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Schrödinger Equation in Phase Space, Irreducible Representations of the Heisenberg Group, and Deformation Quantization

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Abstract. Schrödinger equations in phase space are much discussed and questioned in quantum physics and chemistry. We show that the existence of such an equation is justified by constructing a an extended Weyl representation compatible with Stone and von Neumann's theorem. It turns out that the theory thus obtained is a variant of deformation quantization.

1. Introduction

Just a few decades ago many physicists were still reluctant to accept the idea of a "quantum mechanics in phase space". The usual mantra was that Heisenberg's uncertainty principle forbids us to view points in phase space as having any physical meaning in quantum mechanics (thus overlooking that *mathematics* is insensitive to such ontological considerations). Things have changed, luckily, and phase-space techniques are now widely used, especially in quantum optics and chemistry although the interpretations and methods differ, depending on tribal sensibilities; see [6, 17] for a discussion from a modern point of view. Roughly speaking, there are three ways of doing quantum mechanics in phase space:

- One can use the Weyl–Wigner–Moyal–Groenewold formalism [3, 7, 15], whose hallmark is the Wigner quasi-distribution; from a mathematical point of view this is just the usual Weyl pseudo-differential calculus whose interest comes from its symplectic covariance which links it to Hamiltonian mechanics; this theory is being widely used by physicists working in quantum optics because of its attractive symplectic covariance properties;

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- One can use the beautiful and deep theory of deformation quantization initiated by Bayen *et al.* [1], and based on Moyal's trailblazing work [9]. It is an autonomous full-blown rigorous theory, with deep ramifications in various other parts of mathematics; its hallmark is the star product (of which the Moyal, or Moyal–Groenewold, product is an ancestor). Deformation quantization is essentially the unique associative $\hbar$-deformation of the Poisson brackets of Hamiltonian mechanics and views classical mechanics as a limiting case of quantum mechanics, in the same way as Galilean relativity is viewed as a limiting case of special relativity;
- Finally, one can introduce a Schrödinger equation in phase space; one of the most cited approaches is that of Torres-Vega and Frederick [13, 14] who, using the so-called coherent state representation of wavefunctions, proposed a whole family of Schrödinger equations in phase space, whose prototype is
$$i\hbar\frac{\partial\Psi}{\partial t} = H\left(x + i\hbar\tfrac{\partial}{\partial x}, -i\hbar\tfrac{\partial}{\partial x}\right)\Psi. \tag{1}$$
The work of Torres-Vega and Frederick has been much quoted and discussed by scientists working in quantum chemistry and physics; two recent contributions are for instance [2, 12].

The aim of this paper is to make obvious the following trinity:

(i): We will show that the equation (1), and its symmetrized variant
$$i\hbar\frac{\partial\Psi}{\partial t} = H\left(\tfrac{x}{2} + i\hbar\tfrac{\partial}{\partial p}, \tfrac{p}{2} - i\hbar\tfrac{\partial}{\partial x}\right)\Psi \tag{2}$$
actually correspond to the choice of an irreducible unitary representations of the Heisenberg group in a closed subspace of $L^2(\mathbb{R}^2_{x,p})$ and is thus fully justified by the Stone-von Neumann theorem;

(ii): This unitary representation in phase space corresponds to an extended Weyl calculus in which operators no longer act only on functions defined on configuration space (as is the case for any traditional pseudo-differential calculus), but on functions defined on phase space; this extended Weyl calculus enjoys all the usual symplectic covariance properties when metaplectic operators are themselves extended to phase space;

(iii): We will examine the relationship between equation (2) and deformation quantization; we will see that Torres-Vega and Frederick's theory of Schrödinger equation in phase-space is in fact a *Doppelgänger* of deformation quantization. (This fact does not seem to have been much noticed by authors working on the Schrödinger equation in phase space; I have only found trace of it is the recent preprint [2], although it is already in fact implicit in Torres-Vega and Frederick's paper[14]).

Notations. We denote by σ the canonical symplectic form on the phase space $\mathbb{R}_z^{2n} \equiv \mathbb{R}_x^n \times \mathbb{R}_p^n$:

$$\sigma(z,z') = px' - p'x \text{ if } z = (x,p),\, z' = (x'p')$$

where $x = (x_1, ..., x_1)$, $p = (p_1, ..., p_n)$; we are using the "dotless dot-product" notation $xp = x_1p_1 + \cdots + x_np_n$. The generalized gradients ∂_x and ∂_p are defined by $\partial_x = (\partial/\partial x_1, ..., \partial/\partial x_n)$ and $\partial_p = (\partial/\partial p_1, ..., \partial/\partial p_n)$.

We denote by $Sp(n)$ the real symplectic group; it consists of all linear automorphisms S of $\mathbb{R}_z^{2n}$ such that $\sigma(Sz, Sz') = \sigma(z,z')$ for all z, z'.

$\mathcal{S}(\mathbb{R}^m)$ is the Schwartz space of rapidly decreasing functions on $\mathbb{R}^m$; its dual $\mathcal{S}'(\mathbb{R}^m)$ is the space of tempered distributions. Functions on $\mathbb{R}_x^n$ or $\mathbb{R}_p^n$ will be denoted by small Greek letters $\psi, \phi, ...$ while functions on $\mathbb{R}_z^{2n}$ will be denoted by capital Greek letters, *e.g.*, Ψ.

For the notions of Weyl calculus that are being used here, see Folland [3] or [15]; we are using the notations and normalizations of Littlejohn [7]. For a review of deformation quantization as it was at the end of last millennium, see Sternheimer [11]; this paper in addition contains an exhaustive list of references together with numerous historical comments.

2. Preliminary Considerations

In deriving his equation Schrödinger elaborated on Hamilton's optical–mechanical analogy and was led to integrate the Poincaré–Cartan form

$$\alpha_H = pdx - Hdt \tag{3}$$

in order to obtain a solution of Hamilton-Jacobi's equation for H (see [5]). This allowed him, by an inductive argument, to postulate what we call today the time-independent Schrödinger equation satisfied by a stationary matter-wave ψ_0; later he introduced the wave function $\psi(x,t) = e^{-iEt/\hbar}\psi_0$ which is a solution of the time-dependent equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\left(x, -i\hbar\partial_x\right)\psi. \tag{4}$$

Compared to the Hamilton equations

$$\dot{x} = \partial_p H(x,p) \quad , \quad \dot{p} = -\partial_x H(x,p)$$

from classical mechanics, Schrödinger's equation introduces a deep asymmetry: the variable p has disappeared altogether and has been replaced by the operator $-i\hbar\partial/\partial x$. This asymmetry comes from Schrödinger's honest and totally justifiable use of the action form (3), where the variables p and

x play asymmetric roles. Let us now pause and ask ourselves where the interest of the action form (3) comes from. Well, it mainly comes from the fact that it is a relative integral invariant, that is, its exterior derivative $d\alpha_H$ is an absolute integral invariant. It is precisely this property that allows one to integrate Hamilton–Jacobi's equation in terms of α_H. Now,

$$d\alpha_H = dp \wedge dx - Hdt$$

has α_H as a primitive –among infinitely many other! For instance, every differential form

$$\alpha_H^\lambda = \lambda pdx - (1-\lambda)xdp - Hdt$$

obviously satisfies

$$d\alpha_H^\lambda = dp \wedge dx - Hdt$$

and is hence also a relative integral invariant. Making the particular choice $\lambda = \frac{1}{2}$ we will denote by β_H the corresponding "symmetrized action form":

$$\beta_H = \frac{1}{2}(pdx - xdp) - Hdt = \frac{1}{2}\sigma(z, dz) - Hdt.$$

We claim (somewhat speculatively...) that had Schrödinger used β_H instead of α_H he could very well have landed, not with the equation (4), but rather with the phase-space equation (2), which could hence have led him to deformation quantization's ancestor, Moyal's theory!

Let us justify our claims from a rigorous mathematical point of view.

3. Phase-Space Representation of $\mathbf{H}_n$

Recall that one of the modern ways to justify the Schrödinger quantization rules $x_j \longrightarrow x_j$, $p_j \longrightarrow -i\hbar(\partial/\partial x_j)$ is to construct the Schrödinger representation of the Heisenberg group $\mathbf{H}_n$, that is $\mathbb{R}_z^{2n} \times \mathbb{R}_t$ equipped with the group law

$$(z,t)\cdot(z',t) = (z+z', t+t' + \tfrac{1}{2}\sigma(z,z')). \tag{5}$$

One proceeds as follows: consider the "translation Hamiltonian" $H_{z_0} = \sigma(z, z_0)$; the flow it determines are the translations $T(tz_0) : z \longmapsto z + tz_0$; they act on functions defined on $\mathbb{R}_z^{2n}$ by the rule

$$T(tz_0)\Psi_0(z) = \Psi_0(z - tz_0).$$

In (traditional) quantum mechanics Hilbert spaces and phases play a crucial role; one "quantizes" the operators $T(tz_0)$ by letting them act on $\psi_0 \in L^2(\mathbb{R}_x^n)$ via the Heisenberg–Weyl operators $\widehat{T}(z_0)$ defined by

$$\widehat{T}(tz_0)\psi_0(x) = e^{\frac{i}{\hbar}\varphi(z,t)}T(tz_0)\psi_0(x);$$

here $\varphi(z,t)$ is the increase in action when one goes straight from the point $z - tz_0$ to the point z, that is

$$\varphi(z,t) = \int_{-t}^{0} pdx - H_{z_0}dt = p_0xt - \frac{t^2}{2}p_0x_0; \tag{6}$$

thus

$$\widehat{T}(tz_0)\psi_0(x) = e^{\frac{i}{\hbar}(p_0xt - \frac{t^2}{2}p_0x_0)}\psi_0(x - tx_0). \tag{7}$$

The Schrödinger representation of $\mathbf{H}_n$ in $L^2(\mathbb{R}^n_x)$ is the mapping

$$T_{\mathrm{Sch}} : \mathbf{H}_n \longrightarrow \mathcal{U}(L^2(\mathbb{R}^n_x))$$

($\mathcal{U}(L^2(\mathbb{R}^n_x))$ the unitary operators on $L^2(\mathbb{R}^n_x)$) defined by

$$T_{\mathrm{Sch}}(z_0, t_0)\psi_0(x) = e^{\frac{i}{\hbar}t_0}\widehat{T}(z_0)\psi_0(x); \tag{8}$$

one proves that T_{Sch} is a unitary and irreducible representation; a famous theorem of Stone and von Neumann (see [3, 16] for a proof) asserts that it is, up to unitary equivalences, the *only* irreducible representation of $\mathbf{H}_n$ in $L^2(\mathbb{R}^n_x)$. But this theorem does not prevent us from constructing non-trivial irreducible representations of $\mathbf{H}_n$ in *other* Hilbert spaces; we will come back to this essential point in a moment, but let us first note that Schrödinger's equation for the displacement Hamiltonian $H_{z_0} = \sigma(z, z_0)$, and hence the quantum rules

$$x \longrightarrow x \quad , \quad p \longrightarrow -i\hbar\partial_x \tag{9}$$

now follow from formula (7): an immediate calculation shows that the function $\psi(x,t) = \widehat{T}(tz_0)\psi_0(x)$ is a solution of

$$i\hbar\frac{\partial\psi}{\partial t} = H_{z_0}(x, -i\hbar\partial_x)\,\psi \ \ , \ \ \psi(x,0) = \psi_0(x).$$

Let us quantize the translation operators $T(tz_0)$ in a different way. We *redefine* $\widehat{T}(tz_0)$ by letting it act, not on $L^2(\mathbb{R}^n_x)$, but on $L^2(\mathbb{R}^{2n}_z)$, by the formula

$$\widehat{T}_{\mathrm{ph}}(tz_0)\Psi_0(z) = e^{\frac{i}{\hbar}\varphi'(z,t)}T(tz_0)\Psi_0(z)$$

(the subscript "ph" stands for "*ph*ase space"), and replacing the phase (6) by integrating, not the Poincaré–Cartan form $\alpha_{H_{z_0}}$ but its symmetrized variant

$$\beta_{H_{z_0}} = \frac{1}{2}(pdx - xdp) - H_{z_0}dt.$$

This yields after a trivial calculation

$$\varphi'(z,t) = -\frac{1}{2}H_{z_0}(z)t = -\frac{1}{2}\sigma(z, z_0)t. \tag{10}$$

Summarizing, we have defined

$$\widehat{T}_{\mathrm{ph}}(tz_0)\Psi_0(z) = e^{-\frac{i}{2\hbar}\sigma(z,z_0)t}\Psi_0(z - tz_0). \tag{11}$$

What partial differential equation does the function $\Psi = \widehat{T}_{\mathrm{ph}}(tz_0)\Psi_0$ satisfy? Performing a few calculations one checks that it satisfies the multi-dimensional analogue of the phase-space Schrödinger equation (1) of the introduction, namely

$$i\hbar\frac{\partial\Psi}{\partial t} = H\left(\tfrac{x}{2} + i\hbar\partial_p, \tfrac{p}{2} - i\hbar\partial_x\right)\Psi. \tag{12}$$

We are going to prove the following:

- **(A):** The operators $\widehat{T}_{\mathrm{ph}}(tz_0)$ correspond to a new irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ on a closed subspace of $L^2(\mathbb{R}_z^{2n})$ (which is unitarily equivalent to the Schrödinger representation via Stone–von Neumann's theorem).
- **(B):** The phase-space Schrödinger equation (12) is closely related to deformation quantization, in fact to an extension of the usual Weyl calculus on $L^2(\mathbb{R}_x^n)$ to $L^2(\mathbb{R}_z^{2n})$, for which the operators $H\left(\tfrac{x}{2} + i\hbar\partial_p, \tfrac{p}{2} - i\hbar\partial_x\right)$ are perfectly well-defined.

4. The Irreducible Unitary Representation $\widehat{T}_{\mathrm{ph}}$

We define the phase-space representation of $\mathbf{H}_n$ in analogy with (8) by

$$\widehat{T}_{\mathrm{ph}}(z_0, t_0)\Psi_0(z) = e^{\frac{i}{\hbar}t_0}\widehat{T}_{\mathrm{ph}}(tz_0)\Psi_0(z). \tag{13}$$

Clearly $\widehat{T}_{\mathrm{ph}}(z_0, t_0)$ is a unitary operator; moreover a straightforward calculation shows that

$$\widehat{T}_{\mathrm{ph}}(z_0, t_0)\widehat{T}_{\mathrm{ph}}(z_1, t_1) = e^{\frac{i}{2\hbar}\sigma(z_0,z_1)}\widehat{T}_{\mathrm{ph}}(z_0 + z_1, t_0 + t_1 + \tfrac{1}{2}\sigma(z_0, z_1))$$

so that $\widehat{T}_{\mathrm{ph}}$ is indeed a representation of $\mathbf{H}_n$ on some subspace of $L^2(\mathbb{R}_z^{2n})$. We are going to show that this representation is unitarily equivalent to the Schrödinger representation, and hence irreducible.

Let $\phi \in \mathcal{S}(\mathbb{R}_x^n)$ be normalized to unity:

$$||\phi||^2_{L^2(\mathbb{R}_x^n)} = 1. \tag{14}$$

To that function ϕ we associate the operator $V_\phi : L^2(\mathbb{R}_x^n) \longrightarrow L^2(\mathbb{R}_z^{2n})$ defined by

$$V_\phi\psi(z) = \left(\tfrac{\pi\hbar}{2}\right)^{n/2} W(\psi, \phi)(\tfrac{1}{2}z)$$

where $W(\psi, \overline{\phi})$ is the Wigner–Moyal function (Folland [3]):

$$W(\psi, \phi)(x, p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{\hbar}py}\psi(x + \tfrac{1}{2}y)\overline{\phi}(x - \tfrac{1}{2}y)d^n y.$$

It turns out that V_ϕ is an extension of the "coherent-state representation" to which it reduces,up to the factor $\exp(-ipx/\hbar)$ if one takes for ϕ the real Gaussian

$$\phi_\hbar(x) = \left(\tfrac{1}{\pi\hbar}\right)^{n/4} e^{-\frac{1}{2\hbar}|x|^2}. \tag{15}$$

In fact, a straightforward calculation shows that

$$V_\phi\psi(z) = e^{-\frac{i}{2\hbar}px} U_\phi\psi(z) \tag{16}$$

where the operator U_ϕ is defined by

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

Proposition 1. *(i) The transform V_ϕ is an isometry: the Parseval formula*

$$(V_\phi\psi, V_\phi\psi')_{L^2(\mathbb{R}^{2n}_z)} = (\psi,\psi')_{L^2(\mathbb{R}^n_x)} \tag{18}$$

holds for all $\psi,\psi' \in \mathcal{S}(\mathbb{R}^n_x)$; (ii) V_ϕ extends into an isometric operator $L^2(\mathbb{R}^n_x) \longrightarrow L^2(\mathbb{R}^{2n}_z)$ and

$$V_\phi^* V_\phi = I \quad on \quad L^2(\mathbb{R}^n_x); \tag{19}$$

(iii) The range $\mathcal{H}_\phi$ of V_ϕ is closed in $L^2(\mathbb{R}^{2n}_z)$ (and is hence a Hilbert space), and $P = V_\phi V_\phi^*$ is the orthogonal projection on the Hilbert space $\mathcal{H}_\phi$.

Proof. The operator U_ϕ satisfies the listed properties (see for instance [10], Chapter 2, §2); since $V_\phi\psi(z) = e^{-\frac{i}{2\hbar}px}U_\phi$ we have

$$(V_\phi\psi, V_\phi\psi')_{L^2(\mathbb{R}^{2n}_z)} = (U_\phi\psi, U_\phi\psi')_{L^2(\mathbb{R}^{2n}_z)}$$

and the proposition follows. □

The irreducibility of the representation $\widehat{T}_{\mathrm{ph}}$ is a consequence of the result above:

Corollary 2. *$\widehat{T}_{ph}$ is unitarily equivalent to the Schrödinger representation, and hence irreducible, and we have*

$$\widehat{T}_{ph}(z_0,t_0)V_\phi = V_\phi \widehat{T}_{Sch}(z_0,t_0). \tag{20}$$

Proof. It suffices to show that the operators $\widehat{T}_{\mathrm{ph}}(z_0) = \widehat{T}_{\mathrm{ph}}(z_0,0)$ and $T_{\mathrm{Sch}}(z_0) = T_{\mathrm{Sch}}(z_0,0)$ make the following diagram commutative:

$$\begin{array}{ccc} L^2(\mathbb{R}^n_x) & \xrightarrow{V_\phi} & L^2(\mathbb{R}^{2n}_z) \\ T_{\mathrm{Sch}} \downarrow & & \downarrow \widehat{T}_{\mathrm{ph}} \\ L^2(\mathbb{R}^n_x) & \xrightarrow{V_\phi} & L^2(\mathbb{R}^{2n}_z). \end{array}$$

Now,

$$\begin{aligned}\widehat{T}_{\mathrm{ph}}(z_0)V_\phi\psi(z) &= e^{-\frac{i}{2\hbar}\sigma(z,z_0)}e^{-\frac{i}{2\hbar}px}U_\phi\psi(z-z_0)\\ &= \left(\tfrac{1}{2\pi\hbar}\right)^{n/2}e^{-\frac{i}{\hbar}(p_0x-\frac{1}{2}p_0x_0)}\times\\ &\qquad\int e^{\frac{i}{\hbar}(p-p_0)(x-x_0-x')}\phi(x-x_0-x')\psi(x')d^nx'\end{aligned}$$

and setting $x''=x'+x_0$ in the integral this is

$$\begin{aligned}\widehat{T}_{\mathrm{ph}}(z_0)V_\phi\psi(z) &= \left(\tfrac{1}{2\pi\hbar}\right)^{n/2}e^{-\frac{i}{\hbar}(p_0x-\frac{1}{2}p_0x_0)}\times\\ &\qquad\int e^{\frac{i}{\hbar}(p-p_0)(x-x'')}\phi(x-x'')\psi(x''-x_0)d^nx'\end{aligned}$$

hence

$$\widehat{T}_{\mathrm{ph}}(z_0)(V_\phi\psi)(z)=V_\phi(T_{\mathrm{Sch}}(z_0)\psi)(z)$$

which was to be proven. □

Remark 3. *The Hilbert space $\mathcal{H}_\phi$ is smaller than $L^2(\mathbb{R}^{2n}_z)$; for instance if we chose for ϕ the Gaussian (15) then one proves [10] that the range of the transform U_ϕ defined by (17) consists of all $\Psi\in L^2(\mathbb{R}^{2n}_z)$ such that $\exp(p^2/2\hbar)$ is anti-analytic. It follows that $\mathcal{H}_{\phi_0}$ which is the range of $V_\phi=\exp(-ipx/2\hbar)U_\phi$ consists of all $\Psi\in L^2(\mathbb{R}^{2n}_z)$ for which the following (anti-) Cauchy-Riemann conditions hold:*

$$\frac{\partial}{\partial z_j}(e^{\frac{1}{2\hbar}|z|^2}\Psi(z))=0\ \ ,\ \ 1\leq j\leq n.$$

Moreover, a few calculations, using for instance (16) and (17) show that we have

$$\left(\tfrac{x}{2}+i\hbar\partial_p\right)V_\phi\psi=V_\phi(x\psi)\ \ ,\ \ \left(\tfrac{p}{2}-i\hbar\partial_x\right)V_\phi\psi=V_\phi(-i\hbar\partial_x\psi); \tag{21}$$

the transform V_ϕ thus takes the usual quantization rules (9) to the phase-space quantization rules

$$x\longrightarrow\frac{x}{2}+i\hbar\partial_p\ \ ,\ \ x\longrightarrow\frac{p}{2}-i\hbar\partial_x.$$

Remark 4. *If one uses the transformation U_ϕ instead of V_ϕ and chooses for ϕ the normalized Gaussian $\phi_\hbar$ given by (15) one would get instead the rules*

$$x\longrightarrow x+i\hbar\partial_x\ \ ,\ \ x\longrightarrow -i\hbar\partial_x$$

corresponding to the Torres-Vega and Frederick equation (1).

5. Extended Weyl Calculus

In standard Weyl calculus one associates to a "symbol" a having some some suitable growth properties for $p \to \infty$ class a pseudo-differential operator

$$\widehat{A} = a^w : \mathcal{S}(\mathbb{R}^n_x) \longrightarrow \mathcal{S}(\mathbb{R}^n_x)$$

defined by the kernel

$$K_{\widehat{A}}(x,y) = \left(\tfrac{1}{2\pi\hbar}\right)^{n/2} \int e^{\frac{i}{\hbar}p(x,y)} a(\tfrac{1}{2}(x+y),p)d^N p.$$

One proves that (see *e.g.* [3, 15])

$$\widehat{A}\psi(x) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int \tilde{a}(z_0)\widehat{T}_{\mathrm{Sch}}(z_0)\psi(x)d^{2n}z_0 \tag{22}$$

for $\psi \in \mathcal{S}(\mathbb{R}^n_x)$ (the integral being interpreted as an "oscillatory integral", . In formula (22) $\tilde{a}$ (the "twisted" Weyl symbol) is the symplectic Fourier-transform of a:

$$\tilde{a}(z) = \mathcal{F}_\sigma a(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{\hbar}\sigma(z,z')} a(z')d^{2n}z' \tag{23}$$

and $\widehat{T}_{\mathrm{Sch}}(z_0) = \widehat{T}_{\mathrm{Sch}}(z_0,0)$ is the Heisenberg–Weyl operator (7).

The discussion above suggests that we might now be able to make $\widehat{A}$ to act, not only on functions of x, but also on functions $\Psi \in \mathcal{S}(\mathbb{R}^{2n}_z)$ by defining

$$\widehat{A}_{\mathrm{Sch}}\Psi(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int \tilde{a}(z_0)\widehat{T}_{\mathrm{Sch}}(z_0)\Psi(z)d^{2n}z_0 \tag{24}$$

where we have set

$$\widehat{T}_{\mathrm{Sch}}(z_0)\Psi(z) = e^{\frac{i}{\hbar}(p_0 x - \frac{1}{2}p_0 x_0)}\Psi(z-z_0).$$

It turns out that it is better for our purposes to use instead the operator

$$\widehat{A}_{\mathrm{ph}}\Psi(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int \tilde{a}(z_0)\widehat{T}_{\mathrm{ph}}(z_0)\Psi(z)d^{2n}z_0 \tag{25}$$

obtained by replacing $\widehat{T}_{\mathrm{Sch}}$ by $\widehat{T}_{\mathrm{ph}}$ in (24); somewhat more explicitly:

$$\widehat{A}_{\mathrm{ph}}\Psi(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{2\hbar}\sigma(z,z_0)}\mathcal{F}_\sigma a(z_0)\Psi(z-z_0)d^{2n}z_0. \tag{26}$$

As expected, the operators $\widehat{X}_{\mathrm{ph}}$ and $\widehat{P}_{\mathrm{ph}}$ corresponding to the symbols x and p are just

$$\widehat{X}_{\mathrm{ph}} = \frac{x}{2} + i\hbar\partial_p \ \text{ and } \widehat{P}_{\mathrm{ph}} = \frac{p}{2} - i\hbar\partial_x$$

and we will therefore use the notation

$$\widehat{A}_{\mathrm{ph}} = \widehat{A}(\tfrac{x}{2} + i\hbar\partial_p, \tfrac{p}{2} - i\hbar\partial_x);$$

observe that X_{ph} and P_{ph} obey the usual canonical relations

$$\left[\widehat{X}_{j,\mathrm{ph}}, \widehat{P}_{k,\mathrm{ph}}\right] = i\hbar\delta_{jk}.$$

In a recent paper [4] we have shown, following previous work of Mehlig and Wilkinson [8] that the metaplectic group $Mp(n)$ is generated by the operators

$$\widehat{S}^{(\nu)} = \left(\frac{1}{2\pi\hbar}\right)^n i^\nu \sqrt{|\det(S-I)|} \int e^{-\frac{i}{2\hbar}\sigma(Sz,z)} \widehat{T}((S-I)z) d^{2n}z \qquad (27)$$

where $S \in Sp(n)$, $\det(S-I) \neq 0$, and ν is, modulo 2, the Conley–Zehnder index of a path joining the identity to S in $Sp(n)$; the natural projection $\pi : Mp(n) \longrightarrow Sp(n)$ is defined as the unique epimorphism satisfying $\pi(\widehat{S}^{(\nu)}) = S$. Using the intertwining relation (20) $\widehat{T}_{\mathrm{ph}}(z_0)V_\phi = V_\phi \widehat{T}_{\mathrm{Sch}}(z_0)$ we can define unitary operators $\widehat{S}^{(\nu)}_{\mathrm{ph}} : L^2(\mathbb{R}^{2n}_z) \longrightarrow L^2(\mathbb{R}^{2n}_z)$ by the formula

$$\widehat{S}^{(\nu)}_{\mathrm{ph}} = V_\phi \widehat{S}^{(\nu)} V_\phi^*. \qquad (28)$$

An explicit calculation yields

$$\widehat{S}^{(\nu)}_{\mathrm{ph}} = \left(\frac{1}{2\pi\hbar}\right)^n i^\nu \sqrt{|\det(S-I)|} \int e^{-\frac{i}{2}\sigma(Sz,z)} \widehat{T}_{\mathrm{ph}}((S-I)z) d^{2n}z \qquad (29)$$

so that $\widehat{S}^{(\nu)}_{\mathrm{ph}}$ is independent of the choice of ϕ. The group $Mp_{\mathrm{ph}}(n)$ generated by these operators is trivially isomorphic to the usual group $Mp(n)$, and the usual "metaplectic covariance formula" for Weyl–Heisenberg operators

$$\widehat{S}\widehat{T}_{\mathrm{Sch}}(z) = \widehat{T}_{\mathrm{Sch}}(Sz)\widehat{S} \qquad (30)$$

valid for every $\widehat{S} \in Mp(n)$ with projection $S \in Sp(n)$ extends in a natural way to phase-space Weyl operators:

Proposition 5. *For every $\widehat{S}_{ph} \in Mp_{ph}(n)$ we have*

$$\widehat{S}_{ph}\widehat{T}_{ph}(z) = \widehat{T}_{ph}(Sz)\widehat{S}_{ph}. \qquad (31)$$

Proof. It suffices to prove (31) when $\widehat{S}_{\mathrm{ph}} = \widehat{S}^{(\nu)}_{\mathrm{ph}}$ since the metaplectic operators $\widehat{S}^{(\nu)}_{\mathrm{ph}}$ generate $Mp_{\mathrm{ph}}(n)$. Using successively (28) and (20) we have

$$\widehat{S}^{(\nu)}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z) = V_\phi \widehat{S}^{(\nu)} V_\phi^{-1} \widehat{T}_{\mathrm{ph}}(z) = V_\phi \widehat{S}^{(\nu)} \widehat{T}_{\mathrm{Sch}} V_\phi^{-1}$$

that is, by (30), and again (20),

$$\widehat{S}^{(\nu)}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z) = V_\phi \widehat{T}_{\mathrm{Sch}}(Sz)\widehat{S}^{(\nu)} V_\phi^{-1} = \widehat{T}_{\mathrm{ph}}(Sz) V_\phi \widehat{S}^{(\nu)} V_\phi^{-1}$$

which proves (31). $\square$

The metaplectic covariance for Weyl operators on phase space follows:

Corollary 6. *If $\widehat{A}_{ph}$ has symbol a then $\widehat{S}_{ph}\widehat{A}_{ph}\widehat{S}_{ph}^{-1}$ is the phase-space Weyl operator with symbol $a \circ S^{-1}$.*

Proof. Using (25) we have, using the fact that $\det S = 1$,

$$\begin{aligned}\widehat{S}_{\mathrm{ph}}\widehat{A}_{\mathrm{ph}}\widehat{S}_{\mathrm{ph}}^{-1} &= \left(\tfrac{1}{2\pi\hbar}\right)^n \int \tilde{a}(z)\widehat{S}_{\mathrm{ph}}\widehat{T}_{\mathrm{ph}}(z)\widehat{S}_{\mathrm{ph}}^{-1} d^{2n}z \\ &= \left(\tfrac{1}{2\pi\hbar}\right)^n \int \tilde{a}(z)\widehat{T}_{\mathrm{ph}}(Sz) d^{2n}z \\ &= \left(\tfrac{1}{2\pi\hbar}\right)^n \int \tilde{a}(S^{-1}z)\widehat{T}_{\mathrm{ph}}(z) d^{2n}z;\end{aligned}$$

since by definition (23) of $\tilde{a}$

$$\begin{aligned}\tilde{a}(S^{-1}z) &= \left(\tfrac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{\hbar}\sigma(S^{-1}z,z')} a(z') d^{2n}z' \\ &= \left(\tfrac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{\hbar}\sigma(z,Sz')} a(z') d^{2n}z' \\ &= \left(\tfrac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{\hbar}\sigma(z,Sz')} a(S^{-1}z') d^{2n}z'\end{aligned}$$

this proves our claim. □

5.1. **Relation With Deformation Quantization.** It turns out that formula (26) is the fundamental link between the theory sketched above with deformation quantization. Recall that if $\widehat{A} = a^w$ and $\widehat{B} = b^w$ are the Weyl operators with symbols a and b, respectively, then the twisted symbol $\tilde{c} = \mathcal{F}_\sigma c$ of the compose $\widehat{C} = \widehat{A}\widehat{B}$ is given by the formula

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

since $\mathcal{F}_\sigma$ is an involution, we have $c = \mathcal{F}_\sigma \tilde{c}$ and one verifies that

$$c(z) = \left(\tfrac{1}{4\pi\hbar}\right)^{2n} \int e^{\frac{i}{2\hbar}\sigma(z',z'')} a(z+\tfrac{1}{2}z')b(z-\tfrac{1}{2}z'') d^{2n}z' d^{2n}z'';$$

using expansions in Taylor series and repeated integrations by parts this can be rewritten in terms of the "Janus operator" $\overleftarrow{\partial_x}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_x}$ as

$$c(z) = a(z)\exp\left[\tfrac{i\hbar}{2}(\overleftarrow{\partial_x}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_x}\right] b(z) = a\bigstar b(z)$$

where $\bigstar$ is the star-product. Thus formula (26) says that our extended Weyl calculus can be expressed in terms of the star-product in the following very simple way:

$$\widehat{A}(\tfrac{x}{2} + i\hbar\partial_p, \tfrac{p}{2} - i\hbar\partial_x)\Psi = \mathcal{F}_\sigma(a\bigstar\Psi). \tag{32}$$

Noting that the symplectic Fourier transform satisfies the commutation relations

$$\mathcal{F}_\sigma \circ (\tfrac{x}{2} + i\hbar\partial_p) = (x + \tfrac{i\hbar}{2}\partial_p) \circ \mathcal{F}_\sigma$$
$$\mathcal{F}_\sigma \circ (\tfrac{p}{2} - i\hbar\partial_x) = (p - \tfrac{i\hbar}{2}\partial_x) \circ \mathcal{F}_\sigma$$

and that $\mathcal{F}_\sigma^2 = I$ we have formally

$$\mathcal{F}_\sigma \widehat{A}(\tfrac{x}{2} + i\hbar\partial_p, \tfrac{p}{2} - i\hbar\partial_x) = \widehat{A}(x + \tfrac{i\hbar}{2}\partial_p, p - \tfrac{i\hbar}{2}\partial_x)$$

so that we can rewrite (32) as

$$a\bigstar\Psi = \widehat{A}(x + \tfrac{i\hbar}{2}\partial_p, p - \tfrac{i\hbar}{2}\partial_x)\Psi. \tag{33}$$

This formula is widely used in physics (see Zachos *et al.* [17] and the numerous references therein) and suggests, as it is intended to do, that one passes from our extended Weyl calculus to deformation quantization, and vice-versa, by symplectic Fourier transform.

6. Discussion and Concluding Remarks

There has been some debate among scientists about the relevance or physical significance of a Schrödinger equation in phase space. We have shown that the consideration of such an equation actually is consistent with Stone and von Neumann's theorem on the irreducible representations of the Heisenberg group, and that it is deformation quantization in disguise. One should however not dismiss it too easily as being an uninteresting "souped down" version of a "better" theory. Many quantum physicists –and perhaps even more quantum chemists– are "culturally" closer to the Schrödinger formalism; the solutions Ψ of the equation

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

are interesting objects in themselves, since they contain information about the wavefunction ψ: if $\Psi = V_\phi\psi$ a straightforward calculation shows that

$$\int \Psi(z)d^n p = (2\pi\hbar)^{n/2}\psi(\tfrac{1}{2}x)\overline{\phi(\tfrac{1}{2}x)}$$
$$\int \Psi(z)d^n x = (2\pi\hbar)^{n/2}F\psi(\tfrac{1}{2}p)\overline{F\phi(\tfrac{1}{2}p)}.$$

so that both ψ and its Fourier transform $F\psi$ are immediately obtained from Ψ if $\phi(x) \neq 0$ for all x. It thus appears that Ψ in a sense plays the role of a "joint probability amplitude", as opposed to the Wigner transform $W\psi$ which is not a joint probability density since it can take negative values.

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References

[1] F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, and D. Sternheimer. Deformation Theory and Quantization. I. Deformation of Symplectic Structures. *Annals of Physics* **111**, 6–110, 1978; II Physical Applications **110**, 111–151, 1978.

[2] D. Chruscinski and K. Mtlodawski. Wigner function and Schrödinger equation in phase space representation. Preprint, *arXiv: quant-ph/ 0501163 v1*, 2005.

[3] G. B. Folland. *Harmonic Analysis in Phase space.* Annals of Mathematics studies, Princeton University Press, Princeton, N.J., 1989.

[4] M. de Gosson. On the Weyl Representation of Metaplectic Operators. To appear in *Lett. Math. Phys.*, 2005

[5] M. Jammer. *The Conceptual Development of Quantum Mechanics,* Inst. Series in Pure and Appl. Physics (McGraw-Hill Book Company, *1966).*

[6] Y. S. Kim and M. E. Noz. *Phase space Picture of Quantum Mechanics (Group Theoretical Approach)* World Scientific, Singapore, 1991.

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

[8] B. Mehlig and M. Wilkinson. Semiclassical trace formulae using coherent states. *Ann. Phys.* **18**(10), 6–7, 541–555, 2001.

[9] J. E. Moyal. Quantum mechanics as a statistical theory. *Proc. Camb. Phil. Soc.* **45**:99–124, 1947.

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

[11] D. Sternheimer. Deformation Quantization: Twenty Years After. In *Particles, Fields and Gravitation,* editor J. Rembielenski, Proceedings of a conference held in Łodz, Poland, 15-19 April 1998. AIP Conference Proceedings, Vol. 453, 1998, p.107.

[12] Qian Shu Li, Gong Min Wei, and Li Qiang Lü. Relationship between the Wigner function and the propability density function in quantum phase space representation. *Phys. Rev. A* **70**, 022105, 2004.

[13] G Torres-Vega and J H Frederick, J. Chem. Phys. **93**(12) 8862–8874, 1990.

[14] G Torres-Vega and J H Frederick, J. Chem. Phys. **98**(4) 3103–3120, 1993.

[15] M. W. Wong. *Weyl Transforms.* Springer, 1998.

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

[17] C. K. Zachos, D. B. Fairlie, and T. L. Curtright. *Quantum Mechanics in Phase Space.* World Scientific, Singapore, 2005.

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