

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

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- ② Density Operators
- ③ Weyl Transform
- ④ Wigner Functions
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Quantum Mechanics: An overview

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2 Density Operators

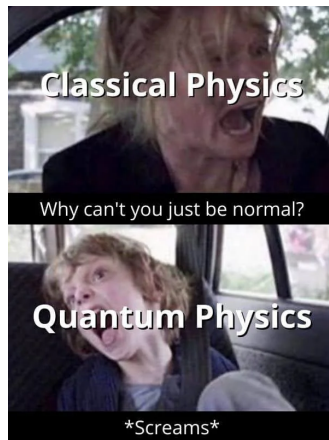
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Motivation



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Hamiltonian Dynamics

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For conservative systems,

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

Hamiltonian Dynamics (continued)

- Time Evolution :

$$\dot{q}_k = \frac{\partial H}{\partial p_k} = \{q_k, H\}$$

$$\dot{p}_k = -\frac{\partial H}{\partial q_k} = \{p_k, H\}$$

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.

Phase space formulation

- Phase space coordinates : (q, p)
- Time evolution \implies Trajectories in phase space
- **An Example** : 1-D Simple Harmonic Oscillator

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

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Bra-Ket Notation

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

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

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- **Inner product** :

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

Linear Operators

- $\hat{A}|\psi\rangle = |\phi\rangle$
- Linearity :
 - ◇ $\hat{A}(|\psi_1\rangle + |\psi_2\rangle) = \hat{A}|\psi_1\rangle + \hat{A}|\psi_2\rangle$
 - ◇ $\hat{A}(c|\psi\rangle) = c\hat{A}|\psi\rangle$
- Linear operator \longleftrightarrow Matrix
 In the basis $\{|\phi_1\rangle, |\phi_2\rangle, \dots, |\phi_n\rangle\}$, the matrix elements of \hat{A} are -

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

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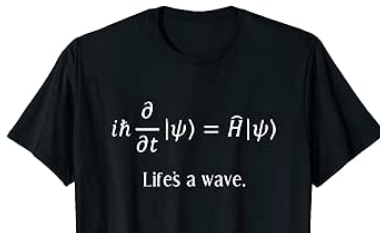
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***Commonly found on t-shirts.*

Describing an infinite dimensional quantum system

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Classical vs Quantum : Summary

	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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Time evolution of density matrices

Liouville-von Neumann equation :

$$i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}]$$

Proof :

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

$$\rho(t) = |\psi(t)\rangle \langle \psi(t)|$$

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

$$i\hbar \frac{d}{dt} \rho(t) = H \rho(t) - \rho(t) H = [H, \rho(t)]$$

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- Weyl transform of an operator \hat{A} is defined as -

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

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

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Weyl-Groenewold-Moyal star product

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

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

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Describing state of the system

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

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

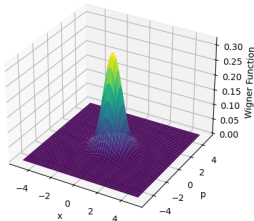
$$\implies W(x, p) = \frac{1}{h} \int e^{-ipy/\hbar} \langle x + \frac{y}{2} | \psi \rangle \langle \psi | x - \frac{y}{2} \rangle dy,$$

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

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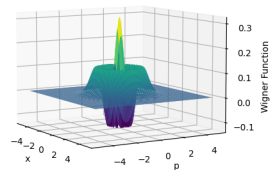
Examples

Wigner Function of the Ground State of a Harmonic Oscillator



(a) Ground state

Wigner Function of the Second Excited State of a Harmonic Oscillator



(b) Second excited state

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

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Properties

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

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

- Marginal distributions :

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

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

Properties (continued)

- Expectation values :

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

- 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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Time evolution of wigner function

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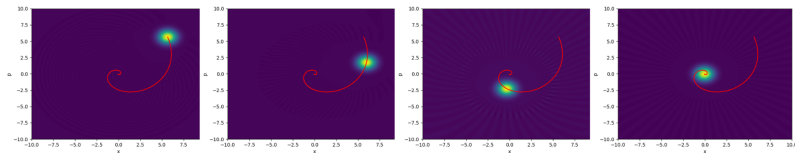


Figure 2: Time evolution of Wigner function for a dissipative quantum system

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Classical limit



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

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

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Summary

- 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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Thanks For Your Attention!!!
Any questions?