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Moyal Bracket and Ehrenfest's Theorem in Born–Jordan Quantization

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Abstract: The usual Poisson bracket $\{A, B\}$ can be identified with the so-called Moyal bracket $\{A, B\}_{\mathrm{M}}$ for larger classes of symbols than was previously thought, provided that one uses the Born–Jordan quantization rule instead of the better known Weyl correspondence. We apply our results to a generalized version of Ehrenfest's theorem on the time evolution of averages of operators.

Keywords: Ehrenfest's theorem; Born-Jordan quantization; Moyal bracket

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Autant de quantifications, autant de religions (Jean Leray (Private communication (1988)), 1906–1998)

1. Introduction

A famous theorem from quantum statistical mechanics says that the evolution of the quantum averages with respect to a state $\widehat{\rho}$ of a quantum observable $\widehat{A}$ under a Hamiltonian evolution obeys the generalized Ehrenfest equation (Messiah [1])

$$\frac{d}{dt}\langle \widehat{A} \rangle = \frac{1}{i\hbar}\langle [\widehat{A}, \widehat{H}] \rangle. \tag{1}$$

If we were able to write the commutator as a quantization of the Poisson bracket $\{A, H\}$ of the classical observables corresponding to $\widehat{A}$ and $\widehat{H}$ by the Weyl correspondence, then we could rewrite Equation (1) as

$$\frac{d}{dt}\langle \widehat{A} \rangle = \int \{A, H\}(x, p)\rho(x, p, t)dpdx \tag{2}$$

where $\rho(x, p, t)$ is the Wigner distribution of the state $\widehat{\rho}$ at time t. This equality is, however, not true in general. In fact, it follows from a classical "no-go" result of Groenewold and van Hove that the Dirac correspondence

$$\{A, H\} \longleftrightarrow \frac{1}{i\hbar}\langle [\widehat{A}, \widehat{H}] \rangle \tag{3}$$

does not hold unless A and H are quadratic polynomials in the x, p variables; Equation (2) has to be replaced with

$$\frac{d}{dt}\langle \widehat{A} \rangle = \int \{A, H\}_{\mathrm{M}}(x, p)\rho(x, p, t)dpdx \tag{4}$$

where $\{A, H\}_{\mathrm{M}}$ is the so-called "Moyal bracket". It was only recently recognized [2,3] that the Dirac correspondence, Equation (3), however, holds for a large class of observables provided that we use the Born–Jordan (BJ) quantization scheme instead of the usual Weyl quantization (this was already noticed but not fully developed by Kauffmann [4] a few years ago). For instance (see Proposition 4 below), for all integers $m, n \geq 0$ we have the exact correspondence

$$\{x^m, p^n\} \overset{\text{BJ}}{\longleftrightarrow} \frac{1}{i\hbar}[\widehat{x}^m, \widehat{p}^n]. \tag{5}$$

Equation (5) is characteristic of BJ quantization as shown in [3]. We emphasize that this fact is not related in any way to Groenewold's and van Hove's result because the latter does not preclude quantizations satisfying Equation (5).

The main result we will prove in this paper is the following (Proposition 6): Let $\rho(z,t)$ be the Wigner distribution at time t and let $\widehat{A}$ be a quantum observable obtained by any quantization procedure from a classical observable (symbol) of the type $A(x,p) = S(x) + V(p)$ with S and V smooth functions of polynomial growth. Then the time-evolution of the quantum average $\langle \widehat{A} \rangle_{\text{qu},t}$ obeys the equation

$$\frac{d}{dt}\langle \widehat{A} \rangle_{\text{qu},t} = \int \{A, H\}(z)\rho(z,t)d^{2n}z. \tag{6}$$

We also mention that Bonet-Luz and Tronci have studied, in [5], Ehrenfest expectation values from a dynamical and geometric point of view focusing on Gaussian states. It would certainly be interesting to develop these techniques using the results in the present paper.

2. The Moyal Star Product

Let $\widehat{A}$ and $\widehat{B}$ be two operators with respective Weyl symbols A and B: $\widehat{A} = \text{Op}^{\text{W}}(A)$ and $\widehat{B} = \text{Op}^{\text{W}}(B)$. Assuming that the product $\widehat{C} = \widehat{A}\widehat{B}$ exists we have $\widehat{C} = \text{Op}^{\text{W}}(C)$ with

$$C(z) = \left(\tfrac{1}{4\pi\hbar}\right)^{2n} \iint e^{\frac{i}{2\hbar}\sigma(z',z'')} A(z + \tfrac{1}{2}z')B(z - \tfrac{1}{2}z'')d^{2n}z'd^{2n}z''; \tag{7}$$

this is "Weyl's product rule". It is customary in quantum mechanical texts to say that the Weyl symbol c is the "Moyal product" [6] (or "star-product") of A and B and to write $c = A \star_\hbar B$. The Moyal bracket of two symbols A and B is defined (when it exists) by

$$\{A, B\}_{\text{M}} = \frac{1}{i\hbar}(A \star_\hbar B - B \star_\hbar A) \tag{8}$$

which is the quantum analogue of the usual Poisson bracket

$$\{A, B\} = \sum_{|\alpha|=1} \partial_x^\alpha A \partial_p^\alpha B - \partial_p^\alpha A \partial_x^\alpha B.$$

The properties of the Moyal product are well documented; we begin with Folland ([7], §39), who studies the case where the symbols A and B belong to the Hörmander class $S^m_{\rho,\delta}(\mathbb{R}^{2n})$ with $\rho > \delta$. We will use here more precise results creditable to Voros [8,9] and Estrada et al. [10]. Before we state them let us introduce the following symbol classes:

- $\mathcal{O}_M(\mathbb{R}^{2n})$ is the space of all C^∞ functions $A : \mathbb{R}^{2n} \longrightarrow \mathbb{C}$ such that for every $\alpha \in \mathbb{N}^n$ there exist $C_\alpha > 0$ and $m_\alpha \in \mathbb{R}$ such that $|\partial_z^\alpha A(z)| \leq C_\alpha(1 + |z|)^{m_\alpha}$;
- $\mathcal{O}_C(\mathbb{R}^{2n})$ is the space of all C^∞ functions $A : \mathbb{R}^{2n} \longrightarrow \mathbb{C}$ such that there exists $m \in \mathbb{R}$ such that for every $\alpha \in \mathbb{N}^n$ there exist $C_\alpha > 0$ such that $|\partial_z^\alpha A(z)| \leq C_\alpha(1 + |z|)^m$;
- $\Gamma^m_\rho(\mathbb{R}^{2n})$ is the Shubin class [11]: $A \in \Gamma^m_\rho(\mathbb{R}^{2n})$ ($\rho \geq 0$) if $|\partial_z^\alpha A(z)| \leq C_\alpha(1 + |z|)^{m-\rho|\alpha|}$; it is sometimes called the "GLS symbol class" in the older literature.

We have the inclusions

$$\mathcal{S}(\mathbb{R}^{2n}) \subset \Gamma^m_\rho(\mathbb{R}^{2n}) \subset \mathcal{O}_C(\mathbb{R}^{2n}) \subset \mathcal{O}_M(\mathbb{R}^{2n}) \subset \mathcal{S}'(\mathbb{R}^{2n}). \tag{9}$$

For $\alpha = (\alpha_1, ..., \alpha_n) \in \mathbb{N}^n$, we write $\partial_z^\alpha = \partial_{z_1}^{\alpha_1} \cdots \partial_{z_{2n}}^{\alpha_{2n}}$ and set

$$\widehat{\partial}_z^\alpha = (-1)^{|\alpha|}(\partial_{z_{n+1}}^{\alpha_1} \cdots \partial_{z_{2n}}^{\alpha_n})(\partial_{z_1}^{\alpha_{n+1}} \cdots \partial_{z_n}^{\alpha_{2n}}).$$

With this notation we have (Estrada et al. [10]):

Proposition 1. *Let $A \in \mathcal{O}_M(\mathbb{R}^{2n})$ and $B \in \mathcal{O}_C(\mathbb{R}^{2n})$ (or vice versa). For every $z = (z_1, ..., z_{2n}) \in \mathbb{R}^{2n}$ and $N \in \mathbb{N}$ we have the pointwise asymptotic expansion*

$$(A \star_\hbar B)(z) = \sum_{|\alpha|=0}^{|\alpha|=N} \left(\frac{i\hbar}{2}\right)^{|\alpha|} \frac{1}{\alpha!} \partial_z^\alpha A(z) \widehat{\partial}_z^\alpha B(z) + O(\hbar^{N+1}) \tag{10}$$

for $\hbar \to 0$. The Moyal bracket has the expansion

$$\{A, B\}_\mathrm{M} = \sum_{|\alpha|=1}^{|\alpha|=N} \left(\frac{i\hbar}{2}\right)^{|\alpha|} \frac{1}{\alpha!} \left[\partial_z^\alpha A(z) \widehat{\partial}_z^\alpha B(z) - \partial_z^\alpha B(z) \widehat{\partial}_z^\alpha A(z)\right] + O(\hbar^{N+1}) \tag{11}$$

In more general cases (when, say, $A \in \mathcal{S}(\mathbb{R}^{2n})$ and $B \in \mathcal{S}'(\mathbb{R}^{2n})$) the expansions above hold in the distributional sense, that is $\langle A \star_\hbar B, c\rangle = \langle S_N, c\rangle + O(\hbar^{N+1})$ for every $c \in \mathcal{S}(\mathbb{R}^{2n})$ where S_N is the sum in the right-hand side of Equation (10). If $\hbar = 0$, we have $A \star_0 B = AB$, the ordinary product of the symbols A and B. Expansion to the second order yields the formulas

$$(A \star_\hbar B)(z) = A(z)B(z) + \frac{i\hbar}{2}\{A, B\}(z) + O(\hbar^2) \tag{12}$$

$$\{A, B\}_\mathrm{M}(z) = \{A, B\}(z) + O(\hbar^2). \tag{13}$$

Moreover, if A or B is a polynomial, the sum in Equation (10) is finite, and is exactly equal to $A \star_\hbar B$.

3. Born–Jordan Quantization

Consider first the case of monomials $x^r p^s$ (we are working with $n = 1$ here). We denote by $\widehat{x}$ and $\widehat{p}$ any operators on $\mathcal{S}(\mathbb{R}^n)$ satisfying the commutation relation $[\widehat{x}, \widehat{p}] = i\hbar$. In the Weyl case we have

$$\mathrm{Op}^\mathrm{W}(x^r p^s) = \frac{1}{2^r} \sum_{k=0}^{r} \binom{r}{k} \widehat{x}^k \widehat{p}^s \widehat{x}^{r-k}.$$

The following is a particular case, taking $\tau = \frac{1}{2}$, of Shubin's [11] τ-odering:

$$\mathrm{Op}^\tau(x^r p^s) = \sum_{k=0}^{r} \binom{r}{k} \tau^k (1-\tau)^{r-k} \widehat{x}^k \widehat{p}^s \widehat{x}^{r-k}.$$

Integrating both sides of this equality from 0 to 1 with respect to the parameter τ, we get, using the properties of the beta function,

$$\mathrm{Op}^\mathrm{BJ}(x^r p^s) = \frac{1}{r+1} \sum_{k=0}^{r} \widehat{x}^k \widehat{p}^s \widehat{x}^{r-k}, \tag{14}$$

which is Born and Jordan's quantization rule [12] for monomials.

Suppose now A is an arbitrary symbol, we assume that $A \in \mathcal{S}(\mathbb{R}^{2n})$ so we can avoid discussing convergence problems at this point. The Weyl operator $\widehat{A} = \mathrm{Op}^\mathrm{W}(A)$ is explicitly given by

$$\widehat{A} = \left(\tfrac{1}{2\pi\hbar}\right)^n \int FA(z_0) \widehat{M}(z_0) d^{2n} z_0 \tag{15}$$

where F is the Fourier transform and $\widehat{M}(z_0)$ is the operator defined, for $z_0 = (x_0, p_0)$, by

$$\widehat{M}(x_0, p_0) = e^{\frac{i}{\hbar}(x_0\widehat{x} + p_0\widehat{p})}. \tag{16}$$

One verifies by a direct calculation (Cohen [13]) that the action of this operator on $\psi \in \mathcal{S}(\mathbb{R}^n)$ is explicitly given by

$$\widehat{M}(x_0, p_0)\psi(x) = e^{\frac{i}{\hbar}(x_0 x + \frac{1}{2}x_0 p_0)}\psi(x + p_0). \tag{17}$$

Introducing the τ-parametrized operators ($\tau \in \mathbb{R}$)

$$\widehat{M}_\tau(x_0, p_0) = e^{\frac{i}{2\hbar}(2\tau - 1)p_0 x_0}\widehat{M}(x_0, p_0), \tag{18}$$

the Shubin τ-operator $\widehat{A}_\tau = \operatorname{Op}^\tau(A)$ [11,14] is defined by

$$\widehat{A}_\tau = \left(\tfrac{1}{2\pi\hbar}\right)^n \int FA(z_0)\widehat{M}_\tau(z_0)d^{2n}z_0 \tag{19}$$

(remark that $\widehat{A}_{1/2} = \operatorname{Op}^{\mathrm{W}}(A)$). Averaging, as in the monomial case, over $\tau \in [0,1]$, we define the Born–Jordan operator $\widehat{A} = \operatorname{Op}^{\mathrm{BJ}}(A)$ by

$$\widehat{A} = \operatorname{Op}^{\mathrm{BJ}}(A) = \int_0^1 \widehat{A}_\tau d\tau. \tag{20}$$

Observing that

$$\int_0^1 e^{\frac{i}{2\hbar}(2\tau-1)px}d\tau = \operatorname{sinc}\left(\frac{px}{2\hbar}\right) = \Phi(z)$$

where $\operatorname{sinc} t = (\sin t)/t$ if $t \neq 0$ and $\operatorname{sinc} 0 = 1$, this definition becomes, in view of Equation (19),

$$\operatorname{Op}^{\mathrm{BJ}}(A) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int FA(z)\Phi(z)\widehat{M}(z)d^{2n}z.$$

Proposition 2. *We have $F^{-1}\Phi \in \mathcal{S}(\mathbb{R}^{2n})$ and*

$$\operatorname{Op}^{\mathrm{BJ}}(A) = (2\pi\hbar)^{-n}\operatorname{Op}^{\mathrm{W}}(A * F^{-1}\Phi) \tag{21}$$

Proof. We recall the convolution formulas

$$F(A * B) = (2\pi\hbar)^n(FA)(FB) \ , \ F(AB) = (2\pi\hbar)^{-n}(FA * FB). \tag{22}$$

We have $\Phi \in C^0(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n})$, hence $F\Phi$ and $F^{-1}\Phi$ exist in the sense of tempered distributions. Equation (21) follows from the first formula, Equation (22): We have

$$(FA)\Phi = (FA)F(F^{-1}\Phi) = (2\pi\hbar)^{-n}F(A * F^{-1}\Phi)$$

and hence

$$\operatorname{Op}^{\mathrm{BJ}}(A) = \left(\tfrac{1}{2\pi\hbar}\right)^{2n} \int F(A * F^{-1}\Phi)(z)\widehat{M}(z)d^{2n}z.$$

□

Let $\psi \in \mathcal{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$ be normalized: $||\psi||_{L^2} = 1$. Let $A \in \mathcal{O}_M(\mathbb{R}^{2n})$ and $\widehat{A} = \operatorname{Op}(A)$ the operator associated to A by some quantization procedure (see next section). The number

$$\langle\widehat{A}\rangle = \int \widehat{A}\psi(x)\overline{\psi(x)}d^n x$$

is by definition the average (or expectation value) of $\widehat{A}$ (in the "state ψ"). It turns out that $\langle\widehat{A}\rangle$ can be calculated in the phase space formalism using both Weyl quantization and Born–Jordan quantization. We denote by $W\psi$ the Wigner transform of ψ:

$$W\psi(x,p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{\hbar}py}\psi(x+\tfrac{1}{2}y)\overline{\psi(x-\tfrac{1}{2}y)}d^ny. \tag{23}$$

Proposition 3. *We have*

$$\langle \mathrm{Op}^{\mathrm{W}}(A)\rangle = \int A(z)W\psi(z)d^{2n}z \tag{24}$$

$$\langle \mathrm{Op}^{\mathrm{BJ}}(A)\rangle = \int A(z)W^{\Phi}\psi(z)d^{2n}z \tag{25}$$

where $W^{\Phi}\psi$ is the quasi-distribution defined by

$$W^{\Phi}\psi = (2\pi\hbar)^{-n}W\psi * F^{-1}\Phi. \tag{26}$$

Proof. Equation (24) is well-known (it is sometimes called the fundamental relation between Weyl pseudodifferential calculus and the Wigner formalism, see [13–16]). Equation (25) follows using Equation (21) (*cf.* [14] Ch. 10, p. 152): We have, using Equation (24),

$$\begin{aligned}\langle \mathrm{Op}^{\mathrm{BJ}}(A)\rangle &= (2\pi\hbar)^{-n}\langle \mathrm{Op}^{\mathrm{W}}(A * F^{-1}\Phi)\rangle \\ &= (2\pi\hbar)^{-n}\int (A * F^{-1}\Phi)(z)W\psi(z)d^{2n}z,\end{aligned}$$

that is, using the Plancherel formula and Equation (22) and recalling that $W\psi$ is real,

$$\begin{aligned}\langle \mathrm{Op}^{\mathrm{BJ}}(A)\rangle &= (2\pi\hbar)^{-n}\int F(A * F^{-1}\Phi)(z)FW\psi(z)d^{2n}z \\ &= \int FA(z)F(F^{-1}\Phi)(z)FW\psi(z)d^{2n}z \\ &= (2\pi\hbar)^{-n}\int FA(z)(F^{-1}\Phi * W\psi)(z)d^{2n}z\end{aligned}$$

which is Equation (25). □

That $W^{\Phi}\psi$ is a quasi-distribution [13,17] is clear: (i) $W^{\Phi}\psi$ is real because $W\psi$ is real and so is $F^{-1}\Phi$ (since $\Phi(-z) = \Phi(z)$); (ii) $W^{\Phi}\psi$ is normalized $W\psi \in L^1(\mathbb{R}^n)$ and $||W\psi||_{L^1} = 1$; then, using Equation (22),

$$\begin{aligned}\int W^{\Phi}\psi(z)d^{2n}z &= (2\pi\hbar)^{-n}\int (W\psi * F^{-1}\Phi)(z)d^{2n}z \\ &= F(W\psi * F^{-1}\Phi)(0) \\ &= (2\pi\hbar)^nFW\psi(0)\Phi(0) = 1,\end{aligned}$$

since $(2\pi\hbar)^nFW\psi(0) = ||W\psi||_{L^1} = 1$ and $\Phi(0) = 1$; (iii) $W^{\Phi}\psi$ satisfies the marginal conditions if $\psi, F\psi \in L^2(\mathbb{R}^n)\cap L^1(\mathbb{R}^n)$:

$$\int W^{\Phi}\psi(z)d^np = |\psi(x)|^2 \ , \ \int W^{\Phi}\psi(z)d^nx = |F\psi(p)|^2 \tag{27}$$

(see [14,17]). The quasi-distribution $W^{\Phi}\psi$ is a particular case of the so-called Cohen class [13,14,17,18], whose elements are characterized by Galilean invariance.

4. The Dirac Correspondence

Let us call "quantization rule" any pseudo-differential calculus

$$\mathrm{Op} : \mathcal{S}'(\mathbb{R}^{2n}) \longrightarrow \mathcal{L}(\mathcal{S}(\mathbb{R}^n), \mathcal{S}'(\mathbb{R}^n)).$$

having the following properties:

(Q1) We have $[\mathrm{Op}(x_j), \mathrm{Op}(p_k)] = i\hbar\delta_{jk}$ for $1 \leq j, k \leq n$;
(Q2) $\mathrm{Op}(1) = I_{\mathrm{d}}$ (the identity operator on $\mathbb{R}^n$);
(Q3) When A is real, $\mathrm{Op}(A)$ is a symmetric operator defined on $\mathcal{S}(\mathbb{R}^n)$;
(Q4) For $U, T \in \mathcal{S}'(\mathbb{R}^n)$, we have $\mathrm{Op}(U \otimes I_{\mathrm{d}})\psi = U\psi$ and $\mathrm{Op}(I_{\mathrm{d}} \otimes T)\psi = F^{-1}(TF\psi)$.

We will write (Q4) as $\mathrm{Op}(U \otimes I_{\mathrm{d}}) = U(\widehat{x})$ and $\mathrm{Op}(I_{\mathrm{d}} \otimes T) = T(\widehat{p})$. Both Weyl and Born–Jordan quantization satisfy these axioms.

The set of Axioms (Q1)–(Q4) is by no means the only possibility for defining a "quantization"; neither are these axioms minimal. Other definitions abound in the literature: See Twareque Ali and Englis [19] for a detailed discussion of the compatibility of various sets of quantization axioms.

In [20], the physicist Dirac suggested that to the Poisson bracket $\{A, B\}$ should correspond, under quantization, the commutator $[\widehat{A}, \widehat{B}] = \widehat{A}\widehat{B} - \widehat{B}\widehat{A}$ (up to a constant). A celebrated "no-go" result, due to Groenewold [21] and improved by van Hove [22,23], however, implies that there exists no quantization Op such that the correspondence

$$\mathrm{Op}(\{A, B\}) = \frac{1}{i\hbar}[\mathrm{Op}(A), \mathrm{Op}(B)] \tag{28}$$

holds for general symbols A and B. They showed, in fact, that Equation (28) cannot hold if A and B are polynomials in x_j, p_k of degree ≥ 2. In fact, let $\mathcal{P}(2n)$ be the Poisson algebra of all polynomials on $\mathbb{R}^{2n}$. Then there exists no quantization Op satisfying Equation (28) outside the particular case of the maximal sub-algebra $\mathcal{P}_2(2n)$ of polynomials of degree at most 2. We refer to Gotay et al. [24] for a comprehensive analysis of obstruction results in quantization. Charles and Chernoff (see [25,26]) have, moreover, proven that there exists no quantization satisfying Equation (28) and such that $\mathrm{Op}(x_j) = x_j$, $\mathrm{Op}(p_j) = -i\hbar\partial/\partial x_j$ (and hence, a fortiori, Axiom (Q4)). It has, however, been shown in [2,3] that the Dirac correspondence holds for a vast class of symbols when one uses the Born–Jordan quantization. Let us begin with an elementary result which already contains the main idea:

Proposition 4. *Let r and s be integers ≥ 0. We have $[\widehat{x}_j{}^r, \widehat{p}_k{}^s] = 0$ for $j \neq k$ and*

$$[\widehat{x}_j{}^r, \widehat{p}_j{}^s] = i\hbar\,\mathrm{Op}^{\mathrm{BJ}}(\{x_j^r, p_j^s\}). \tag{29}$$

Proof. The case $j \neq k$ is trivial. Assume $j = k$. One easily proves by induction on r and s and by repeated use of the relations $[\widehat{x}_j, \widehat{p}_j] = i\hbar$ that

$$[\widehat{x}_j{}^{r+1}, \widehat{p}_j{}^{s+1}] = (s+1)i\hbar \sum_{k=0}^{r} \widehat{x}_j{}^{r-k}\widehat{p}_j{}^{s}\widehat{x}_j{}^{k}. \tag{30}$$

Equation (14), defining the Born–Jordan quantization of $x_j,^r\, p_j^s$ can hence be rewritten

$$\mathrm{Op}^{\mathrm{BJ}}(x_j^r p_j^s) = \frac{1}{i\hbar(r+1)(s+1)}[\widehat{x}_j{}^{r+1}, \widehat{p}_j{}^{s+1}]. \tag{31}$$

On the other hand, we have

$$\{x_j^{r+1}, p_j^{s+1}\} = (r+1)(s+1)x_j^r p_j^s, \tag{32}$$

hence Equation (29). $\square$

More generally, Proposition 5 was proven in [2,3].

Proposition 5. *Let the symbols $A, B \in \mathcal{O}_M(\mathbb{R}^{2n})$ be of the type*

$$A(x,p) = S(p) + U(x) \ , \ B(x,p) = T(p) + V(x) \tag{33}$$

and set $\widehat{A} = S(\widehat{p}) + U(\widehat{x})$, $\widehat{A} = T(\widehat{p}) + V(\widehat{x})$. We have

$$\mathrm{Op}^{\mathrm{BJ}}(\{A,B\}) = \frac{1}{i\hbar}[\widehat{A},\widehat{B}]. \tag{34}$$

Note that the condition $A, B \in \mathcal{O}_M(\mathbb{R}^{2n})$ holds when f and g belong to the space $\mathcal{O}_M(\mathbb{R}^n)$ of all C^∞ functions on $\mathbb{R}^n$ such that $|\partial_x^\alpha f(x)| \leq C_\alpha(1+|x|)^{m_\alpha}$; this is in particular the case when A and B are physical Hamiltonians of the type "kinetic energy $\frac{1}{2}p^2$ plus potential $U(x)$" as soon as the derivatives $\partial_x^\alpha U(x)$ are polynomially bounded. In addition, note that the Weyl and Born–Jordan quantizations of symbols of the type $A = S + U$ are identical since we have in both cases $\widehat{S} = S(\widehat{p})$ and $\widehat{U} = U(\widehat{x})$; the distinction between both quantizations only appears when one passes to the commutator of two such Hamiltonians, since we have

$$[\widehat{S}+\widehat{U}, \widehat{T}+\widehat{V}] = [\widehat{S},\widehat{V}] + [\widehat{U},\widehat{T}]$$

and, by Proposition 5,

$$\mathrm{Op}^{\mathrm{BJ}}(\{S,V\}) = \frac{1}{i\hbar}[\widehat{S},\widehat{V}] \ , \ \mathrm{Op}^{\mathrm{BJ}}(\{U,T\}) = \frac{1}{i\hbar}[\widehat{U},\widehat{T}].$$

5. Ehrenfest's Theorem: Schrödinger Picture

Let $A \in \mathcal{O}_M(\mathbb{R}^{2n})$ be real; interpreting A as a "classical observable", its average (or expectation value) with respect to a probability density ρ_0 on $\mathbb{R}^{2n}$ is, when defined,

$$\langle A \rangle_{\mathrm{cl}} = \int A(z)\rho_0(z)d^{2n}z. \tag{35}$$

The time evolution of $\langle A \rangle_{\mathrm{cl}}$ under the action of a Hamiltonian flow (f_t^H) is given by

$$\langle A \rangle_{\mathrm{cl},t} = \int A(z)\rho(z,t)d^{2n}z \tag{36}$$

where $\rho(z,t)$ is a solution of Liouville's equation

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} \ , \ \rho(\cdot, 0) = \rho_0. \tag{37}$$

It satisfies the equation (Royer [27])

$$\frac{d}{dt}\langle A \rangle_{\mathrm{cl},t} = \int \{A,H\}(z)\rho(z,t)d^{2n}z = \langle \{A,H\} \rangle_{\mathrm{cl},t}. \tag{38}$$

In the quantum case one proceeds as follows: Let $\widehat{A} = \mathrm{Op}^{\mathrm{W}}(A)$ be obtained from A by Weyl quantization, and $\widehat{\rho}_0$ be a density operator (i.e., a nonnegative operator with trace one); by definition

$$\langle \widehat{A} \rangle_{\mathrm{qu}}^{\mathrm{W}} = \int A(z)\rho_0(z)d^{2n}z \tag{39}$$

where ρ_0 is the Wigner distribution of $\widehat{\rho}_0$, that is $\widehat{\rho}_0 = (2\pi\hbar)^n \operatorname{Op}^{\mathrm{W}}(\rho_0)$. Replacing Liouville's Equation (37) with the Wigner equation

$$\frac{\partial \rho}{\partial t} = \{H, \rho\}_{\mathrm{M}} \ , \ \rho(\cdot, 0) = \rho_0 \tag{40}$$

we have the analogue of the classical Equation (36)

$$\langle \widehat{A} \rangle^{\mathrm{W}}_{\mathrm{qu},t} = \int A(z)\rho(z,t)d^{2n}z. \tag{41}$$

One shows (Royer [27], Messiah [1], V-19) that $\widehat{\rho}$ satisfies von Neumann's equation

$$\frac{\partial \widehat{\rho}}{\partial t} = \frac{1}{i\hbar}[\widehat{H}, \widehat{\rho}] \ , \ \widehat{\rho}(0) = \widehat{\rho}_0 \tag{42}$$

and that the time evolution of the quantum average $\langle \widehat{A} \rangle_{\mathrm{qu}}$ is given by

$$\frac{d}{dt}\langle \widehat{A} \rangle^{\mathrm{W}}_{\mathrm{qu},t} = \frac{1}{i\hbar}\langle [\widehat{A}, \widehat{H}] \rangle_{\mathrm{qu},t}.$$

Now comes the crucial point. We have, in view of Equation (7),

$$\frac{d}{dt}\langle \widehat{A} \rangle^{\mathrm{W}}_{\mathrm{qu},t} = \int \{A, H\}_{\mathrm{M}}(z)\rho(z,t)d^{2n}z,$$

where $\{A, H\}_{\mathrm{M}}$ is the Moyal bracket of A and H. However, in the Born–Jordan case we have a stronger result. Let us define the distribution

$$\rho^{\Phi} = (2\pi\hbar)^{-n}\rho * F^{-1}\Phi, \tag{43}$$

where F is the Fourier transform on $\mathbb{R}^{2n}$. Since a density operator is a convex sum of orthogonal projections on normalized vectors $\psi_j \in L^2(\mathbb{R}^n)$, we can always write

$$\rho = \sum_j \alpha_j W\psi_j \ , \ \alpha_j > 0 \ , \ \sum_j \alpha_j = 1,$$

hence, recalling Equation (26) of $W^{\Phi}\psi$

$$\rho^{\Phi} = \sum_j \alpha_j W^{\Phi}\psi_j \, , \alpha_j > 0 \ , \ \sum_j \alpha_j = 1.$$

It follows that the function ρ^{Φ} is real and normalized to one, as is ρ.

Proposition 6. *Let H and A both be of the type of Equation (33), that is $H = I_{\mathrm{d}} \otimes T + U \otimes I_{\mathrm{d}}$ and $A = I_{\mathrm{d}} \otimes S + V \otimes I_{\mathrm{d}}$, where S, T, U, V are smooth polynomially bounded functions. The average*

$$\langle \widehat{A} \rangle^{\mathrm{BJ}}_{\mathrm{qu},t} = \int A(z)\rho^{\Phi}(z,t)d^{2n}z$$

satisfies the time-evolution equation

$$\frac{d}{dt}\langle \widehat{A} \rangle^{\mathrm{BJ}}_{\mathrm{qu},t} = \int \{A, H\}(z)\rho^{\Phi}(z,t)d^{2n}z \tag{44}$$

provided that $\{A, H\}\rho \in L^1(\mathbb{R}^{2n})$.

Proof. This immediately follows from Equation (34) in Proposition 5 together with Equation (25) in Proposition 3. □

It immediately follows that the average of the moments are given, in the case $n=1$, by the relations

$$\frac{d}{dt}\langle\widehat{x}^k\rangle_{\mathrm{qu},t} = k\int x^{k-1}\partial_p H(z)\rho^{\Phi}(z,t)d^{2n}z \tag{45}$$

$$\frac{d}{dt}\langle\widehat{p}^k\rangle_{\mathrm{qu},t} = -k\int p^{k-1}\partial_x H(z)\rho^{\Phi}(z,t)d^{2n}z \tag{46}$$

for every $k\in\mathbb{N}$. Let us illustrate this on a simple example; consider the quartic oscillator Hamiltonian

$$H=\frac{1}{2}p^2+\lambda x^4.$$

Choose first $A=x^k$ ($k\geq 1$); we have $\{A,H\}=kx^{k-1}p$, hence Equation (44) yields

$$\frac{d}{dt}\langle\widehat{x}^k\rangle_{\mathrm{qu},t} = k\langle\widehat{x}^{k-1}\widehat{p}\rangle_{\mathrm{qu},t}$$

and this result is in perfect accord with the prediction obtained by Weyl theory since we have here

$$\{A,H\}_{\mathrm{M}} = kx^{k-1}p = \{A,H\}.$$

Choose now $A=p^k$. Then $\{A,H\}=-4\lambda kx^3p^{k-1}$ and hence

$$\frac{d}{dt}\langle\widehat{p}^k\rangle_{\mathrm{qu},t} = -4\lambda k\langle\widehat{x}^3\widehat{p}^{k-1}\rangle_{\mathrm{qu},t}.$$

This relation is different from that predicted by Weyl theory; in the latter we have

$$\{A,H\}_{\mathrm{M}} = -4\lambda kx^3p^{k-1} + \text{lower order terms} \neq \{A,H\}.$$

6. Ehrenfest's Theorem: Heisenberg Picture

The approach to Ehrenfest's theorem becomes much simpler if one uses the Heisenberg picture. In the latter the state is fixed, but the quantum observables vary in time. Defining $\widehat{A}(t)=(\widehat{U}_t^H)^*\widehat{A}\widehat{U}_t^H$ where $\widehat{U}_t^H=e^{-i\widehat{H}t/\hbar}$ is the evolution operator determined by the Hamiltonian operator $\widehat{H}$, we have

$$\frac{d}{dt}\widehat{A}(t) = -\frac{1}{i\hbar}[\widehat{H},\widehat{A}(t)].$$

Taking the average with respect to an arbitrary state $\widehat{\rho}$ we get

$$\langle\frac{d}{dt}\widehat{A}(t)\rangle_{\mathrm{qu}} = -\frac{1}{i\hbar}\langle[\widehat{H},\widehat{A}(t)]\rangle_{\mathrm{qu}}.$$

Assuming again that $\widehat{A}=S(\widehat{p})+U(\widehat{x})$, $\widehat{A}=T(\widehat{p})+V(\widehat{x})$ the commutator $[\widehat{H},\widehat{A}(t)]$ is the Born–Jordan quantization of the Poisson bracket $\{H,A\}$ so that we have

$$\frac{d}{dt}\mathrm{Op}^{\mathrm{BJ}}(A(t)) = -\frac{1}{i\hbar}\mathrm{Op}^{\mathrm{BJ}}(\{H,A\}).$$

7. Comments and Discussion

Expectation values are the objects in quantum physics that can be compared with the results of measurements [28] (this should be contrasted with the fact that the state function ψ (or ρ) is not directly observable). It would perhaps be possible to test the physical validity of our results experimentally; one could consider for this purpose the Hamiltonians which occur in the study of spreading of a wavepacket passing through a nonlinear optical medium ("Kerr medium" [28]); such Hamiltonians are no longer of the classical type $\frac{1}{2}p^2 + U$ but contain quartic terms $p^4 + x^4$; our results thus immediately apply to them. There is also a strong obvious relation between the Moyal bracket and deformation quantization in flat space [29,30]; in [31–33] we have hinted at this relation using the notion of Bopp calculus, introduced by one of us in [34]. It would certainly be useful to develop these results from the point of view of the results presented here.

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References

1. Messiah, A. *Quantum Mechanics*; North–Holland Publ. Co.: Amsterdam, The Netherlands, 1991; Volume 1.
2. De Gosson, M. Bypassing the Groenewold–van Hove obstruction on: A new argument in favor of Born–Jordan quantization. *J. Phys. A Math. Theor.* **2016**, *49*, 39LT01. [CrossRef]
3. De Gosson, M.; Nicola, F. Born–Jordan pseudodifferential operators and the Dirac correspondence: Beyond the Groenewold–van Hove Theorem. *Bull. Sci. Math.* **2018**, *144*, 64–81. [CrossRef]
4. Kauffmann, S.K. Unambiguous quantization from the maximum classical correspondence that is self-consistent: The slightly stronger canonical commutation rule Dirac missed. *Found. Phys.* **2011**, *41*, 805–819. [CrossRef]
5. Bonet-Luz, E.; Tronci, C. Hamiltonian approach to Ehrenfest expectation values and Gaussian quantum states. *Proc. R. Soc. Lond. Ser. A* **2016**, *472*, 2015077. [CrossRef] [PubMed]
6. Moyal, J.E. Quantum mechanics as a statistical theory. *Proc. Camb. Philos. Soc.* **1949**, *45*, 99–124. [CrossRef]
7. Folland, G.B. *Harmonic Analysis in Phase Space*; Princeton University Press: Princeton, NJ, USA, 1989.
8. Voros, A. Asymptotic $\hbar$-expansions of stationary quantum states. *Ann. Inst. Henri Poincaré A* **1977**, *26*, 343–403.
9. Voros, A. An algebra of pseudodifferential operators and the asymptotics of quantum mechanics. *J. Funct. Anal.* **1978**, *29*, 104–132. [CrossRef]
10. Estrada, R.; Gracia-Bondia, J.M.; Várilly, J. On asymptotic expansions of twisted products. *J. Math. Phys.* **1989**, *30*, 2789–2796. [CrossRef]
11. Shubin, M.A. *Pseudodifferential Operators and Spectral Theory*; Springer: Berlin/Heidelberg, Germany, 1987.
12. Born, M.; Jordan, P. Zur Quantenmechanik. *Z. Phys.* **1925**, *34*, 858–888. [CrossRef]
13. Cohen, L. *The Weyl Operator and Its Generalization*; Springer Science & Business Media: Berlin/Heidelberg, Germany, 2012.
14. De Gosson, M. *Introduction to Born–Jordan Quantization: Theory and Applications*; series Fundamental Theories of Physics; Springer: Berlin/Heidelberg, Germany, 2016.
15. De Gosson, M. *Symplectic Methods in Harmonic Analysis and in Mathematical Physics*; Birkhäuser: Basel, Switzerland, 2011.
16. Littlejohn, R.G. The semiclassical evolution of wave pckets. *Phys. Rep.* **1986**, *138*, 193–291. [CrossRef]
17. Boggiatto, P.; de Donno, G.; Oliaro, A. Time-Frequency Representations of Wigner Type and Pseudo-Differential Operators. *Trans. Am. Math. Soc.* **2010**, *362*, 4955–4981. [CrossRef]
18. Cohen, L. *Time-Frequency Analysis*; Prentice-Hall: New York, NY, USA, 1995.
19. Ali, S.T.; Englis, M. Quantization Methods: A Guide for Physicists and Analysts. *Rev. Math. Phys.* **2005**, *17*, 391–490. [CrossRef]
20. Dirac, P.A.M. *Principles of Quantum Mechanics*; Oxford University Press: Oxford, UK, 1982.
21. Groenewold, H.J. On the principles of elementary quantum mechanics. *Physics* **1946**, *12*, 405–460.
22. Van Hove, L. Sur certaines représentations unitaires d'un group infini de transformations. *Proc. R. Acad. Sci. Belg.* **1951**, *26*, 1–102.
23. Van Hove, L. Sur le problème des relations entre les transformations unitaires de la mécanique quantique et les transformations canoniques de la mécanique classique. *Acad. R. Belg. Bull.* **1951**, *37*, 610–620.

24. Gotay, M.J.; Grundling, H.B.; Tuynman, G.M. Obstruction Results in Quantization Theory. *J. Nonlinear Sci.* **1996**, *6*, 469–498. [CrossRef]
25. Abraham, R.; Marsden, J. *Foundations of Mechanics*, 2nd ed.; The Benjamin/Cummings Publ. Company: San Francisco, CA, USA, 1978.
26. Plebanski, J.F.; Przanowski, M.; Tosiek, J. The Weyl–Wigner formalism II. The Moyal Bracket. *Acta Phys. Pol. B* **1996**, *27*, 1961–1990.
27. Royer, A. Ehrenfest's Theorem Reinterpreted and Extended with Wigner's Function. *Found. Phys.* **1992**, *22*, 727–736. [CrossRef]
28. George, L.T.; Sudheesh, C.; Lakshmibala, S.; Balakrishnan, V. Ehrenfest's theorem and nonclassical states of light. *Resonance* **2012**, *17*, 23–32. [CrossRef]
29. Bayen, F.; Flato, M.; Fronsdal, C.; Lichnerowicz, A.; Sternheimer, D. Deformation Theory and Quantization. I. Deformation of Symplectic Structures. *Ann. Phys.* **1978**, *111*, 6–110. [CrossRef]
30. Bayen, F.; Flato, M.; Fronsdal, C.; Lichnerowicz, A.; Sternheimer, D. Deformation Theory and Quantization. II Physical Applications. *Ann. Phys.* **1978**, *110*, 111–151. [CrossRef]
31. De Gosson, M.; Luef, F. A new approach to the $\star$-genvalue equation. *Lett. Math. Phys.* **2008**, *85*, 173–183. [CrossRef]
32. De Gosson, M.; Luef, F. Spectral and Regularity properties of a Pseudo-Differential Calculus Related to Landau Quantization. *J. Pseudo-Differ. Oper. Appl.* **2010**, *1*, 3–34. [CrossRef]
33. De Gosson, M.; Luef, F. Born–Jordan Pseudodifferential Calculus, Bopp Operators and Deformation Quantization. *Integr. Equ. Oper. Theory* **2016**, *84*, 463–485. [CrossRef]
34. De Gosson, M. Spectral Properties of a Class of Generalized Landau Operators. *Commun. Partial Differ. Oper.* **2008**, *33*, 2096–2104. [CrossRef]