The 1 – D Dirac equation in the phase space quantum mechanics

Jaromir Tosiek

(in collaboration with Luca Campobasso)

Institute of Physics, Lodz University of Technology, Poland

XXXIX WGMP, Białystok 2022

Prof. Bogdan Mielnik

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Motivation

- The phase space approach to systems with both: classical degrees of freedom and purely quantum ones (e.g. spin)
  In the Hilbert space version of quantum mechanics they are modelled on $L^2(\mathbb{R}^n) \otimes \mathbb{C}^{(s+1)}$
- Representation of relativistic quantum mechanics on a phase space
- Continuity equation in terms of Wigner function

M. Przanowski, J. Tosiek, F. J. Turrubiates, *The Weyl – Wigner – Moyal Formalism on a Discrete Phase Space. I. A Wigner Function for a Nonrelativistic Particle with Spin*, Fortschr. Phys. **67**, 1900080 (2019).

1 – D Dirac equation

A general shape of the free Hamilton operator for a Dirac particle in one dimension is

$$\hat{H} = \alpha(c\hat{p}) + \beta mc^2\hat{\mathbf{1}} \tag{1}$$

where α and β are some square matrices. Because of the requirement

$$\hat{H}^2 = c^2\hat{p}^2 + m^2c^4\hat{\mathbf{1}}$$

we can see that there must be

$$\alpha^2 = \mathbf{1} \ , \ \alpha \cdot \beta + \beta \cdot \alpha = \mathbf{0} \ , \ \beta^2 = \mathbf{1}.$$

1 – D Dirac equation

On the contrary to the 3 – D case this system of conditions can be fulfilled by 2×2 square matrices e.g.

$$\alpha = \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad \beta = \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The time – dependent Dirac equation is of the form

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

Vector $|\Psi(t)\rangle$ is a two – component object $|\Psi(t)\rangle = \begin{bmatrix} |\Psi_1(t)\rangle \\ |\Psi_0(t)\rangle \end{bmatrix}$ from the tensor product of Hilbert spaces $\mathcal{H} \otimes \mathbb{C}^2$, where the space $\mathcal{H}$ is isomorphic to $L^2(\mathbb{R})$.

Eigenvalues of energy in the 1 – D Dirac equation

Possible eigenvalues of the Hamilton operator (1) belong to the sum of intervals

$$E \in (-\infty, -mc^2) \cup (mc^2, +\infty)$$

and satisfy the dispersion relation:

$$E^2 = (cp)^2 + (mc^2)^2, \qquad E_\pm = \pm\sqrt{(cp)^2 + (mc^2)^2},$$

where $p \in \mathbb{R}$.

Eigenvectors of the Hamilton operator in the 1 – D Dirac equation

Eigenfunctions of the Hamilton operator (1) are of the form

$$\psi_{p\pm}(x) = \frac{1}{\sqrt{2\pi\hbar}} \begin{pmatrix} \frac{cp}{E_\pm - mc^2} \\ 1 \end{pmatrix} \left(\frac{(cp)^2}{(E_\pm - mc^2)^2} + 1 \right)^{-\frac{1}{2}} e^{ipx/\hbar}.$$

and fulfill orthonormality conditions

$$\int_{\mathbb{R}} \psi^\dagger_{p'+}(x)\psi_{p+}(x)dx = \delta(p - p'),$$

$$\int_{\mathbb{R}} \psi^\dagger_{p'-}(x)\psi_{p-}(x)dx = \delta(p - p')$$

$$\int_{\mathbb{R}} \psi^\dagger_{p'+}(x)\psi_{p-}(x)dx = 0.$$

Solutions are parametrised by exclusively the momentum p and the sign of energy.

Phase space for classical degrees of freedom

Hilbert space $L^2(\mathbb{R}^1)$ can be equipped with a basis generated by eigenstates of the position operator $\hat{q}$

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

Another basis can be spanned by eigenvectors of the momentum operator $\hat{p}$

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

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

Phase space for classical degrees of freedom

Operators of position and of momentum

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

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

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

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

$$= \exp\{i(\lambda\hat{p} + \mu\hat{q})\} \quad \text{displacement operator}$$

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 $\mathbb{R}^2$

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

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 $\mathcal{H}^{(s+1)} \cong \mathbb{C}^{(s+1)}$ equipped with an orthonormal basis

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

We introduce another orthonormal basis

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

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

with

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

We put the phase $\phi_0 = 0$.

Phase space for internal discrete degrees of freedom

Define then two hermitian operators

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

and

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

which enable us to construct the following unitary operators (Schwinger operators)

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

and

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

Phase space for internal discrete degrees of freedom

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

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

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

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

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

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

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

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

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

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

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

Consequently,

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

Representation of states

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

- It is a real function

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

- Its trace is equal to one

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

- It gives the marginal distribution

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

Phase space model of the 1 – D Dirac equation

In this case $s = 1$.

Two states referring to the internal degree of freedom are

$$\sigma_z|0\rangle = -1\,|0\rangle \quad , \quad \sigma_z|1\rangle = 1\,|1\rangle.$$

Therefore the operators

$$\hat{n} = |1\rangle\langle 1| \quad , \quad \hat{\phi} = \pi|\phi_1\rangle\langle\phi_1|$$

are (up to a factor) projection operators on the directions $|1\rangle$ and $|\phi_1\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)$ respectively.

The Schwinger operators are

$$\widehat{V} = |0\rangle\langle 0| - |1\rangle\langle 1| \quad \text{and}$$

$$\widehat{R} = |\phi_0\rangle\langle\phi_0| - |\phi_1\rangle\langle\phi_1| = |0\rangle\langle 1| + |1\rangle\langle 0|.$$

Phase space model of the 1 – D Dirac equation

The family of unitary operators $\widehat{D}(k,l)$ consists of four elements

$$\widehat{D}(0,0) = \hat{\mathbf{1}} = |0\rangle\langle 0| + |1\rangle\langle 1|, \qquad \widehat{D}(1,0) = \widehat{R} = |0\rangle\langle 1| + |1\rangle\langle 0|$$
$$\widehat{D}(0,1) = \widehat{V} = |0\rangle\langle 0| - |1\rangle\langle 1|, \quad \widehat{D}(1,1) = -i\widehat{R}\widehat{V} = i|0\rangle\langle 1| - i|1\rangle\langle 0|.$$

Our choice of kernels

$$\mathcal{P}\left(\frac{\hbar\lambda\mu}{2}\right) = 1 \quad \text{the} \quad \text{Weyl} \quad \text{ordering}$$

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

One cannot put $\mathcal{K}\left(\frac{\pi kl}{2}\right) = 1$.

Phase space model of the 1 – D Dirac equation

The Hamilton function on the quantum phase space $\mathbb{R} \times \Gamma^2$ equals

$$\begin{aligned} H(p,x,\phi_0,0) &= cp - mc^2, \quad H(p,x,\phi_1,0) = -cp - mc^2 \\ H(p,x,\phi_0,1) &= cp + mc^2, \quad H(p,x,\phi_1,1) = -cp + mc^2. \end{aligned} \tag{2}$$

Components of the Wigner function of a free particle with the momentum $\tilde{p}$ are

$$\begin{cases} W_\pm(p,x,\phi_0,0) &= \frac{1}{4\pi\hbar}\delta(p-\tilde{p})\frac{(E_\pm - mc^2)(c\tilde{p}+E_\pm - mc^2)}{(c\tilde{p})^2+(E_\pm - mc^2)^2}, \\ W_\pm(p,x,\phi_1,0) &= \frac{1}{4\pi\hbar}\delta(p-\tilde{p})\frac{(E_\pm - mc^2)(E_\pm - mc^2 - c\tilde{p})}{(c\tilde{p})^2+(E_\pm - mc^2)^2}, \\ W_\pm(p,x,\phi_0,1) &= \frac{1}{4\pi\hbar}\delta(p-\tilde{p})\frac{c\tilde{p}(c\tilde{p}+E_\pm - mc^2)}{(c\tilde{p})^2+(E_\pm - mc^2)^2}, \\ W_\pm(p,x,\phi_1,1) &= \frac{1}{4\pi\hbar}\delta(p-\tilde{p})\frac{c\tilde{p}(c\tilde{p}-E_\pm + mc^2)}{(c\tilde{p})^2+(E_\pm - mc^2)^2}. \end{cases}$$

Star product for $s = 1$

$$
\begin{aligned}
(f*g)(p,q,\phi_m,n,t) = \frac{1}{(\pi\hbar)^2} \sum_{m',n',m'',n''=0}^{1} \int_{\mathbb{R}\times\mathbb{R}\times\mathbb{R}\times\mathbb{R}} dp'dq'dp''dq'' \\
\times f(p',q',\phi_{m'},n',t) g(p'',q'',\phi_{m''},n'',t) \\
\exp\left\{\frac{2i}{\hbar}[(q-q')\cdot(p-p'') - (q-q'')\cdot(p-p')]\right\} \\
\Big\{(1+(-1)^{m'+m''})(1+(-1)^{n'+n''}) + (-1)^m((-1)^{m'} + (-1)^{m''}) \\
+ (-1)^{m+n}((-1)^{m'+n'} + (-1)^{m''+n''}) \\
+(-1)^n((-1)^{n'} + (-1)^{n''}) + i\Big[(-1)^m(-1)^{n'+n''}((-1)^{m'} - (-1)^{m''}) \\
+ (-1)^{m+n}((-1)^{m''+n'} - (-1)^{m'+n''}) \\
+(-1)^n(-1)^{m'+m''}((-1)^{n''} - (-1)^{n'})\Big]\Big\}.
\end{aligned}
$$

Star product – differential formula

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

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

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

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

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

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

The Liouville – von Neumann – Wigner equation

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

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

The Moyal bracket is defined as

$$\{W[\mathcal{P},\mathcal{K}],H\}_M:=\frac{1}{i\hbar}\Big(W[\mathcal{P},\mathcal{K}]*H-H*W[\mathcal{P},\mathcal{K}]\Big)$$

Time evolution of spatial density of probability

The change of spatial density of probability $\rho(\vec{r}_0, t)$ with time combined with the Liouville – von Neumann – Wigner equation leads to the relation

$$\frac{\partial}{\partial t} \sum_{m,n=0}^{s} \int_{\mathbb{R}^3} d\vec{p}\, W[\mathcal{P}, \mathcal{K}](\vec{p}, \vec{r}, \phi_m, n, t)$$

$$+ \sum_{m,n=0}^{s} \int_{\mathbb{R}^3} d\vec{p}\, \{W[\mathcal{P}, \mathcal{K}](\vec{p}, \vec{r}, \phi_m, n, t), H(\vec{p}, \vec{r}, \phi_m, n, t)\}_M = 0.$$

The continuity equation takes the form

$$\frac{\partial \rho(\vec{r}_0, t)}{\partial t} + \mathrm{div}\vec{j}(\vec{r}, t) = 0.$$

Current density in the 1 – D Dirac equation

The expression

$$\sum_{m,n=0}^{s} \int_{\mathbb{R}^3} d\vec{p}\,\{W[\mathcal{P},\mathcal{K}](\vec{p},\vec{r},\phi_m,n,t), H(\vec{p},\vec{r},\phi_m,n,t)\}_M$$

represents the element $\mathrm{div}\vec{j}(\vec{r},t)$.

The current density for the 1 – D Dirac equation is of the form

$$\vec{j}(x,t) = \int_{\mathbb{R}} dp\, c\Big(W(p,x,\phi_0,0,t)$$

$$+W(p,x,\phi_0,1,t) - W(p,x,\phi_1,0,t) - W(p,x,\phi_1,1,t)\Big).$$