The Weyl-Wigner-Moyal formalism on a discrete phase space

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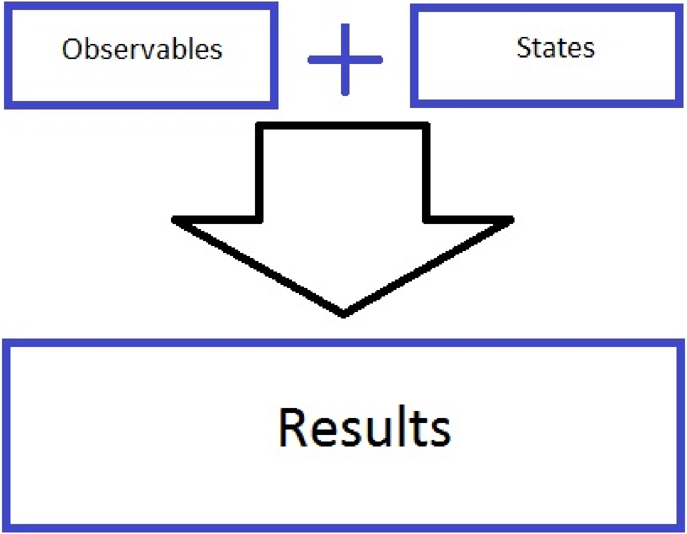
Motivation

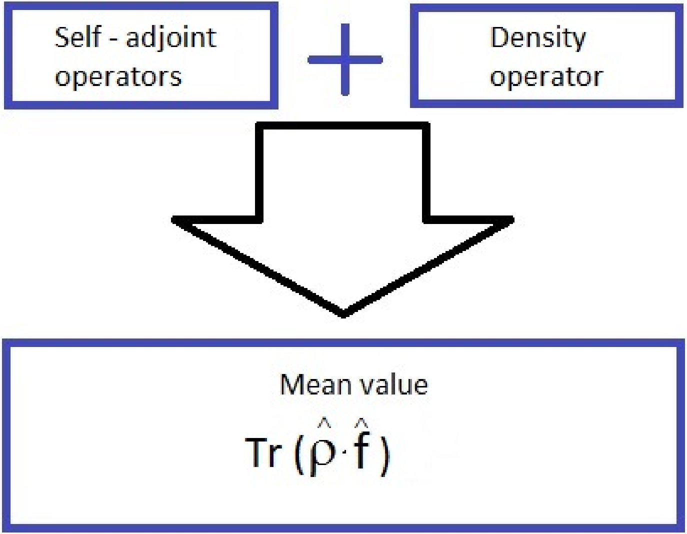
The phase space approach to systems with both: classical degrees of freedom and purely quantum ones (spin)

In the Hilbert space version of quantum mechanics they are modelled on $L^2(\mathbb{R}^n) \otimes \mathcal{H}^{(s+1)}$

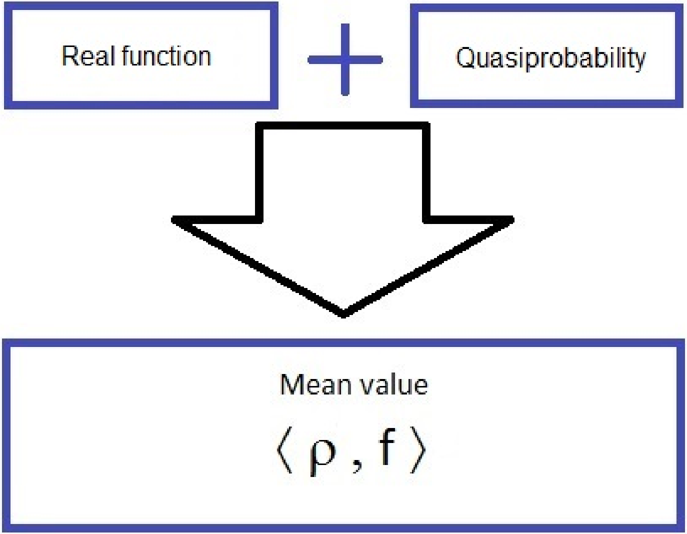
General scheme



Quantum mechanics – the Hilbert space approach



Quantum mechanics – the phase space formulation



Phase space for classical degrees of freedom

Hilbert space $L^2(\mathbb{R}^1)$ can be equipped with a basis

$$\langle q|q'\rangle = \delta(q'-q), \quad q, q' \in \mathbb{R}$$

Another basis can be spanned by vectors

$$|p\rangle = \int_{\mathbb{R}} \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipx}{\hbar}\right) |q\rangle dq,$$

$$\langle p|p'\rangle = \delta(p'-p), \quad p, p' \in \mathbb{R}$$

Phase space for classical degrees of freedom

Let us define two operators

$$\hat{q} = \int_{\mathbb{R}} q|q\rangle dq\langle q|$$

and

$$\hat{p} = \int_{\mathbb{R}} p|p\rangle dp\langle p|$$

with the commutation relation

$$[\hat{q}, \hat{p}] = i\hbar\hat{\mathbf{1}}.$$

Phase space for classical degrees of freedom

Applying them we introduce two families of unitary operators:

$$\exp(i\lambda\hat{p}) \quad \text{and} \quad \exp(i\mu\hat{q}), \quad \lambda, \mu \in \mathbb{R},$$

satisfying the commutation rule

$$\exp\left(-\frac{i\hbar\lambda\mu}{2}\right)\exp(i\lambda\hat{p})\exp(i\mu\hat{q})$$

$$= \exp\left(\frac{i\hbar\lambda\mu}{2}\right)\exp(i\mu\hat{q})\exp(i\lambda\hat{p}) =: \hat{\mathcal{U}}(\lambda, \mu)$$

$$= \exp\{i(\lambda\hat{p} + \mu\hat{q})\}.$$

Phase space for classical degrees of freedom

One can establish a correspondence between operators in $\mathcal{H} \cong L^2(\mathbb{R}^1)$ and functions on $\mathbb{R}^2$

$$f(p,q) = \frac{\hbar}{2\pi}\int_{\mathbb{R}\times\mathbb{R}} d\lambda d\mu \mathcal{P}^{-1}\left(\frac{\hbar\lambda\mu}{2}\right)\exp\{i(\lambda\cdot p+\mu\cdot q)\}\mathrm{Tr}\left\{\widehat{f}\widehat{\mathcal{U}}^{+}(\lambda,\mu)\right\}.$$

By $\mathcal{P}\left(\frac{\hbar\lambda\mu}{2}\right)$ we mean a function related to the operator ordering.

This formula shows that the phase space used for representation of classical degrees of freedom is $\mathbb{R}^{2n}$.

Phase space for internal discrete degrees of freedom

Consider an $(s+1)$ – dimensional Hilbert space $\mathcal{H}^{(s+1)}$ equipped with an orthonormal basis

$$\{|0\rangle, |1\rangle, \ldots, |s\rangle\}, \;\; \langle n|n'\rangle = \delta_{nn'}, \;\; n, n' = 0, 1, \ldots, s.$$

We introduce another orthonormal basis

$$|\phi_m\rangle := \frac{1}{\sqrt{s+1}} \sum_{n=0}^{s} \exp(in\phi_m)|n\rangle,$$

$$\langle \phi_m|\phi_{m'}\rangle = \delta_{mm'} \;\; , \;\; m, m' = 0, 1, \ldots, s$$

with

$$\phi_m = \phi_0 + \frac{2\pi}{s+1} m, \;\; m = 0, 1, \ldots, s.$$

Phase space for internal discrete degrees of freedom

Define then two hermitian operators

$$\hat{n} := \sum_{n=0}^{s} n|n\rangle\langle n|$$

and

$$\hat{\phi} := \sum_{m=0}^{s} \phi_m|\phi_m\rangle\langle\phi_m|$$

which enable us to construct the following unitary operators

$$\hat{V} := \exp\left(i\frac{2\pi}{s+1}\hat{n}\right)$$

satisfying $\hat{V}^{s+1} = \hat{\mathbf{1}}$ and

$$\hat{U} := \exp(i\hat{\phi})$$

fulfilling the equality $\hat{U}^{s+1} = \exp\left\{i(s+1)\phi_0\right\}\hat{\mathbf{1}}$.

These operators fulfill the commutation relation

$$\exp\left(-i\frac{\pi kl}{s+1}\right)\hat{U}^k\hat{V}^l = \exp\left(i\frac{\pi kl}{s+1}\right)\hat{V}^l\hat{U}^k =: \hat{\mathcal{D}}(k,l), \quad k,l\in\mathbb{Z}.$$

Hence one can construct a formula

$$f(\phi_m,n) = \frac{1}{s+1}\sum_{k,l=0}^{s}\mathcal{K}^{-1}(k,l)\exp\left\{i\left(k\phi_m + \frac{2\pi}{s+1}ln\right)\right\}$$

$$\times \mathrm{Tr}\left\{\hat{f}\,\hat{\mathcal{D}}^{+}(k,l)\right\}$$

assigning a function $f(\phi_m,n)$ on a discrete phase space (a grid) $\{(\phi_m,n)\}_{m,n=0}^{s}$ denoted by $\Gamma^{(s+1)}$ to the operator $\hat{f}$.

Phase space for internal discrete degrees of freedom

The inverse formula is of the form

$$\hat{f} = \frac{1}{s+1} \sum_{m,n=0}^{s} f(\phi_m, n) \hat{\Omega}[\mathcal{K}](\phi_m, n),$$

where the Stratonovich – Weyl quantizer

$$\hat{\Omega}[\mathcal{K}](\phi_m, n) := \frac{1}{s+1} \sum_{k,l=0}^{s} \mathcal{K}(k,l) \hat{\mathcal{D}}(k,l) \exp\left\{-i\left(k\phi_m + \frac{2\pi}{s+1} ln\right)\right\}.$$

Phase space for internal discrete degrees of freedom

$\mathcal{K}(k,l)$ is called a kernel and it should satisfy some properties.

- It depends on the product $k \times l$ so we put $\mathcal{K}\left(\frac{\pi kl}{s+1}\right)$
- To give a one – to – one correspondence between functions and operators

$$\mathcal{K}\left(\frac{\pi kl}{s+1}\right) \neq 0 \;\; \forall k,l \in \{0,...,s\}$$

- For any function f on which depends on one variable i.e. $f = f(\phi_m)$ or $f = f(n)$ the associated operator $\widehat{f} = f(\widehat{\phi})$ or $\widehat{f} = f(\widehat{n})$, respectively.

$$\mathcal{K}(0) = 1$$

Phase space for internal discrete degrees of freedom

- For any real function $f(p,q,\phi_m,n)$ the corresponding operator $\widehat{f}$ is Hermitian.

$$\mathcal{K}^*\left(\frac{\pi kl}{s+1}\right) = (-1)^{s+1-k-l}\mathcal{K}\left(\frac{\pi(s+1-k)(s+1-l)}{s+1}\right),$$

$$1 \leq k,l \leq s,$$

$$\mathcal{K}^*(0) = \mathcal{K}(0).$$

- Sometimes one adds the condition

$$\mathrm{Tr}\left\{\widehat{\Omega}[\mathcal{K}](\phi_m,n)\widehat{\Omega}[\mathcal{K}](\phi_{m'},n')\right\} = (s+1)\delta_{mm'}\delta_{nn'}$$

implying

$$\left|\mathcal{K}\left(\frac{\pi kl}{s+1}\right)\right| = 1 \ \forall \ 0 \leq k,l \leq s.$$

Phase space for internal discrete degrees of freedom

Possible choices of the kernel

One cannot put $\mathcal{K}\left(\frac{\pi kl}{s+1}\right) = 1$ for all $0 \leq k, l \leq s$.

The simplest one seems to be $\mathcal{K}(0) = 1$ and $\mathcal{K}\left(\frac{\pi kl}{s+1}\right) = \pm 1$ for $kl \neq 0$.

- If $s+1 =$ odd number one puts

$$\mathcal{K}\left(\frac{\pi kl}{s+1}\right) = (-1)^{kl}$$

- If $s+1$ is even and $\frac{s+1}{2}$ is an odd number one assumes

$$\mathcal{K}\left(\frac{\pi kl}{s+1}\right) = \begin{cases} -1 & \text{for} \quad kl = \text{odd number} \\ -1 & \text{for} \quad kl = 2p, \quad p = \text{odd number} \\ +1 & \text{for} \quad kl = 4r \end{cases}$$

Phase space for systems with continuous and internal degrees of freedom

Putting together formalism for continuous and discrete degrees of freedom we can see that

$$\mathbb{R}^3 \times \mathbb{R}^3 \times \Gamma^{(s+1)} \ni f(p, q, \phi_m, n) \overset{(\mathcal{P},\mathcal{K})}{\longleftrightarrow} \widehat{f} \in L^2(\mathbb{R}^3) \otimes \mathcal{H}^{(s+1)}$$

$$f(p, q, \phi_m, n) = \left(\frac{\hbar}{2\pi}\right)^3 (s+1)^{-1} \sum_{k,l=0}^{s} \int_{\mathbb{R}^3 \times \mathbb{R}^3} d\lambda d\mu$$

$$\left(\mathcal{P}\left(\frac{\hbar\lambda \cdot \mu}{2}\right) \mathcal{K}\left(\frac{\pi k l}{s+1}\right)\right)^{-1}$$

$$\exp\{i(\lambda \cdot p + \mu \cdot q)\} \exp\left\{i \frac{2\pi}{s+1}(km + ln)\right\} \mathrm{Tr}\left\{\widehat{f}\widehat{\mathcal{U}}^{+}(\lambda, \mu)\widehat{\mathcal{D}}^{+}(k, l)\right\}$$

Phase space for systems with continuous and internal degrees of freedom

$$\widehat{f} = \frac{1}{(2\pi)^6(s+1)^2} \sum_{k,l,m,n=0}^{s} \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} d\lambda d\mu dp dq$$

$$\mathcal{P}\left(\frac{\hbar\lambda\cdot\mu}{2}\right)\mathcal{K}\left(\frac{\pi kl}{s+1}\right)$$

$$\exp\{-i(\lambda\cdot p+\mu\cdot q)\}\exp\left\{-i\frac{2\pi}{s+1}(km+ln)\right\}$$

$$f(p,q,\phi_m,n)\widehat{\mathcal{U}}(\lambda,\mu)\widehat{\mathcal{D}}(k,l)$$

Star product

For a spin $\frac{1}{2}$ nonrelativistic particle we choose the orthonormal basis $\{|n\rangle\}_{n=0,1}$ in $\mathcal{H}^{(2)}$ in a standard way

$$\widehat{\sigma}_3|0\rangle = 1 \cdot |0\rangle, \qquad \widehat{\sigma}_3|1\rangle = -1 \cdot |1\rangle.$$

The phase space representation of our quantum system is

$$\{(p, q, \phi_m, n)\} = \mathbb{R}^3 \times \mathbb{R}^3 \times \{(\phi_m, n)\}_{m,n=0,1}$$

and a simple kernel

$$\mathcal{K}\left(\frac{\pi k l}{2}\right) = (-1)^{kl}, \qquad k, l = 0, 1$$

Star product

$$(f * g)(p, q, \phi_m, n) =$$

$$\frac{1}{16} \sum_{m', n', m'', n''=0}^{1} f(p, q, \phi_{m'}, n') \exp\left\{ \frac{i\hbar}{2} \overleftrightarrow{\mathcal{P}} \right\} g(p, q, \phi''_m, n'')$$

$$\Big\{ (1 + (-1)^{m'+m''})(1 + (-1)^{n'+n''}) + (-1)^m((-1)^{m'} + (-1)^{m''}) +$$

$$(-1)^{m+n}((-1)^{m'+n'} + (-1)^{m''+n''}) + (-1)^n((-1)^{n'} + (-1)^{n''}) +$$

$$i \Big[(-1)^m(-1)^{n'+n''}((-1)^{m'} - (-1)^{m''}) + (-1)^{m+n}((-1)^{m''+n'} -$$

$$(-1)^{m'+n''}) + (-1)^n(-1)^{m'+m''}((-1)^{n''} - (-1)^{n'}) \Big] \Big\} .$$

Representation of states

If $\widehat{\rho}$ is a density operator of the quantum system then the average value of an observable $\widehat{f}$

$$\langle \widehat{f} \rangle = \mathrm{Tr}\{\widehat{f}\,\widehat{\rho}\}$$

Hence, we define the Wigner function of the state $\widehat{\rho}$ for the kernels $(\mathcal{P}, \mathcal{K})$ as

$$\rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n) := \frac{1}{(2\pi\hbar)^3(s+1)} \mathrm{Tr}\left\{\widehat{\rho}\,\widehat{\Omega}[\mathcal{P},\mathcal{K}](p,q,\phi_m,n)\right\}$$

Consequently,

$$\langle \widehat{f} \rangle = \sum_{m,n=0}^{s} \int_{\mathbb{R}^3\times\mathbb{R}^3} dpdqf(p,q,\phi_m,n)\rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n)$$

Representation of states

Properties of $\rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n)$

- It is a real function

$$\rho_W^*[\mathcal{P},\mathcal{K}] = \rho_W[\mathcal{P},\mathcal{K}]$$

- Its trace is equal to one

$$\sum_{m,n=0}^{s} \int_{\mathbb{R}^3\times\mathbb{R}^3} dpdq\rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n) = \mathrm{Tr}\{\widehat{\rho}\} = 1$$

- It gives the marginal distributions

$$\sum_{m,n=0}^{s} \int_{\mathbb{R}^3} dp \rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n) = \mathrm{Tr}\{\widehat{\rho}|q\rangle\langle q|\}$$

$$\sum_{m,n=0}^{s} \int_{\mathbb{R}^3} dq \rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n) = \mathrm{Tr}\{\widehat{\rho}|p\rangle\langle p|\}$$

$$\sum_{m=0}^{s} \int_{\mathbb{R}^3\times\mathbb{R}^3} dp dq \rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n) = \mathrm{Tr}\{\widehat{\rho}|n\rangle\langle n|\}$$

$$\sum_{n=0}^{s} \int_{\mathbb{R}^3\times\mathbb{R}^3} dp dq \rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n) = \mathrm{Tr}\{\widehat{\rho}|\phi_m\rangle\langle \phi_m|\}$$

The Liouville – von Neumann – Wigner equation

The evolution equation for the Wigner function $\rho_W[\mathcal{P},\mathcal{K}](p,q,\phi_m,n;t)$ reads

$$\frac{\partial \rho_W[\mathcal{P},\mathcal{K}]}{\partial t} + \frac{1}{i\hbar}\Big(\rho_W[\mathcal{P},\mathcal{K}] * H - H * \rho_W[\mathcal{P},\mathcal{K}]\Big) = 0,$$

where the Hamiltonian $H = H(p,q,\phi_m,n)$ is defined as

$$H(p,q,\phi_m,n) = \mathrm{Tr}\left\{\widehat{H}\widehat{\Omega}[\mathcal{P},\mathcal{K}](p,q,\phi_m,n)\right\}.$$