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Harmonizing Classical and Quantum Mechanics: A semi-classical approach to quantum systems

Ashlin V Thomas

School of Physical Sciences National Institute of Science Education and Research

November 8, 2024



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School of Physical Sciences National Institute of Science Education and Research

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• State of the system : $(q_1, q_2, \dots, q_{3n}, p_1, p_2, \dots, p_{3n})$

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Hamiltonian Dynamics

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• State of the system : $(q_1, q_2, \cdots, q_{3n}, p_1, p_2, \cdots, p_{3n})$

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• Observables : $f(q_1, q_2, \dots, q_{3n}, p_1, p_2, \dots, p_{3n})$

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- State of the system : $(q_1, q_2, \cdots, q_{3n}, p_1, p_2, \cdots, p_{3n})$
- Observables : $f(q_1, q_2, \dots, q_{3n}, p_1, p_2, \dots, p_{3n})$

Weyl Transform

• Hamiltonian :

$$H(q, p, t) = \sum_{k=1}^{3n} p_k \dot{q_k} - \mathcal{L}(q, \dot{q}, t)$$

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- State of the system : $(q_1, q_2, \cdots, q_{3n}, p_1, p_2, \cdots, p_{3n})$
- Observables : $f(q_1, q_2, \dots, q_{3n}, p_1, p_2, \dots, p_{3n})$

Weyl Transform

• Hamiltonian :

$$H(q, p, t) = \sum_{k=1}^{3n} p_k \dot{q_k} - \mathcal{L}(q, \dot{q}, t)$$

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For conservative systems,

$$H(q,p,t) = T(q,\dot{q}) + V(q,t)$$

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• Time Evolution :

$$\dot{q}_{k} = rac{\partial H}{\partial p_{k}} = \{q_{k}, H\}$$

 $\dot{p}_{k} = -rac{\partial H}{\partial q_{k}} = \{p_{k}, H\}$

where, $\{F, G\} = \sum_{i} \frac{\partial F}{\partial q_{i}} \frac{\partial G}{\partial p_{i}} - \frac{\partial F}{\partial p_{i}} \frac{\partial G}{\partial q_{i}}$ is called the Poisson bracket.

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Phase space formulation

Density Operators

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- Phase space coordinates : (q, p)
- Time evolution \implies Trajectories in phase space

Weyl Transform

• An Example : 1-D Simple Harmonic Oscillator

$$H=\frac{1}{2m}p^2+\frac{1}{2}kq^2$$

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• Ket vector :
$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \\ \psi_n \end{pmatrix}$$

where, n is called the dimension of the vector space.

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• Ket vector :
$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \end{pmatrix}$$

where, n is called the dimension of the vector space.

• Bra vector :
$$\langle \psi | = (\psi_1^* \ \psi_2^* \ \cdots \ \psi_n^*)$$

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• Ket vector :
$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \end{pmatrix}$$

where, n is called the dimension of the vector space.

- Bra vector : $\langle \psi | = \left(\psi_1^* \ \psi_2^* \ \cdots \ \psi_n^* \right)$
- Inner product :

$$\langle \phi | \psi \rangle = \begin{pmatrix} \phi_1^* \ \phi_2^* \ \cdots \ \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \\ \psi_n \end{pmatrix} = \sum_{k=1}^n \phi_k^* \psi_k$$

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- $\hat{A} \left| \psi \right\rangle = \left| \phi \right\rangle$
- Linearity :

$$\diamond \ \hat{A}(|\psi_1\rangle + |\psi_2\rangle) = \hat{A} |\psi_1\rangle + \hat{A} |\psi_2\rangle \diamond \ \hat{A}(c |\psi\rangle) = c \hat{A} |\psi\rangle$$

• Linear operator \longleftrightarrow Matrix In the basis $\{ |\phi_1\rangle, |\phi_2\rangle, \cdots, |\phi_n\rangle \}$, the matrix elements of \hat{A} are -

$$A_{ij} = \langle \phi_i | \hat{A} | \phi_j \rangle$$

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• State of the system : $|\psi
angle$ with $\langle\psi|\psi
angle=1$

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• Observables : Hermitian linear operators $(\hat{A}^*)^T = A$

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• Expectation values : $\langle A
angle = \langle \psi | \, \hat{A} \, | \psi
angle$

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- Expectation values : $\left< A \right> = \left< \psi \right| \hat{A} \left| \psi \right>$
- Time evolution : Schrödinger equation**

Density Operators

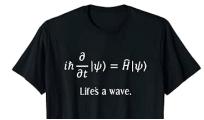
Introduction

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- State of the system : $|\psi\rangle$ with $\langle\psi|\psi\rangle=1$

Weyl Transform

- Observables : Hermitian linear operators $(\hat{A}^*)^T = A$
- Expectation values : $\langle A
 angle = \langle \psi | \, \hat{A} \, | \psi
 angle$
- Time evolution : Schrödinger equation**



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**Commonly found on t-shirts.

Density Operators

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• State of the system : $|\psi\rangle \longleftrightarrow \psi(\vec{r},t)$ with

Weyl Transform

$$\langle \psi | \psi
angle = \int d^3 x \; \psi^*(ec{r},t) \; \psi(ec{r},t) = 1$$

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• State of the system : $|\psi
angle \longleftrightarrow \psi(ec{r},t)$ with

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$$\langle \psi | \psi
angle = \int d^3 x \; \psi^*(ec{r},t) \; \psi(ec{r},t) = 1$$

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• Observables : Self-adjoint linear operators

$$\left\langle \hat{A}\phi \middle| \psi \right\rangle = \left\langle \phi \middle| \hat{A}\psi \right\rangle$$

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• State of the system : $|\psi
angle \longleftrightarrow \psi(\vec{r},t)$ with

Weyl Transform

$$\langle \psi | \psi
angle = \int d^3 x \; \psi^*(ec{r},t) \; \psi(ec{r},t) = 1$$

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• Observables : Self-adjoint linear operators

$$\left\langle \hat{A}\phi \middle| \psi \right\rangle = \left\langle \phi \middle| \hat{A}\psi \right\rangle$$

• Expectation values :

Density Operators

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$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \int d^3 x \ \psi^*(\vec{r},t) \ \hat{A} \ \psi(\vec{r},t)$$

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• State of the system : $|\psi
angle \longleftrightarrow \psi(\vec{r},t)$ with

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$$\langle \psi | \psi
angle = \int d^3 x \; \psi^*(ec{r},t) \; \psi(ec{r},t) = 1$$

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• Observables : Self-adjoint linear operators

$$\left\langle \hat{A}\phi \middle| \psi \right\rangle = \left\langle \phi \middle| \hat{A}\psi \right\rangle$$

• Expectation values :

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$$\langle A
angle = \langle \psi | \hat{A} | \psi
angle = \int d^3 x \; \psi^*(\vec{r},t) \; \hat{A} \; \psi(\vec{r},t)$$

• Time evolution : Schrödinger equation

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	Classical Mechanics	Quantum Mechanics
State of the system	Phase space variables	Ket states
Observables	Functions of phase space variables	Self-adjoint operators
Time Evolution	Trajectories in phase space (Hamilton's equations)	Schrödinger equation

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• Definition for pure state : $\hat{\rho} = \left|\psi\right\rangle \left\langle\psi\right|$



- Definition for pure state : $\hat{
 ho} = \left|\psi\right\rangle \left\langle\psi\right|$
- Hermiticity : $\hat{\rho}^{\dagger} = (\ket{\psi} \bra{\psi})^{\dagger} = \ket{\psi} \bra{\psi} = \hat{\rho}$

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- Definition for pure state : $\hat{\rho} = \left|\psi\right\rangle \left\langle\psi\right|$
- Hermiticity : $\hat{\rho}^{\dagger} = (\ket{\psi} \bra{\psi})^{\dagger} = \ket{\psi} \bra{\psi} = \hat{\rho}$

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• Trace normalisation : $Tr[\hat{\rho}] = 1$

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- Definition for pure state : $\hat{
 ho} = \left|\psi\right\rangle \left\langle\psi\right|$
- Hermiticity : $\hat{\rho}^{\dagger} = (\ket{\psi} \bra{\psi})^{\dagger} = \ket{\psi} \bra{\psi} = \hat{\rho}$

Weyl Transform

- Trace normalisation : $Tr[\hat{\rho}] = 1$
- Expectation value : $\langle A \rangle = Tr[\hat{\rho}\hat{A}]$

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- Definition for pure state : $\hat{\rho}=\left|\psi\right\rangle \left\langle\psi\right|$
- Hermiticity : $\hat{\rho}^{\dagger} = (\ket{\psi} \bra{\psi})^{\dagger} = \ket{\psi} \bra{\psi} = \hat{\rho}$

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- Trace normalisation : $Tr[\hat{\rho}] = 1$
- Expectation value : $\langle A \rangle = Tr[\hat{\rho}\hat{A}]$
- Definition for mixed states : $\hat{\rho} = \sum_{m} P_{m} \left| \psi_{m} \right\rangle \left\langle \psi_{m} \right|$

Density Operators

Introduction

- Definition for pure state : $\hat{\rho}=\left|\psi\right\rangle \left\langle\psi\right|$
- Hermiticity : $\hat{\rho}^{\dagger} = (\ket{\psi} \bra{\psi})^{\dagger} = \ket{\psi} \bra{\psi} = \hat{\rho}$

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- Trace normalisation : $Tr[\hat{\rho}] = 1$
- Expectation value : $\langle A \rangle = Tr[\hat{\rho}\hat{A}]$
- Definition for mixed states : $\hat{\rho} = \sum_{m} P_{m} \left| \psi_{m} \right\rangle \left\langle \psi_{m} \right|$

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Time evolution of density matrices

Density Operators

Liouville-von Neumann equation :

Weyl Transform

$$i\hbar \frac{\mathrm{d}\hat{
ho}}{\mathrm{d}t} = [\hat{H}, \hat{
ho}]$$

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Proof :

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Schrödinger equation :
$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

 $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$
 $i\hbar \frac{d}{dt}\rho(t) = \left(i\hbar \frac{d}{dt} |\psi(t)\rangle\right)\langle\psi(t)| + |\psi(t)\rangle\left(i\hbar \frac{d}{dt}\langle\psi(t)|\right)$
 $i\hbar \frac{d}{dt}\rho(t) = H\rho(t) - \rho(t)H = [H, \rho(t)]$

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• Operators \rightarrow Functions of phase space variables

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- Operators \rightarrow Functions of phase space variables
- Weyl transform of an operator \hat{A} is defined as -

$$\begin{split} \tilde{A}(x,p) &= \int dy \; \exp\left(-\frac{ipy}{\hbar}\right) \langle x + \frac{y}{2} \mid \hat{A} \mid x - \frac{y}{2} \rangle \\ &= \int du \; \exp\left(\frac{ixu}{\hbar}\right) \langle p + \frac{u}{2} \mid \hat{A} \mid p - \frac{u}{2} \rangle \end{split}$$

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• Examples :

$$\hat{1} \rightarrow 1$$

 $\hat{X} \rightarrow x$
 $\hat{P} \rightarrow p$
 $\hat{X}\hat{P} \rightarrow xp + \frac{i\hbar}{2}$

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• Examples :

$$\hat{1}
ightarrow 1$$

 $\hat{X}
ightarrow x$
 $\hat{P}
ightarrow p$
 $\hat{X}\hat{P}
ightarrow xp + rac{i\hbar}{2}$

But what about $\hat{P}\hat{X}$?

$$\hat{P}\hat{X} \to xp - rac{i\hbar}{2}$$

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• Examples :

$$\hat{1}
ightarrow 1$$

 $\hat{X}
ightarrow x$
 $\hat{P}
ightarrow p$
 $\hat{X}\hat{P}
ightarrow xp + rac{i\hbar}{2}$

But what about $\hat{P}\hat{X}$?

$$\hat{P}\hat{X} \to xp - \frac{i\hbar}{2}$$

$$Tr[\hat{A}\hat{B}] = \frac{1}{h} \int \int \tilde{A}(x,p)\tilde{B}(x,p) \, dx \, dp$$

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• Let us denote the weyl transform of \hat{A} as $\mathcal{W}(\hat{A})$. Then,

$$\mathcal{W}(\hat{A}\hat{B}) = \mathcal{W}(\hat{A}) \star \mathcal{W}(\hat{B})$$



Weyl-Groenewold-Moyal star product

Density Operators

• Let us denote the weyl transform of \hat{A} as $\mathcal{W}(\hat{A})$. Then,

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$$\mathcal{W}(\hat{A}\hat{B}) = \mathcal{W}(\hat{A}) \star \mathcal{W}(\hat{B})$$

where,

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$$f(x,p)\star g(x,p) = f(x,p) \exp\left(\frac{i\hbar}{2} (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)\right) g(x,p)$$

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Weyl-Groenewold-Moyal star product

Density Operators

• Let us denote the weyl transform of \hat{A} as $\mathcal{W}(\hat{A})$. Then,

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$$\mathcal{W}(\hat{A}\hat{B}) = \mathcal{W}(\hat{A}) \star \mathcal{W}(\hat{B})$$

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where,

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$$f(x,p)\star g(x,p) = f(x,p) \exp\left(\frac{i\hbar}{2} (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)\right) g(x,p)$$

• It is non-commutative and associative.

Weyl-Groenewold-Moyal star product

Density Operators

• Let us denote the weyl transform of \hat{A} as $\mathcal{W}(\hat{A})$. Then,

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$$\mathcal{W}(\hat{A}\hat{B}) = \mathcal{W}(\hat{A}) \star \mathcal{W}(\hat{B})$$

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where,

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$$f(x,p)\star g(x,p) = f(x,p) \exp\left(\frac{i\hbar}{2} (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)\right) g(x,p)$$

- It is non-commutative and associative.
- Moyal bracket OR \star -commutator : $[f,g]_{\star} = f \star g g \star f$

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- Wigner function : Analogue of wave function
- Weyl transform of density operator

$$W(x,p) = \frac{1}{h} \int e^{-ipy/\hbar} \langle x + \frac{y}{2} | \hat{\rho} | x - \frac{y}{2} \rangle \, dy,$$

$$\implies W(x,p) = \frac{1}{h} \int e^{-ipy/\hbar} \langle x + \frac{y}{2} | \psi \rangle \, \langle \psi | \, x - \frac{y}{2} \rangle \, dy,$$

$$\implies W(x,p) = \frac{1}{h} \int e^{-ipy/\hbar} \, \psi \left(x + \frac{y}{2} \right) \, \psi^* \left(x - \frac{y}{2} \right) \, dy.$$

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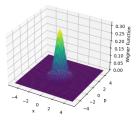
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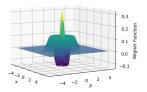
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Wigner Function of the Ground State of a Harmonic Oscillator



Wigner Function of the Second Excited State of a Harmonic Oscillator



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(a) Ground state (b) Second excited state

Figure 1: Wigner functions for different states of the quantum harmonic oscillator

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- Real valued function
- Quasi-probability distribution
- Normalization :

$$\int \int W(x,p)\,dx\,dp=1$$

• Marginal distributions :

$$\int W(x,p) dp = \psi^*(x)\psi(x) = |\psi(x)|^2$$
$$\int W(x,p) dx = \psi^*(p)\psi(p) = |\psi(p)|^2$$

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• Expectation values :

$$\langle \hat{A}
angle = \int \int W(x,p) \, ilde{A}(x,p) \, dx \, dp$$

• Orthogonality :

$$\int \int W_{a}(x,p) W_{b}(x,p) \, dx \, dp = \frac{1}{h} |\langle \psi_{a} | \psi_{b} \rangle|^{2}$$

• Bound on the distribution :

$$|W(x,p)| \leq \frac{2}{h}$$

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$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{1}{i\hbar} [H, W]_{\star}$$

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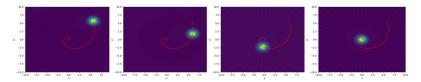


Figure 2: Time evolution of Wigner function for a dissipative quantum system

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$$\lim_{\hbar \to 0} \frac{1}{i\hbar} [f,g]_{\star} = \{f,g\}$$

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$$\lim_{\hbar \to 0} \frac{1}{i\hbar} [f,g]_{\star} = \{f,g\}$$

• Hence, in the classical limit wigner function evolves as-

$$\frac{\partial W}{\partial t} = \{H, W\}$$

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• Does this really work??

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• Does this really work??

 $\diamond\,$ Wigner function being negative in regions of phase space.





• Does this really work??

◊ Wigner function being negative in regions of phase space.

 \diamond Dependence of spread of distribution on \hbar .

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• Does this really work??

♦ Wigner function being negative in regions of phase space.
 ♦ Dependence of spread of distribution on ħ.

$$f \star g = fg + \frac{i\hbar}{2} \{f, g\}$$
$$-\frac{\hbar^2}{8} \left(\frac{\partial^2 f}{\partial x^2} \frac{\partial^2 g}{\partial p^2} + \frac{\partial^2 f}{\partial p^2} \frac{\partial^2 g}{\partial x^2} - 2 \frac{\partial^2 f}{\partial x \partial p} \frac{\partial^2 g}{\partial x \partial p} \right) + \mathcal{O}(\hbar^3)$$

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• Wigner and Weyl presents a completely equivalent formulation of quantum mechanics in phase space, with its own strange features.



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- "It is the way in which physical results are extracted, using not only the Wigner function, but also the Weyl transform of the desired operator and the star product algebra, which accounts for the quantum behaviour."^[1]



- Wigner and Weyl presents a completely equivalent formulation of quantum mechanics in phase space, with its own strange features.
- It naturally incorporates mixed states in it.
- "It is the way in which physical results are extracted, using not only the Wigner function, but also the Weyl transform of the desired operator and the star product algebra, which accounts for the quantum behaviour."^[1]
- "In some other part of the universe, wigner-weyl approach might be the method of doing quantum mechanics discovered first."^[2]

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