Wigner Quantum Mechanics : A phase space formalism

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June, 3, 2025

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M2 PhyQS

QMat YIG Symposium

QMat QUANTUM SCIENCE AND NANOMATERIALS

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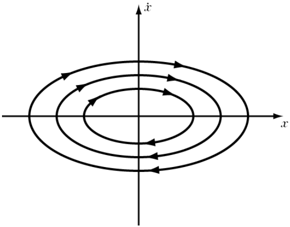
What we know :

- Classical mechanics
- Schrödinger quantum mechanics

What we want :

- Express quantum mechanics in phase space
- Study the quantum-classical correspondence



A bit of history

Foundations (~ 1930) :

Figure 1 – Hermann Weyl (1885-1955)

Figure 2 – Eugene Wigner (1902-1995)

Weyl quantization

Phase space variables

$\Updownarrow$

Weyl (symmetric) ordered observables

Quantum corrections to classical thermodynamic

$\Updownarrow$

Wigner function and Wigner map

Full description (End of WW2) :

Figure 3 – Hildebrand Groenewold (1910 - 1996)

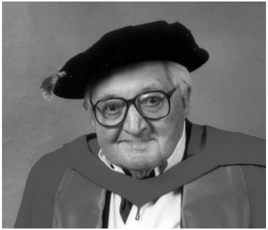


Figure 4 – Jose Enrique Moyal (1910 - 1998)

Creation in parallel of the same theory of phase space quantum mechanics gathering Weyl quantization and Wigner map

Wigner-Weyl transform

Opposition :

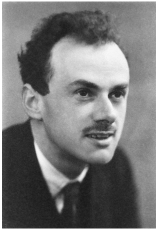


Figure 5 – Paul Adrien Maurice Dirac (1902-1984)

"I think it is obvious that there cannot be any distribution function $F(p, q)$ which would give correctly the mean value of any $f(p, q)$ ..." (1945)

E. Wigner did it in 1932

(Wigner = Dirac's brother-in-law)

Never changed opinion

"[vN density operator] existence is rather surprising in view of the fact that phase space has no meaning in quantum mechanics, there being no possibility of assigning numerical values simultaneously to the q's and p's."

"I think your kind of work would be valuable only if you can put it in a very neat form."

Reminder of classical mechanics

System described by an Hamiltonian :

$$H(x,p)$$

Time evolution :

$$\frac{\mathrm{d}\Omega}{\mathrm{d}t} = \{\Omega, H\}$$

Quantum-classical correspondence :

$$\{\,,\,\} \sim [\,,\,]$$

Classical-quantum difference ?

Take :

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1, x_2)$$

Then :

$$\begin{aligned}\frac{\mathrm{d}x_1 p_2}{\mathrm{d}t} &= p_2 \frac{p_1}{m} - x_1 \frac{\partial V}{\partial x_2} \\ &= p_2 \dot{x}_1 + x_1 \dot{p}_2\end{aligned}$$

No supplementary information

Phase space variables remain **factorized**

Phase-point operators :

$$\hat{A}(x,p) = \int_{\mathbb{R}} \mathrm{d}y \, e^{\frac{i}{\hbar}py} \left| x + \frac{y}{2} \right\rangle \left\langle x - \frac{y}{2} \right|$$

Hilbert space $L^2(\mathbb{R})$

Operators $\hat{\Omega}(\hat{x},\hat{p})$

$\Longleftrightarrow$

Phase space Γ

Weyl symbols $\Omega_W(x,p)$

Weyl quantization

$$\hat{\Omega}(\hat{x},\hat{p}) = \iint_{\mathbb{R}^2} \mathrm{d}x\mathrm{d}p \, \Omega_W(x,p)\hat{A}(x,p)$$

Wigner transform

$$\Omega_W(x,p) = \frac{1}{2\pi\hbar} \operatorname{Tr}\left(\hat{\Omega}(\hat{x},\hat{p})\hat{A}(x,p)\right)$$

Properties for a good transform :

$$\operatorname{Tr}\Big(\hat{A}(x,p)\Big) = 1, \; \operatorname{Tr}\Big(\hat{A}(x,p)\hat{A}(x',p')\Big) = 2\pi\hbar\delta(x-x')\delta(p-p')$$

Weyl-Wigner transform

Examples :

$$\hat{n} = \frac{1}{2}(\hat{x}^2 + \hat{p}^2 - 1) \implies n_W = \frac{1}{2}(x^2 + p^2 - 1)$$

$$\hat{x}\hat{p} \implies xp + \frac{i\hbar}{2}$$

Easier transform : **Bopp operators**

$$\hat{x} \to x + \frac{i\hbar}{2}\overrightarrow{\partial_p},\ \hat{p} \to p - \frac{i\hbar}{2}\overrightarrow{\partial_x}$$

$\hbar \to 0$: recovery of the classical limit

Respect of commutation relations :

$$[\hat{x}, \hat{p}] = \left(x + \frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\left(p + \frac{i\hbar}{2}\frac{\partial}{\partial x}\right) - \left(p + \frac{i\hbar}{2}\frac{\partial}{\partial x}\right)\left(x + \frac{i\hbar}{2}\frac{\partial}{\partial p}\right) = i\hbar$$

Generalization to many particles

Phase-point operators :

$$\hat{A}(\mathbf{x},\mathbf{p}) = \bigotimes_{i=1}^{N} \hat{A}(x_i, p_i)$$

Weyl quantization

$$\hat{\Omega}(\hat{\mathbf{x}},\hat{\mathbf{p}}) = \iint_{\mathbb{R}^2} \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{p}\,\Omega_W(\mathbf{x},\mathbf{p})\hat{A}(\mathbf{x},\mathbf{p})$$

Wigner transform

$$\Omega_W(x,p) = \frac{1}{(2\pi\hbar)^N}\,\mathrm{Tr}\left(\hat{\Omega}(\hat{\mathbf{x}},\hat{\mathbf{p}})\hat{A}(\mathbf{x},\mathbf{p})\right)$$

Projection properties :

$$\frac{1}{2\pi\hbar}\int \mathrm{d}p_j\,\hat{A}(\mathbf{x},\mathbf{p}) = |x_j\rangle\langle x_j| \otimes \left(\bigotimes_{i\neq j}^{N} \hat{A}(x_i,p_i)\right),$$

$$\frac{1}{2\pi\hbar}\int \mathrm{d}x_j\,\hat{A}(\mathbf{x},\mathbf{p}) = |p_j\rangle\langle p_j| \otimes \left(\bigotimes_{i\neq j}^{N} \hat{A}(x_i,p_i)\right)$$

Hilbert space		Phase space
Density matrix $\hat{\rho}$	$\Longleftrightarrow$	Wigner function $W(x,p)$

$$W(x,p) = \frac{1}{2\pi\hbar}\int \mathrm{d}y \, \left\langle x - \frac{y}{2}\middle|\hat{\rho}\middle|x + \frac{y}{2}\right\rangle$$

Important properties :

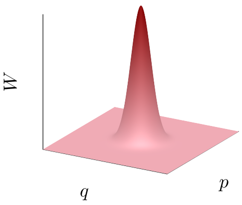
$$\int \mathrm{d}x\mathrm{d}p \, W(x,p) = \mathrm{Tr}(\rho) = 1$$

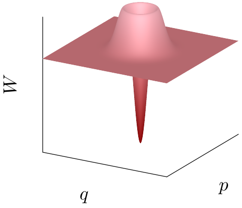
$$\int \mathrm{d}p \, W(x,p) = \langle x|\hat{\rho}|x\rangle \, , \int \mathrm{d}x \, W(x,p) = \langle p|\hat{\rho}|p\rangle$$

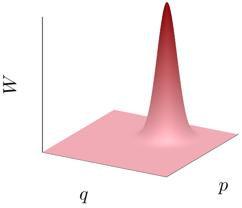
Integration measure in phase space :

$$\left\langle \hat{\Omega} \right\rangle = \int \mathrm{d}x\mathrm{d}p \, W(x,p)\Omega_W(x,p)$$

Example : Harmonic Oscillator







$$\rho = |0\rangle\langle 0| \implies W = \frac{1}{\pi\hbar} e^{-(x^2+p^2)}$$

$$\rho = |1\rangle\langle 1| \implies W = -\frac{1}{\pi\hbar} e^{-(x^2+p^2)}(1 - 2(x^2 + p^2))$$

$$\rho = |\alpha\rangle\langle \alpha| \implies W = \frac{1}{\pi\hbar} e^{-((x-\sqrt{2}\Re(\alpha))^2+(p-\sqrt{2}\Im(\alpha))^2)}$$

Uncertainty principle : $\sigma_x \sigma_p = \frac{1}{2}$ for Gaussian states

Hilbert space

Heisenberg equation

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

Liouville-von Neumann equation

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

$$\Longleftrightarrow$$

Phase space

Moyal equation

$$\frac{\mathrm{d}\Omega_W}{\mathrm{d}t} = \frac{i}{\hbar}\{\{H_W, \Omega_W\}\}$$

Liouville-von Neumann-Wigner equation

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{i}{\hbar}\{\{W, H_W\}\}$$

$$\{\{A, B\}\} = \frac{2}{\hbar} A \sin\left(\frac{\hbar}{2}\left(\overleftrightarrow{\partial_x \partial_p} - \overleftrightarrow{\partial_p \partial_x}\right)\right) B$$

Classical limit = Classical mechanics

$$\{\{A, B\}\} = \{A, B\} + \mathcal{O}(\hbar^2)$$

Let :

$$\hat{H} = \frac{\hat{p}^2}{2m} + V\hat{x}^3$$

Quantum phase space :

$$\frac{\mathrm{d}p^3}{\mathrm{d}t} = -9Vx^2p^2 + \frac{3}{2}V\hbar^2$$

Classical phase space :

$$\frac{\mathrm{d}p^3}{\mathrm{d}t} = -9Vx^2p^2$$

Weyl symbols do not factorize

$\Downarrow$

Quantum part in the equation of motion

Truncated Wigner Approximation

Neglect the quantum part

Then :

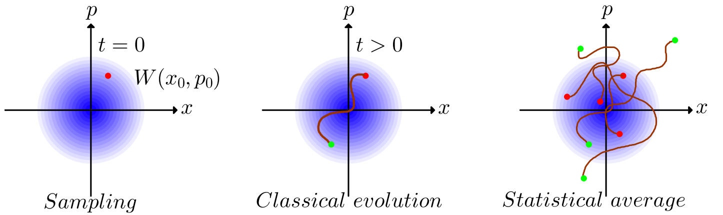
$$\frac{\mathrm{d}W}{\mathrm{d}t} = \{W, H_W\}$$

$$\{\{\,,\,\}\} \rightarrow \{\,,\,\}$$

Liouville equation !

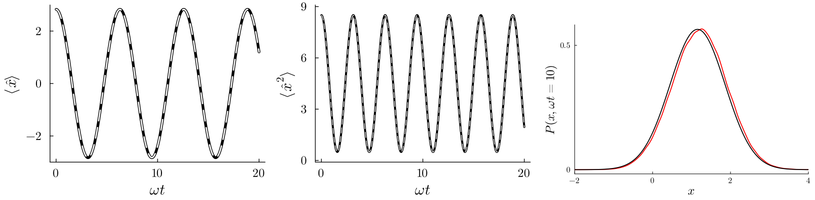
Conservation of the volume in phase space along trajectories

$$\langle \hat{\Omega} \rangle = \int \mathrm{d}x\mathrm{d}p\, W(x(0), p(0), (0))\Omega_W(x, p)$$

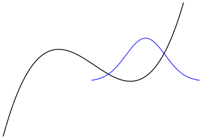


Exact for harmonic oscillator

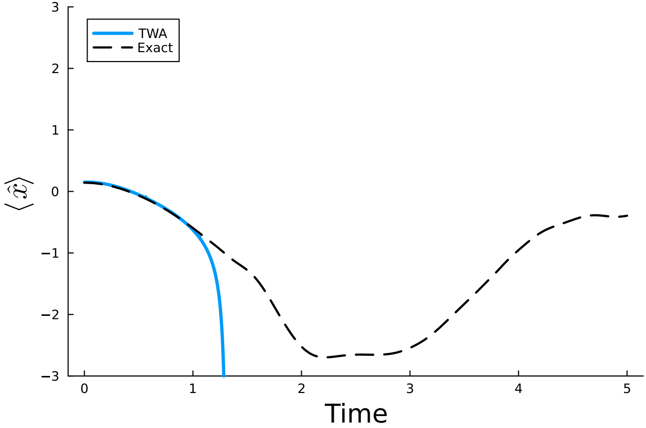
$$V(x) = \frac{1}{2}\omega^2 x^2$$



Anharmonic oscillator

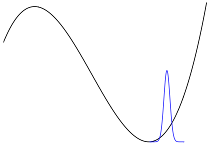


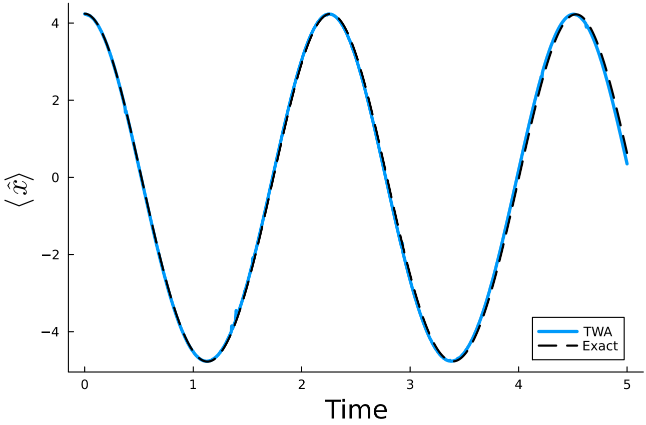
$$V(x) = x^3 + x^2$$



Anharmonic oscillator

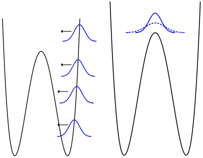
$$V(x) = 0.1x^3 + 4x^2$$

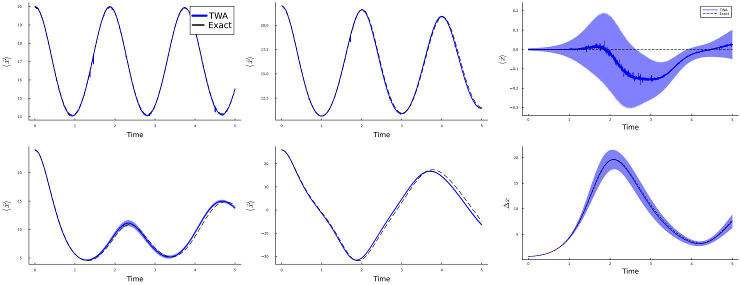


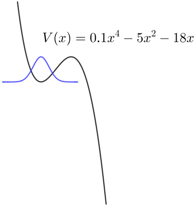


Quartic potential

$$V(x) = 0.005x^4 - 3x^2$$

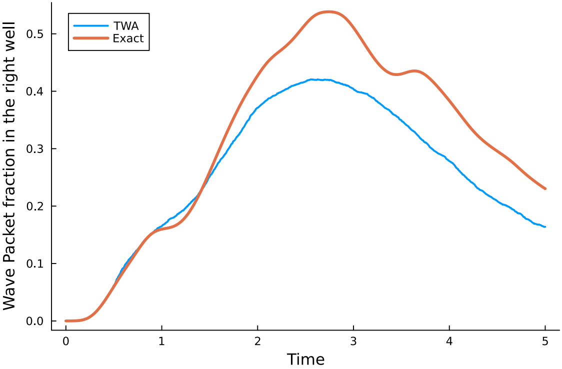






Quartic potential

$$V(x) = 0.1x^4 - 5x^2 - 18x$$



Reconstruction of the density matrix/Wigner function :

- Measurements on an ensemble of identical quantum states
- Measured operators must form a basis on the Hilbert space
- Easy for discrete systems
- Hard for continuous systems (homodyne tomography)

Example : Two-level system

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 + s_z & s_x - is_y \\ s_x + is_y & 1 - s_z \end{pmatrix}.$$

Single-qubit Pauli measurements : z measurement then H gate and x measurement then P+H gates and y measurement

Use : quantum computing, quantum information theory (determine actual state of quibts), quantum optics (state of signals)

Integration of W over any line $\alpha x + \beta p \implies$ distribution for $\alpha\hat{x} + \beta\hat{p}$

Cannot measure over usual phase space lines in experiments...

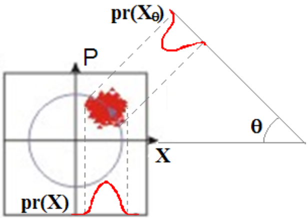
$\Downarrow$

Measurements over rotated directions $\implies W(q, \theta)$

$\Downarrow$

Radon transform $\implies W(q, p)$

$$\left(\begin{array}{c} \Downarrow \\ \text{Weyl quantization} \implies \hat{\rho} \end{array} \right)$$



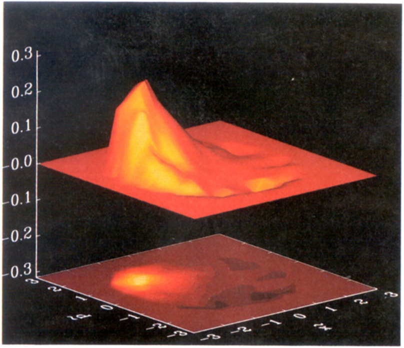


Figure 6 – Experimental reconstruction of a classical-like coherent state of a harmonic oscillator [3]

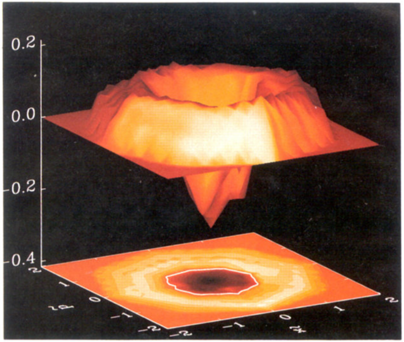


Figure 7 – Experimental reconstruction of the first excited energy eigenstate of a harmonic oscillator [3]

A unique phase space?

Normal order $\hat{a}^\dagger \hat{a} \implies$ Glauber-Sudarshan P distribution

$$P(\alpha, \alpha^*) = \frac{1}{\pi^2} \int \mathrm{d}\beta \mathrm{d}\beta^* \ \mathrm{Tr}\left(\hat{\rho} e^{i\beta^* \hat{a}^\dagger} e^{i\beta \hat{a}}\right) e^{-i\beta^* \alpha^* - i\beta\alpha}$$

Anti-normal order $\hat{a}\hat{a}^\dagger \implies$ Husimi Q distribution

$$Q(\alpha, \alpha^*) = \frac{1}{\pi^2} \int \mathrm{d}\beta \mathrm{d}\beta^* \ \mathrm{Tr}\left(\hat{\rho} e^{i\beta \hat{a}} e^{i\beta^* \hat{a}^\dagger}\right) e^{-i\beta^* \alpha^* - i\beta\alpha}$$

Symmetric order $\hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger \implies$ Wigner W distribution

$$W(\alpha, \alpha^*) = \frac{1}{\pi^2} \int \mathrm{d}\beta \mathrm{d}\beta^* \ \mathrm{Tr}\left(\hat{\rho} e^{i\beta \hat{a} + i\beta^* \hat{a}^\dagger}\right) e^{-i\beta^* \alpha^* - i\beta\alpha}$$

Still an open question

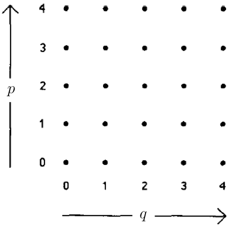
A phase space is easily defined in dimension N :

$$(q, p) \in [\![0, N-1]\!]^2$$

From discrete position and momentum basis :

$$|q\rangle \, , \; q \in [\![0, N-1]\!], \;\; |p\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} e^{\frac{2i\pi}{N} qp} \, |q\rangle$$

Problem : the transform is not unique for all N



Conclusion

A powerful framework to :

- Understand quantum-classical correspondence
- Compute quantum dynamics
- Determine the state of a system

A lot of links with **Path Integrals** !

Still needs development for the discrete phase space

Thank you for your attention !

References

[1] A. Polkovnikov, Phase space representation of quantum dynamics, Annals of Physics, 325(8) :1790-1852, (2010).

[2] C. Zachos, D. Fairlie and T. Curtright. A concise treatise on quantum mechanics in phase space. World Scientific, 12 (2016).

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[4] W. K. Wooters. A Wigner-Function Formulation of Finite-State Quantum Mechanics. Annals of Physics 176. 1-21 (1987)