(z,z') = \left(\frac{1}{2\pi\hbar}\right)^N \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}z\wedge z'}\mathcal{F}_\sigma A(z-z').$$

In view of the standard theory of integral operators, $\widehat{A}_{\mathrm{ph}}$ is self-adjoint if and only if $K(z,z') = \overline{K(z',z)}$; in view of the antisymmetry of the symplectic product, we have

$$\overline{K(z',z)} = \left(\frac{1}{2\pi\hbar}\right)^N \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}z\wedge z'}\overline{\mathcal{F}_\sigma A(z'-z)}.$$

Hence, our claim since by definition (32) of the symplectic Fourier transform

$$\overline{\mathcal{F}_\sigma A(z'-z)} = \left(\tfrac{1}{2\pi\hbar}\right)^N \int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(z-z')\wedge z''}\overline{A(z'')}\,\mathrm{d}^{2N}z'' = \mathcal{F}_\sigma \overline{A}(z-z').$$

(ii) Assume that $\widehat{A}_{\mathrm{Sch}}\psi = \lambda\psi$; choosing $\phi \in \mathcal{S}(\mathbb{R}_x^N)$ we have, using the intertwining formula (42),

$$U_\phi(\widehat{A}_{\mathrm{Sch}}\psi) = \widehat{A}_{\mathrm{ph}}(U_\phi\psi) = \lambda U_\phi\psi;$$

hence, λ is an eigenvalue of $\widehat{A}_{\mathrm{ph}}$. $\qquad\square$

Note that there is no reason for an arbitrary eigenvalue of $\widehat{A}_{\mathrm{ph}}$ to be an eigenvalue of $\widehat{A}_{\mathrm{Sch}}$; this is only the case if the corresponding eigenvector belongs to the range of a Wigner wavepacket transform.

5.3. The case of quadratic Hamiltonians

There is an interesting application of the theory of the metaplectic group outlined in section 4 to the Schrödinger's equation in phase space. Assume that H is a quadratic Hamiltonian (for instance, the harmonic oscillator Hamiltonian); the flow determined by the associated Hamilton equations is linear and consists of symplectic matrices S_t. Letting time vary, thus obtain a curve $t \longmapsto S_t$ in the symplectic group $Sp(N)$ passing through the identity I at time $t = 0$; following general principles to that curve we can associate (in a unique way) a curve $t \longmapsto \widehat{S}_t$ of metaplectic operators. Let now $\psi_0 = \psi_0(x)$ be some square-integrable function and set $\psi(x,t) = \widehat{S}_t\psi_0(x)$. Then, ψ is just the solution of the standard Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi, \qquad \psi(t=0) = \psi_0 \tag{60}$$

associated with the quadratic Hamiltonian function H. (Equivalently, $\widehat{S}_t$ is just the propagator for (60).) This observation allows us to solve explicitly the phase-space Schrödinger equation for any such H, as explained below. Since the wavepacket transform U automatically takes the solution ψ of (60) to a solution of the phase-space Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}_{\mathrm{ph}}\Psi,$$

we have

$$\Psi(z,t) = (\widehat{S}_t)_{\mathrm{ph}}\Psi(z,0).$$

Assume now that the symplectic matrix S_t is free and $\det(S_t - I) \neq 0$. Then, by (51),

$$\Psi(z, t) = \left(\frac{1}{2\pi\hbar}\right)^{N/2} \frac{\mathrm{i}^{m(t) - \mathrm{Inert}\, W_{xx}(t)}}{\sqrt{|\det(S_t - I)|}} \int \mathrm{e}^{\frac{\mathrm{i}}{2\hbar} z_0^T M_S(t) z_0} \widehat{T}_{\mathrm{ph}}(z_0) \Psi(z, 0)\, \mathrm{d}^{2N} z_0, \tag{61}$$

where $m(t)$, $W_{xx}(t)$ and $M_S(t)$ correspond to S_t. If t is such that S_t is not free, or $\det(S_t - I) = 0$, then it suffices to write the propagator $\widehat{S}_t$ as the product of two operators (50); note however that such values of t are exceptional and that the solution (61) can be extended by taking the limit near such t provided that takes some care in calculating the Maslov indices.

Let us illustrate this when H is the harmonic oscillator Hamiltonian function (57). The one-parameter group (S_t) is in this case given by

$$S_t = \begin{bmatrix} \cos \omega t & \sin \omega t \\ -\sin \omega t & \cos \omega t \end{bmatrix}$$

and the Hamilton principal function by

$$W(x, x'; t) = \frac{1}{2 \sin \omega t} ((x^2 + x'^2) \cos \omega t - 2xx').$$

A straightforward calculation yields

$$M_S(t) = \begin{bmatrix} \frac{\sin \omega t}{-2 \cos \omega t + 2} & 0 \\ 0 & \frac{\sin \omega t}{-2 \cos \omega t + 2} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \cot\left(\frac{\omega t}{2}\right) & 0 \\ 0 & \cot\left(\frac{\omega t}{2}\right) \end{bmatrix}$$

and

$$\det(S_t - I) = 2(1 - \cos \omega t) = 4 \sin^2\left(\frac{\omega t}{2}\right);$$

moreover,

$$W_{xx}(t) = -\tan\left(\frac{\omega t}{2}\right).$$

Insertion in formula (61) yields the explicit solution

$$\Psi(z, t) = \frac{\mathrm{i}^{\nu(t)}}{2\left|2\pi\hbar \sin\left(\frac{\omega t}{2}\right)\right|^{1/2}} \int \exp\left[\frac{\mathrm{i}}{4\hbar}\left(x_0^2 + p_0^2\right) \cot\left(\frac{\omega t}{2}\right)\right] \widehat{T}_{\mathrm{ph}}(z_0) \Psi(z, 0)\, \mathrm{d}^2 z_0,$$

with

$$\nu(t) = \begin{cases} 0, & \text{if} \quad 0 < t < \dfrac{\pi}{\omega}, \\ -2, & \text{if} \quad -\dfrac{\pi}{\omega} < t < 0. \end{cases}$$

6. Interpretation of the phase-space wavefunction Ψ

Let us shortly discuss the probabilistic interpretation of the solutions Ψ of the phase-space Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial \Psi}{\partial t} = \widehat{H}_{\mathrm{ph}} \Psi;$$

we will in particular elucidate the role played by ϕ.

6.1. Marginal probabilities

Let ψ be in $L^2(\mathbb{R}_x^N)$; if ψ is normalized, $\|\psi\| = 1$, then so is $\Psi = U_\phi \psi$ in view of the Parseval formula (21): $\|\Psi\| = 1$. It follows that $|\Psi|^2$ is a probability density in phase space. It turns out that by an appropriate choice of ϕ the marginal probabilities can be chosen arbitrarily close to $|\psi|^2$ and $|F\psi|^2$.

Theorem 12. *Let $\psi \in L^2(\mathbb{R}_x^N)$ and set $\Psi = U_\phi \psi$. (i) We have*

$$\int |\Psi(x, p)|^2 \, \mathrm{d}^N p = (|\phi|^2 * |\psi|^2)(x), \tag{62}$$

$$\int |\Psi(x, p)|^2 \, \mathrm{d}^N x = (|F\phi|^2 * |F\psi|^2)(p). \tag{63}$$

(ii) Let $\langle A \rangle_\psi = (A_{\mathrm{Sch}} \psi, \psi)$ be the mathematical expectation of the symbol A in the normalized quantum state ψ. We have

$$\langle A \rangle_\psi = ((A_{\mathrm{ph}} \Psi, \Psi)), \qquad \Psi = U_\phi \psi. \tag{64}$$

Proof. We have, by definition of Ψ,

$$|\Psi(z)|^2 = \left(\frac{1}{2\pi\hbar}\right)^N \iint e^{-\frac{i}{\hbar} p \cdot (x' - x'')} \overline{\phi}(x - x') \phi(x - x'') \psi(x') \overline{\psi}(x'') \, \mathrm{d}^N x' \, \mathrm{d}^N x''.$$

Since we have, by the Fourier inversion formula,

$$\int e^{-\frac{i}{\hbar} p \cdot (x' - x'')} \, \mathrm{d}^N p = (2\pi\hbar)^N \delta(x' - x''),$$

it follows that

$$\int |\Psi(z)|^2 \, \mathrm{d}^N p = \iiint \delta(x' - x'') |\phi(x - x')|^2 |\psi(x')|^2 \, \mathrm{d}^N x' \, \mathrm{d}^N x''$$

$$= \int \left[\int \delta(x' - x'') \, \mathrm{d}^N x'' \right] |\phi(x - x')|^2 |\psi(x')|^2 \, \mathrm{d}^N x'$$

$$= \int |\phi(x - x')|^2 |\psi(x')|^2 \, \mathrm{d}^N x',$$

hence formula (62). To prove (63), we note that in view of the metaplectic covariance formula (48) for the wavepacket transform we have

$$U_{\widehat{J}\phi}(\widehat{J}\psi)(x, p) = U_\phi \psi(-p, x),$$

where $\widehat{J} = i^{-N/2} F$ is the metaplectic Fourier transform. It follows that

$$U_{F\phi}(F\psi)(x, p) = i^{-N} U_\phi \psi(-p, x)$$

and hence changing $(-p, x)$ into (x, p):

$$U_\phi \psi(x, p) = i^N U_{F\phi}(F\psi)(p, -x).$$

Hence, using (62),

$$\int |\Psi(x, p)|^2 \, \mathrm{d}^N x = \int |U_{F\phi}(F\psi)(p, -x)|^2 \, \mathrm{d}^N x$$

$$= \int |U_{F\phi}(F\psi)(p, x)|^2 \, \mathrm{d}^N x$$

$$= (|F\phi|^2 * |F\psi|^2)(p),$$

which concludes the proof of (63). To prove (64), it suffices to note that in view of the intertwining formula (42) and the fact that $U_\phi^* = U_\phi^{-1}$, we have

$$
\begin{aligned}
((A_{\mathrm{ph}}\Psi, \Psi)) &= ((\widehat{A}_{\mathrm{ph}} U_\phi \psi, U_\phi \psi)) \\
&= (U_\phi^* \widehat{A}_{\mathrm{ph}} U_\phi \psi, \psi) \\
&= (\widehat{A}_{\mathrm{Sch}}\psi, \psi).
\end{aligned}
$$
$\square$

The above result shows that the marginal probabilities of $|\Psi|^2$ are just the traditional position and momentum probability densities $|\psi|^2$ and $|F\psi|^2$ 'smoothed out' by convoluting them with $|\phi|^2$ and $|F\phi|^2$, respectively.

6.2. The limit $\hbar \to 0$

Assume now that we choose for ϕ the Gaussian (20):

$$
\phi(x) = \phi_\hbar(x) = \left(\frac{1}{\pi\hbar}\right)^{N/4} \exp\left(-\frac{1}{2\hbar}|x|^2\right).
$$

The Fourier transform of ϕ is identical to ϕ

$$
F\phi_\hbar(p) = \left(\frac{1}{\pi\hbar}\right)^{N/4} \exp\left(-\frac{1}{2\hbar}|p|^2\right) = \phi_\hbar(p);
$$

hence, setting $\Psi_\hbar = U_{\phi_\hbar}\psi$ and observing that $|\phi_\hbar|^2 \to \delta$ when $\hbar \to 0$,

$$
\int |\Psi_\hbar(x, p)|^2 \, d^N p = (|\psi|^2 * |\phi_\hbar|^2)(x) \xrightarrow{\hbar \to 0} |\psi(x)|^2,
$$

$$
\int |\Psi_\hbar(x, p)|^2 \, d^N x = (|F\psi|^2 * |\phi_\hbar|^2)(p) \xrightarrow{\hbar \to 0} |F\psi(p)|^2.
$$

Thus, in the limit $\hbar \to 0$, the square of the modulus of the phase-space wavefunction becomes a true joint probability density for the probability densities $|\psi|^2$ and $|F\psi|^2$.

7. Discussion and remarks

We have exposed some theoretical background for a mathematical justification of the phase-space Schrödinger equation

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

The aesthetic appeal of this equation is obvious—at least if one likes the Hamiltonian formulation of mechanics. But is this equation *useful*? While the notion of 'usefulness' in science more than often has a relative and subjective character, one of the main practical appeals of the phase-space Schrödinger equation is that it governs the quantum evolution of both pure and mixed states, while the solutions of the usual Schrödinger equation are, by definition, only pure states. Another of the advantages of the phase-space approach is, as pointed out in [19], the availability of factorization methods for the Hamiltonian, for instance, SUSY. From a practical point of view, it could be held against Schrödinger equations in $2N$-dimensional phase space that they are uninteresting because they involve solving a partial differential equation in $2N + 1$ variables instead of $N + 1$ as for the ordinary Schrödinger equation. But this is perhaps a somewhat stingy reservation especially in times where modern computing techniques allow an efficient processing of large strings of independent variables.

It would perhaps be interesting to make explicit the relationship between the theory of the Schrödinger equation in phase space we have sketched and other approaches to quantum mechanics in phase space, for instance, the 'deformation quantization' of Bayen *et al* [3], and whose master equation is the 'quantum Liouville equation'.

We would like to end this section—and paper!—by discussing a little bit the possible physical interpretation of the phase-space Schrödinger equation. Recall that we showed in theorem 4 that a phase-space Gaussian

$$\Psi_G(z) = \exp\left(-\frac{1}{2\hbar}Gz^2\right), \qquad G = G^T > 0$$

is in the range of any of the Wigner wavepacket transforms U_ϕ if and only if $G \in Sp(N)$ and that in this case

$$W\psi(z) = |\Psi_G(z)|^2 = \exp\left(-\frac{1}{\hbar}Gz^2\right)$$

for some (pure) Gaussian state ψ. Let us more generally consider Gaussians

$$\Psi_M(z) = \exp\left(-\frac{1}{\hbar}Mz^2\right),$$

where M is a positive-definite symmetric real matrix. One proves that Ψ_M is the Wigner transform $W(\hat{\rho})$ of a (usually mixed) quantum state if and only if $M^{-1} + iJ$ is positive definite and Hermitian:

$$(M^{-1} + iJ)^* = M^{-1} + iJ \geqslant 0. \tag{65}$$

The probabilistic meaning of this condition is the following: defining as usual the covariance matrix of the state $\hat{\rho}$ by

$$\Sigma = \frac{\hbar}{2}M^{-1},$$

condition (65) can be rewritten as

$$\left(\Sigma + i\frac{\hbar}{2}J\right)^* = \Sigma + i\frac{\hbar}{2}J \geqslant 0, \tag{66}$$

which is equivalent to the uncertainty principle of quantum mechanics (see [26, 27]; we have also discussed this in [10]). For instance, when $N = 1$, the matrix

$$\Sigma = \begin{bmatrix} \Delta x^2 & \Delta(x, p) \\ \Delta(x, p) & \Delta p^2 \end{bmatrix}$$

satisfies (66) if and only if

$$\Delta x^2 \Delta p^2 \geqslant \tfrac{1}{4}\hbar^2 + \Delta(x, p),$$

which is the form of the Heisenberg inequality that should be used as soon as correlations are present, and not the usual textbook inequality $\Delta x \Delta p \geqslant \tfrac{1}{2}\hbar$.

It turns out that conditions (65) and (66) have a simple topological interpretation: we have shown in our previous work [10, 11] that they are equivalent to the third condition.

The phase-space ball $B(\sqrt{\hbar}) : |z| \leqslant \hbar$ can be embedded into the 'Wigner ellipsoid' $W_M : Mz^2 \leqslant \hbar$ using symplectic transformations (linear or not). Equivalently, the symplectic capacity (or 'Gromov width') of W_M is at least $\pi\hbar = \tfrac{1}{2}h$, one half of the quantum of action: $c(W_M) \geqslant \tfrac{1}{2}h$.

We have discussed in some detail in [10, 11] how this result allows a 'coarse graining' of phase space by symplectic quantum cells, which we dubbed 'quantum blobs'. It appears

that it is precisely this coarse graining that prevents Gaussians Ψ_M with Wigner ellipsoids smaller than a 'quantum blob' to represent a quantum state. Is this to say that if the Wigner ellipsoid of Ψ_M has exactly symplectic capacity $\frac{1}{2}h$ then Ψ_M is a pure state? No, because such states are characterized by the fact that the associated Wigner ellipsoid is exactly the image of the ball $B(\sqrt{\hbar})$ by a symplectic transformation since they are described by the inequality $Gz^2 = (Sz)^2 \leqslant \hbar$ in view of theorem 4, and there are infinitely many ellipsoids with symplectic capacity $\frac{1}{2}h$ which are not the image of $B(\sqrt{\hbar})$ by a symplectic transformation. However, we have shown in [10, 11] that if the ellipsoid $W_M : Mz^2 \leqslant \hbar$ has symplectic capacity $\frac{1}{2}h$ then one can associate with W_M a unique pure Gaussian state. The argument goes as follows: if $c(W_M) = \frac{1}{2}h$, then S and S' in $Sp(N)$ are such that

$$S(B(\sqrt{\hbar})) \subset W_M, \qquad S'(B(\sqrt{\hbar})) \subset W_M;$$

then, there exists $R \in U(N) = Sp(N) \cap O(2N)$ such that $S = RS'$ (the proof of this property is not entirely trivial) and hence $S^T S = (S')^T S'$. It follows that the ellipsoid $W_G : Gz^2 \leqslant \hbar, G = S^T S$, is uniquely determined by W_M and that the pure Gaussian state corresponding to

$$\Psi_G(z) = \exp\left(-\frac{1}{2\hbar}Gz^2\right)$$

is canonically associated with the mixed state Ψ_M, which does not in general belong to the range of any Wigner wavepacket transform U_ϕ. It would be interesting to generalize this result to arbitrary functions $\Psi \in L^2(\mathbb{R}_z^{2N})$ by defining, in analogy with the Gaussian case, a 'Wigner set' W_Ψ associated with Ψ. One could then perhaps prove that Ψ represents an arbitrary (mixed) quantum state provided that W_Ψ has a symplectic capacity at least $\frac{1}{2}h$. But enough is enough! We hope to come back to these possibilities in the future.

Acknowledgments

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