

Phase Space Quantum Mechanics

Canonical Regime

Part 1

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Classical Hamiltonian systems

Phase space

Phase space — a *Poisson manifold*, i.e. a smooth manifold M endowed with a two times contravariant antisymmetric tensor field \mathcal{P} (a *Poisson tensor*) satisfying the below relation

$$\mathcal{L}_{\zeta_f} \mathcal{P} = 0,$$

for every vector fields ζ_f (*Hamiltonian fields*) defined as

$$\zeta_f := \mathcal{P} df, \quad f \in C^\infty(M).$$

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Algebra of observables

Algebra of observables — an algebra $\mathcal{A}_C = C^\infty(M)$, with respect to a point-wise product, of all (complex valued) smooth functions on M .

Admissible observables

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Lie structure on $C^\infty(M)$

A *Poisson bracket*

$$\{f, g\}_{\mathcal{P}} := \mathcal{P}(df, dg), \quad f, g \in C^\infty(M)$$

introduces a structure of a Lie algebra on $C^\infty(M)$. Indeed, the Poisson bracket is a properly defined Lie bracket. In fact, it has the following properties

$$\begin{aligned} \{f, g\} &= -\{g, f\} && \text{(antisymmetry),} \\ \{f, gh\} &= \{f, g\}h + g\{f, h\} && \text{(Leibniz's rule),} \\ 0 &= \{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} && \text{(Jacobi's identity).} \end{aligned}$$

The algebra $C^\infty(M)$ endowed with the Poisson bracket is called a *Poisson algebra*.

Classical Hamiltonian system

Classical Hamiltonian system — a triple (M, \mathcal{P}, H) , where $H \in \mathcal{O}_C$ is some distinguished observable called a *Hamiltonian*.

Canonical coordinates

Local coordinates q^i, p_i ($i = 1, \dots, N$) in which a Poisson tensor \mathcal{P} have (locally) a form

$$\mathcal{P} = \frac{\partial}{\partial q^i} \wedge \frac{\partial}{\partial p_i} = \frac{\partial}{\partial q^i} \otimes \frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_i} \otimes \frac{\partial}{\partial q^i} \quad \text{i.e.} \quad \mathcal{P}^{ij} = \begin{pmatrix} 0_N & \mathbb{I}_N \\ -\mathbb{I}_N & 0_N \end{pmatrix}$$

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are called *canonical coordinates*.

In the canonical coordinates a Hamiltonian field ζ_f and a Poisson bracket take a form

$$\zeta_f = \frac{\partial f}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial f}{\partial q^i} \frac{\partial}{\partial p_i},$$

$$\{f, g\} = \frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i}.$$

Pure states, mixed states and expectation values of observables

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Mixed states

Mixed states — probability distribution functions defined on the phase space, i.e. functions $\rho \in C^\infty(M)$ such that

- $0 \leq \rho(\xi) \leq 1$ for $\xi \in M$,
- $\int_M \rho(\xi) d\xi = 1$.

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- $\int_M \rho(\xi) d\xi = 1$.

In this picture pure states can be defined as Dirac delta distributions, i.e.

$$\xi_0 \in M \longleftrightarrow \delta(\xi - \xi_0).$$

Expectation values of observables

Expectation value of observable $A \in \mathcal{A}_C$ in a state ρ :

$$\langle A \rangle_\rho := \int_M A(\xi) \rho(\xi) d\xi.$$

For a pure state $\rho(\xi) = \delta(\xi - \xi_0)$:

$$\langle A \rangle_\rho = \int_M A(\xi) \delta(\xi - \xi_0) d\xi = A(\xi_0).$$

Time evolution of classical Hamiltonian systems

The Hamiltonian H governs the time evolution of the system:

$$H \longrightarrow \zeta_H \longrightarrow \Phi_t^H$$

\implies

$$\xi(t + \Delta t) = \Phi_{\Delta t}^H(\xi(t))$$

$$\Updownarrow$$

$$\dot{\xi} = \zeta_H$$

$$\Updownarrow$$

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}$$

(Hamilton equations)

$$\rho(t) = (\Phi_{\Delta t}^H)^* \rho(t + \Delta t)$$

$$\Updownarrow$$

$$L(H, \rho) := \frac{\partial \rho}{\partial t} - \{H, \rho\} = 0$$

(Liouville equation)

For $\rho(\xi) = \delta(\xi - \xi_0)$ the Liouville equation induces the Hamilton equations.

Time dependent expectation value of observables

A time dependent expectation value of an observable $A \in \mathcal{A}_C$ in a state $\rho(t)$, i.e. $\langle A \rangle_{\rho(t)}$, fulfills the following equation of motion

$$\langle A \rangle_{L(H,\rho)} = 0 \iff \frac{d}{dt} \langle A \rangle_{\rho(t)} - \langle \{A, H\} \rangle_{\rho(t)} = 0.$$

Time development of observables

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Time development of $A \in \mathcal{A}_C$:

$$A(t) = U_t^H A(0) = e^{t\mathcal{L}_{\zeta_H}} A(0) = e^{t\zeta_H} A(0) \iff \frac{\partial A}{\partial t}(t) - \{A(t), H\} = 0.$$

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Both presented approaches to the time development yield equal predictions concerning the results of measurements:

$$\langle A(0) \rangle_{\rho(t)} = \langle A(t) \rangle_{\rho(0)}.$$

Basics of deformation quantization

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Quantization of the Poisson algebra of observables

Quantization of (M, \mathcal{P}) :

Deformation with respect to \hbar of the classical algebra of observables \mathcal{A}_C to some noncommutative quantum algebra of observables \mathcal{A}_Q , i.e.

$$\begin{aligned} \cdot &\longrightarrow \star, \\ \{\cdot, \cdot\} &\longrightarrow [|\cdot, \cdot|] = \frac{1}{i\hbar}[\cdot, \cdot], \end{aligned}$$

where $[\cdot, \cdot]$ is a \star -commutator.

\star -product

The deformed noncommutative multiplication on \mathcal{A}_Q should satisfy such natural conditions

- ① $f \star (g \star h) = (f \star g) \star h$ (associativity),
- ② $f \star g = fg + o(\hbar)$,
- ③ $[[f, g]] = \{f, g\} + o(\hbar)$,
- ④ $f \star 1 = 1 \star f = f$,
- ⑤ $f \star g = \sum_{k=0}^{\infty} \hbar^k B_k(f, g)$,

where $f, g, h \in \mathcal{A}_Q$ and $B_k: \mathcal{A}_Q \times \mathcal{A}_Q \rightarrow \mathcal{A}_Q$ are bilinear operators.

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From the construction of the \star -product it can be immediately seen that in the limit $\hbar \rightarrow 0$ the quantized algebra of observables reduces to the classical algebra of observables.

The bracket $[[\cdot, \cdot]]$ is a well-defined Lie bracket. In fact, it satisfies

$$[[f, g]] = -[[g, f]] \quad (\text{antisymmetry}),$$

$$[[f, g \star h]] = [[f, g]] \star h + g \star [[f, h]] \quad (\text{Leibniz's rule}),$$

$$0 = [[f, [[g, h]]]] + [[h, [[f, g]]]] + [[g, [[h, f]]]] \quad (\text{Jacobi's identity}).$$

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In this case

$$\mathcal{P} = \sum_{i=1}^N X_i \wedge Y_i = \sum_{i=1}^N (X_i \otimes Y_i - Y_i \otimes X_i),$$

where X_i, Y_i ($i = 1, \dots, N$) are some pair-wise commuting vector fields on M .

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Also

$$\begin{aligned} \{f, g\}_{\mathcal{P}} &= f \left(\sum_{i=1}^N (X_i \otimes Y_i - Y_i \otimes X_i) \right) g = f \left(\sum_{i=1}^N (\overleftarrow{X}_i \overrightarrow{Y}_i - \overleftarrow{Y}_i \overrightarrow{X}_i) \right) g \\ &= \sum_{i=1}^N (X_i(f) Y_i(g) - Y_i(f) X_i(g)). \end{aligned}$$

Space of states and properties of canonical $\star_{\sigma,\alpha,\beta}$ -products

In the rest of the presentation the case of $\star_{\sigma,\alpha,\beta}$ -products related to the canonical Poisson tensor $\mathcal{P} = \partial_x \wedge \partial_p$ on a manifold $M = \mathbb{R}^2$ will be considered.

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Canonical $\star_{\sigma,\alpha,\beta}$ -products

The $\star_{\sigma,\alpha,\beta}$ -product takes the form

$$\begin{aligned} f \star_{\sigma,\alpha,\beta} g &= f \exp \left(i\hbar \overleftarrow{\partial}_x \overrightarrow{\partial}_p - i\hbar \overleftarrow{\partial}_p \overrightarrow{\partial}_x + \hbar \alpha \overleftarrow{\partial}_x \overrightarrow{\partial}_x + \hbar \beta \overleftarrow{\partial}_p \overrightarrow{\partial}_p \right) g \\ &= \sum_{n,m,r,s=0}^{\infty} (-1)^m (i\hbar)^{n+m} \hbar^{r+s} \frac{\sigma^n \bar{\sigma}^m \alpha^r \beta^s}{n! m! r! s!} \\ &\quad \cdot (\partial_x^{n+r} \partial_p^{m+s} f) (\partial_x^{m+r} \partial_p^{n+s} g). \end{aligned}$$

Particular cases of the $\star_{\sigma,\alpha,\beta}$ -product

The well-known particular cases of the $\star_{\sigma,\alpha,\beta}$ -product are

- ① for $\sigma = \alpha = \beta = 0$, the Kupershmidt-Manin product,
- ② for $\sigma^{ij} = \frac{1}{2}\delta^{ij}$, $\alpha = \beta = 0$, the Moyal (or Groenewold) product

$$\begin{aligned} f \star_{\frac{1}{2}} g &= f \exp \left(\frac{1}{2} i \hbar (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x) \right) g \\ &= f \exp \left(\frac{1}{2} i \hbar \partial_x \wedge \partial_p \right) g. \end{aligned}$$

- ③ for $\sigma = \frac{1}{2}$, $\alpha = \frac{2\lambda-1}{2\omega}$, $\beta = \omega^2\alpha$ where $\omega, \lambda \in \mathbb{R}$ and $\omega > 0$

$$f \star g = f \exp \left(\hbar \lambda \overleftarrow{\partial}_a \overrightarrow{\partial}_{\bar{a}} - \hbar \bar{\lambda} \overleftarrow{\partial}_{\bar{a}} \overrightarrow{\partial}_a \right) g,$$

where the new coordinates $a(x, p) = (\omega x + ip)/\sqrt{2\omega}$,
 $\bar{a}(x, p) = (\omega x - ip)/\sqrt{2\omega}$ called *holomorphic coordinates* were used.

Theorem

Let $f, g \in \mathcal{A}_Q$ be such that $f \star_{\sigma,\alpha,\beta} g$ and $g \star_{\sigma,\alpha,\beta} f$ are integrable functions. Then there holds

$$\iint (f \star_{\sigma,\alpha,\beta} g)(x, p) dx dp = \iint (g \star_{\sigma,\alpha,\beta} f)(x, p) dx dp.$$

Moreover, for the Moyal \star -product (the case of $\sigma = \frac{1}{2}$ and $\alpha = \beta = 0$) there holds

$$\iint (f \star_{\frac{1}{2}} g)(x, p) dx dp = \iint f(x, p) g(x, p) dx dp.$$

Space of states

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It is possible to extend the \star_{σ} -product to the \star_{σ} -product between functions from $L^2(\mathbb{R}^2)$, as to make from $L^2(\mathbb{R}^2)$ a Hilbert algebra with respect to the \star_{σ} -multiplication.

Space of states for the general $\star_{\sigma,\alpha,\beta}$ -multiplication

For $\alpha \neq 0, \beta \neq 0$ the space of states for the general $\star_{\sigma,\alpha,\beta}$ -multiplication can be defined by

$$\mathcal{H} = S_{\alpha,\beta}(L^2(\mathbb{R}^2)).$$

where for appropriate $f \in L^2(\mathbb{R}^2)$:

$$S_{\alpha,\beta}f(x, p) = \frac{1}{2\pi\hbar\sqrt{\alpha\beta}} \iint f(x', p') e^{-\frac{1}{2\hbar\alpha}(x-x')^2} e^{-\frac{1}{2\hbar\beta}(p-p')^2} dx' dp'.$$

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The scalar product and the $\star_{\sigma,\alpha,\beta}$ -product on \mathcal{H} can be defined by

$$\begin{aligned}\langle \Psi | \Phi \rangle_{\mathcal{H}} &= \langle S_{\alpha,\beta}^{-1} \Psi | S_{\alpha,\beta}^{-1} \Phi \rangle_{L^2}, \quad \Psi, \Phi \in \mathcal{H}, \\ \Psi \star_{\sigma,\alpha,\beta} \Phi &= S_{\alpha,\beta}^{-1} \Psi \star_{\sigma} S_{\alpha,\beta}^{-1} \Phi, \quad \Psi, \Phi \in \mathcal{H}.\end{aligned}$$

Hence, \mathcal{H} is also a Hilbert algebra.

Theorem

The scalar product on \mathcal{H} can be written in a form

$$\langle \Psi | \Phi \rangle_{\mathcal{H}} = \iint (\mathcal{F}\Psi(\xi, \eta))^* \mathcal{F}\Phi(\xi, \eta) d\mu(\xi, \eta),$$

where

$$d\mu(\xi, \eta) = e^{\frac{1}{\hbar}\alpha\xi^2} e^{\frac{1}{\hbar}\beta\eta^2} d\xi d\eta.$$

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Theorem

For any function $A \in \mathcal{A}_Q$ there holds

$$\begin{aligned} A_L \star_{\sigma,\alpha,\beta} &= A_{\sigma,\alpha,\beta}(\hat{q}_{\sigma,\alpha}, \hat{p}_{\sigma,\beta}), \\ A_R \star_{\sigma,\alpha,\beta} &= A_{\sigma,\alpha,\beta}(\hat{q}_{\bar{\sigma},\alpha}^*, \hat{p}_{\bar{\sigma},\beta}^*), \end{aligned}$$

where

$$\begin{aligned} \hat{q}_{\sigma,\alpha} &:= x + i\hbar\sigma\partial_p + \hbar\alpha\partial_x = x_L \star_{\sigma,\alpha,\beta}, \\ \hat{p}_{\sigma,\beta} &:= p - i\hbar\bar{\sigma}\partial_x + \hbar\beta\partial_p = p_L \star_{\sigma,\alpha,\beta}, \end{aligned}$$

and

$$\begin{aligned} \hat{q}_{\bar{\sigma},\alpha}^* &:= x - i\hbar\bar{\sigma}\partial_p + \hbar\alpha\partial_x = x_R \star_{\sigma,\alpha,\beta}, \\ \hat{p}_{\bar{\sigma},\beta}^* &:= p + i\hbar\sigma\partial_x + \hbar\beta\partial_p = p_R \star_{\sigma,\alpha,\beta}. \end{aligned}$$

(σ, α, β) -ordered operator functions

The symbol $A_{\sigma,\alpha,\beta}(\hat{q}, \hat{p})$ denotes a (σ, α, β) -ordered operator function defined by

$$A_{\sigma,\alpha,\beta}(\hat{q}, \hat{p}) := A(-i\hbar\partial_\xi, i\hbar\partial_\eta) e^{\frac{i}{\hbar}(\xi\hat{q} - \eta\hat{p} + (\frac{1}{2} - \sigma)\xi\eta) + \frac{1}{2\hbar}(\alpha\xi^2 + \beta\eta^2)} \Big|_{\xi=\eta=0}.$$

Examples of operator functions

- For $A(x, p) = x^2 + p^2$

$$\begin{aligned}A_{\sigma,\alpha,\beta}(\hat{q}, \hat{p}) &= (\hat{q}^2 + \hat{p}^2)_{\sigma,\alpha,\beta} = \hat{q}^2 + \hat{p}^2 - \hbar\alpha - \hbar\beta \\ &= \hat{q}^2 + \hat{p}^2 + i(\alpha + \beta)\hat{q}\hat{p} - i(\alpha + \beta)\hat{p}\hat{q}.\end{aligned}$$

In particular, the case when $\alpha = \beta = 0$ gives

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$$(\hat{q}^2 + \hat{p}^2)_{\sigma,\alpha,\beta} = \hat{q}^2 + \hat{p}^2.$$

- For $A(x, p) = xp$

$$A_{\sigma,\alpha,\beta}(\hat{q}, \hat{p}) = (\hat{q}\hat{p})_{\sigma,\alpha,\beta} = \hat{q}\hat{p} - i\hbar\sigma = \bar{\sigma}\hat{q}\hat{p} + \sigma\hat{p}\hat{q}.$$

In particular, the case when $\sigma = 0, \frac{1}{2}, 1$ gives

$$(\hat{q}\hat{p})_{\sigma=0,\alpha,\beta} = \hat{q}\hat{p} \quad (\text{normal ordering}),$$

$$(\hat{q}\hat{p})_{\sigma=\frac{1}{2},\alpha,\beta} = \frac{1}{2}\hat{q}\hat{p} + \frac{1}{2}\hat{p}\hat{q} \quad (\text{Weyl ordering}),$$

$$(\hat{q}\hat{p})_{\sigma=1,\alpha,\beta} = \hat{p}\hat{q} \quad (\text{anti-normal ordering}).$$

Adjoint of $\star_{\sigma,\alpha,\beta}$ -multiplication

It is possible to introduce adjoint of left and right $\star_{\sigma,\alpha,\beta}$ -multiplication in a standard way

$$\langle (A_L \star_{\sigma,\alpha,\beta})^\dagger \Psi_1 | \Psi_2 \rangle_{\mathcal{H}} = \langle \Psi_1 | A_L \star_{\sigma,\alpha,\beta} \Psi_2 \rangle_{\mathcal{H}},$$

$$\langle (A_R \star_{\sigma,\alpha,\beta})^\dagger \Psi_1 | \Psi_2 \rangle_{\mathcal{H}} = \langle \Psi_1 | A_R \star_{\sigma,\alpha,\beta} \Psi_2 \rangle_{\mathcal{H}}.$$

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$$\langle (A_R \star_{\sigma,\alpha,\beta})^\dagger \Psi_1 | \Psi_2 \rangle_{\mathcal{H}} = \langle \Psi_1 | A_R \star_{\sigma,\alpha,\beta} \Psi_2 \rangle_{\mathcal{H}}.$$

From this it then follows that

$$(A_L \star_{\sigma,\alpha,\beta})^\dagger = A_{\sigma,\alpha,\beta}^\dagger(\hat{q}_{\sigma,\alpha}, \hat{p}_{\sigma,\beta}) = A_{\bar{\sigma},\alpha,\beta}^*(\hat{q}_{\sigma,\alpha}, \hat{p}_{\sigma,\beta}),$$

$$(A_R \star_{\sigma,\alpha,\beta})^\dagger = A_{\sigma,\alpha,\beta}^\dagger(\hat{q}_{\bar{\sigma},\alpha}^*, \hat{p}_{\bar{\sigma},\beta}^*) = A_{\bar{\sigma},\alpha,\beta}^*(\hat{q}_{\bar{\sigma},\alpha}^*, \hat{p}_{\bar{\sigma},\beta}^*).$$

Pure states, mixed states and expectation values of observables

Pure states

Pure states are functions $\Psi_{\text{pure}} \in \mathcal{H}$ which satisfy the following conditions

- ① $\Psi_{\text{pure}} \star_{\sigma,\alpha,\beta} = (\Psi_{\text{pure}} \star_{\sigma,\alpha,\beta})^\dagger$ (hermiticity),
- ② $\Psi_{\text{pure}} \star_{\sigma,\alpha,\beta} \Psi_{\text{pure}} = \frac{1}{\sqrt{2\pi\hbar}} \Psi_{\text{pure}}$ (idempotence),
- ③ $\|\Psi_{\text{pure}}\|_{\mathcal{H}} = 1$ (normalization).

Mixed states

Mixed states $\Psi_{\text{mix}} \in \mathcal{H}$ are defined as linear combinations of some families of pure states $\Psi_{\text{pure}}^{(\lambda)}$

$$\Psi_{\text{mix}} := \sum_{\lambda} p_{\lambda} \Psi_{\text{pure}}^{(\lambda)},$$

where $0 \leq p_{\lambda} \leq 1$ and $\sum_{\lambda} p_{\lambda} = 1$.

Quantum distribution functions

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$$\iint \rho(x, p) dx dp = 1.$$

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Marginal distributions

Marginal distributions

$$P(x) := \int \rho(x, p) dp, \quad P(p) := \int \rho(x, p) dx,$$

are probabilistic distribution functions.

Expectation value of observables

The expectation value of an observable $A \in \mathcal{A}_Q$ in an admissible state $\Psi \in \mathcal{H}$:

$$\langle A \rangle_{\Psi} = \iint (A \star_{\sigma,\alpha,\beta} \rho)(x, p) dx dp,$$

where

$$\rho = \frac{1}{\sqrt{2\pi\hbar}} \Psi.$$

Time evolution of quantum Hamiltonian systems

The time evolution of a quantum Hamiltonian system is governed by a Hamiltonian H . It will be assumed that $H \in \mathcal{O}_Q$ and that H is self-adjoint in \mathcal{H} , i.e. $H = H^*$ and $H_{L,R} \star_{\sigma,\alpha,\beta} = (H_{L,R} \star_{\sigma,\alpha,\beta})^\dagger$.

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Time evolution equation

The time evolution of a quantum distribution function ρ :

$$L(H, \rho) := \frac{\partial \rho}{\partial t} - [H, \rho] = 0$$

$$\Updownarrow$$

$$i\hbar \frac{\partial \rho}{\partial t} - [H, \rho] = 0.$$

Stationary states

Stationary states Ψ satisfy

$$[H, \Psi] = 0.$$

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For pure states the above equation is equivalent to a pair of $\star_{\sigma,\alpha,\beta}$ -genvalue equations

$$H \star_{\sigma,\alpha,\beta} \Psi = E\Psi, \quad \Psi \star_{\sigma,\alpha,\beta} H = E\Psi,$$

for some $E \in \mathbb{R}$.

The formal solution of the time evolution equation takes the form

$$\rho(t) = U(t) \star_{\sigma,\alpha,\beta} \rho(0) \star_{\sigma,\alpha,\beta} U(-t),$$

where

$$U(t) = e_{\star_{\sigma,\alpha,\beta}}^{-\frac{i}{\hbar}tH} := \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{i}{\hbar}t\right)^k \underbrace{H \star_{\sigma,\alpha,\beta} \dots \star_{\sigma,\alpha,\beta} H}_k$$

is an unitary function in \mathcal{H} as H is self-adjoint.

Time dependent expectation value

A time dependent expectation value of an observable $A \in \mathcal{A}_Q$ in a state $\rho(t)$, i.e. $\langle A \rangle_{\rho(t)}$, fulfills the following equation of motion

$$\langle A \rangle_{L(H, \rho)} = 0 \iff \frac{d}{dt} \langle A \rangle_{\rho(t)} - \langle [A, H] \rangle_{\rho(t)} = 0.$$

Time development of observables

The time development of $A \in \mathcal{A}_Q$:

$$A(t) = U(-t) \star_{\sigma,\alpha,\beta} A(0) \star_{\sigma,\alpha,\beta} U(t) \iff \frac{\partial A}{\partial t}(t) - [A(t), H] = 0.$$

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The time development of $A \in \mathcal{A}_Q$:

$$A(t) = U(-t) \star_{\sigma,\alpha,\beta} A(0) \star_{\sigma,\alpha,\beta} U(t) \iff \frac{\partial A}{\partial t}(t) - [A(t), H] = 0.$$

Both presented approaches to the time development yield equal predictions concerning the results of measurements:

$$\langle A(0) \rangle_{\rho(t)} = \langle A(t) \rangle_{\rho(0)}.$$

The end of Part 1