Canonical Coordinate Transformations in Quantum Mechanics

Part 1

Maciej Błaszak and Ziemowit Domański

Adam Mickiewicz University, Faculty of Physics
Division of Mathematical Physics

June 21–22, 2012

Motivation

Classical harmonic oscillator

Hamiltonian:

$$H(x,p) = \frac{1}{2}\left(p^2 + \omega^2 x^2\right)$$

Born's quantization rule

$$x \to \hat{q} = x, \quad p \to \hat{p} = -i\hbar\partial_x, \quad \text{symmetric ordering of } \hat{q},\ \hat{p}$$

After applying it to the Hamiltonian of the harmonic oscillator:

$$\hat{H} = H(\hat{q},\hat{p}) = \frac{1}{2}\left(\hat{p}^2 + \omega^2 \hat{q}^2\right)$$

Motivation

Perform a classical canonical transformation of coordinates $T\colon (\mathbb{R}\setminus\{0\})\times\mathbb{R}\to(\mathbb{R}\setminus\{0\})\times\mathbb{R}$, $T(x',p')=(x,p)$ where

$$x=\begin{cases}\sqrt{|2x'|}, & x'>0\\ -\sqrt{|2x'|}, & x'<0\end{cases}, \quad p=p'\sqrt{|2x'|}$$

receiving

$$H'(x',p')=H(T(x',p'))=|x'|p'^2+\omega^2|x'|.$$

Born's quantization rule:

$$\hat{H}'=H'(\hat{q}',\hat{p}')=\frac{1}{2}|\hat{q}'|\hat{p}'^2+\frac{1}{2}\hat{p}'^2|\hat{q}'|+\omega^2|\hat{q}'|.$$

Hamiltonians $\hat{H}$ and $\hat{H}'$ are not unitarily equivalent — they describe different quantum systems. Inconsistency of the quantization of classical Hamiltonian systems?

Quantum mechanics on phase space

The idea of a quantization of a classical Hamiltonian system

A deformation, with respect to the Planck's constant $\hbar$, of a classical Hamiltonian system:

- a deformation of a phase space (a Poisson manifold) to a noncommutative phase space (a noncommutative Poisson manifold),
- a deformation of a classical space of states to a quantum space of states.

A deformation of a phase space

A Poisson manifold $(M, \mathcal{P})$ ($\mathcal{P}$ being a Poisson tensor) is fully described by a Poisson algebra $\mathcal{A}_C = (C^\infty(M), \cdot, \{\cdot, \cdot\})$. By deforming $\mathcal{A}_C$ to some noncommutative algebra $\mathcal{A}_Q = (C^\infty(M), \star, [\![\cdot, \cdot]\!])$, where $\star$ is some noncommutative associative product of functions being a deformation of a point-wise product $\cdot$ and $[\![\cdot, \cdot]\!]$ is a deformation of the Poisson bracket $\{\cdot, \cdot\}$, we can think of $\mathcal{A}_Q$ as describing a noncommutative Poisson manifold.

Quantum mechanics on phase space

Moyal quantization scheme

Let $M = \mathbb{R}^2$ and $\mathcal{P} = \partial_x \wedge \partial_p$. Define the $\star$-product by

$$f \star g = f \exp\left(\frac{1}{2} i\hbar \overleftarrow{\partial}_x \overrightarrow{\partial}_p - \frac{1}{2} i\hbar \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right) g, \quad f, g \in C^\infty(\mathbb{R}^2)$$

and the deformed Poisson bracket by

$$[\![f, g]\!] = \frac{1}{i\hbar}[f, g] = \frac{1}{i\hbar}(f \star g - g \star f), \quad f, g \in C^\infty(\mathbb{R}^2).$$

Space of states

Define a quantum space of states as a Hilbert space $\mathcal{H} = L^2(\mathbb{R}^2)$. It is possible to define the $\star$-product on $\mathcal{H}$ by extending it from the algebra $C^\infty(\mathbb{R}^2)$.

Quantum mechanics on phase space

Observables and states as operators

Observables $A \in C^\infty(\mathbb{R}^2)$ and states $\Psi \in L^2(\mathbb{R}^2)$ can be treated as operators $\hat{A}$ and $\hat{\Psi}$ defined on the Hilbert space of states $L^2(\mathbb{R}^2)$ by the following prescription

$$\hat{A} = A \star, \quad \hat{\Psi} = \sqrt{2\pi\hbar}\Psi \star .$$

The operator $\hat{A}$ can be written as a symmetrically-ordered function A of operators of position $\hat{q}_M = x \star = x + \frac{1}{2} i\hbar\partial_p$ and momentum $\hat{p}_M = p \star = p - \frac{1}{2} i\hbar\partial_x$:

$$\hat{A} = A \star = A_M(\hat{q}_M, \hat{p}_M).$$

Canonical transformations of coordinates in phase space quantum mechanics

Transformations of phase space coordinates

A transformation of phase space coordinates is defined as in classical mechanics, i.e. as a smooth bijective map

$$T\colon \mathbb{R}^2 \supset U \ni (x', p') \to (x, p) \in W \subset \mathbb{R}^2.$$

We will assume that T is defined on almost the whole phase space, i.e. $\mathbb{R}^2 \setminus U$ and $\mathbb{R}^2 \setminus W$ are sets of measure zero.

Observables $A \in C^\infty(\mathbb{R}^2)$ and states $\Psi \in L^2(\mathbb{R}^2)$ transform according to the formulae

$$A'(x', p') = A(T(x', p')), \quad \Psi'(x', p') = \Psi(T(x', p')).$$

Canonical transformations of coordinates in phase space quantum mechanics

The $\star$-product has to transform according to the formula

$$(f \star g) \circ T = (f \circ T) \star'_T (g \circ T), \quad f, g \in C^\infty(\mathbb{R}^2).$$

The $\star'_T$-product is in fact given by the following equation

$$f \star'_T g = f \exp\left(\frac{1}{2} i\hbar \overleftarrow{D_{x'}} \overrightarrow{D_{p'}} - \frac{1}{2} i\hbar \overleftarrow{D_{p'}} \overrightarrow{D_{x'}}\right) g,$$

where vector fields $D_{x'}$, $D_{p'}$ are derivations ∂_x, ∂_p transformed by the transformation T according to the formulae

$$(\partial_x f) \circ T = D_{x'}(f \circ T), \quad f \in C^\infty(\mathbb{R}^2),$$
$$(\partial_p f) \circ T = D_{p'}(f \circ T), \quad f \in C^\infty(\mathbb{R}^2).$$

Canonical transformations of coordinates in phase space quantum mechanics

Example: Linear transformations

$$(x,p) = T(x',p') = (dx' - bp', -cx' + ap'),$$

where $a,b,c,d \in \mathbb{R}$, $ad - bc = 1$. The linear transformation T is generated by a function $F(x,x') = \frac{1}{b}xx' - \frac{a}{2b}x^2 - \frac{d}{2b}x'^2$, i.e.

$$p = \frac{\partial F}{\partial x}(x,x'), \quad p' = -\frac{\partial F}{\partial x'}(x,x').$$

The linear transformation T preserves the $\star$-product, i.e.

$$(f \star g) \circ T = (f \circ T) \star' (g \circ T), \quad f,g \in C^\infty(\mathbb{R}^2),$$

where

$$\star' = \exp\left(\frac{1}{2} i\hbar \overleftarrow{\partial}_{x'} \overrightarrow{\partial}_{p'} - \frac{1}{2} i\hbar \overleftarrow{\partial}_{p'} \overrightarrow{\partial}_{x'}\right).$$

Canonical transformations of coordinates in phase space quantum mechanics

Example: A class of nonlinear transformations

$$(x, p) = T(x', p') = (-ap' - a\phi'(x'), a^{-1}x').$$

where $a \in \mathbb{R}$, $a \neq 0$, ϕ is an arbitrary smooth function. The transformation T is generated by the function $F(x, x') = a^{-1}xx' + \phi(x')$. The Moyal $\star$-product transforms to the following product

$$\star'_T = \exp\left(\frac{1}{2}i\hbar\overleftarrow{D_{x'}}\overrightarrow{D_{p'}} - \frac{1}{2}i\hbar\overleftarrow{D_{p'}}\overrightarrow{D_{x'}}\right),$$

where

$$D_{x'} = -a^{-1}\partial_{p'}, \quad D_{p'} = a\partial_{x'} - a\phi''(x')\partial_{p'}.$$

Canonical transformations of coordinates in phase space quantum mechanics

Example: Nonlinear point transformations

$$(x,p) = T(x',p') = (\phi(x'), (\phi'(x'))^{-1}p')$$

where ϕ is an arbitrary smooth bijective function. The transformation T is generated by the function $F(x',p) = -p\phi(x')$, i.e.

$$x = -\frac{\partial F}{\partial p}(x',p), \quad p' = -\frac{\partial F}{\partial x'}(x',p).$$

The Moyal $\star$-product transforms to the following product

$$\star'_T = \exp\left(\frac{1}{2}i\hbar\overleftarrow{D_{x'}}\overrightarrow{D_{p'}} - \frac{1}{2}i\hbar\overleftarrow{D_{p'}}\overrightarrow{D_{x'}}\right),$$

where

$$D_{x'} = (\phi'(x'))^{-1}\partial_{x'} + (\phi'(x'))^{-2}\phi''(x')p'\partial_{p'}, \quad D_{p'} = \phi'(x')\partial_{p'}.$$

Special case of the previous example

For

$$\phi(x') = \begin{cases} \sqrt{|2x'|}, & x' > 0 \\ -\sqrt{|2x'|}, & x' < 0 \end{cases}$$

we receive the following point transformation

$$(x, p) = T(x', p') = \begin{cases} (\sqrt{|2x'|}, p'\sqrt{|2x'|}), & x' > 0 \\ (-\sqrt{|2x'|}, p'\sqrt{|2x'|}), & x' < 0 \end{cases}.$$

The transformed Moyal product takes the form

$$\star'_T = \exp\left(\frac{1}{2}i\hbar\overleftarrow{D_{x'}}\overrightarrow{D_{p'}} - \frac{1}{2}i\hbar\overleftarrow{D_{p'}}\overrightarrow{D_{x'}}\right),$$

where

$$D_{x'} = \sqrt{|2x'|}\partial_{x'} - \frac{\operatorname{sgn}(x')}{\sqrt{|2x'|}}p'\partial_{p'}, \quad D_{p'} = \frac{1}{\sqrt{|2x'|}}\partial_{p'}.$$

Classical canonical transformations

A transformation T of coordinates is a classical canonical transformation if

$$\{x', p'\}' = 1,$$

where $\{\cdot\,,\,\cdot\}'$ denotes a Poisson bracket transformed to the new coordinate system:

$$\{f, g\}' = \{f \circ T^{-1}, g \circ T^{-1}\} \circ T, \quad f, g \in C^\infty(\mathbb{R}^2).$$

Quantum canonical transformations

A transformation T of coordinates is a quantum canonical transformation if

$$[\![x', p']\!]' = 1,$$

where $[\![\cdot\,,\,\cdot]\!]'$ denotes a deformed Poisson bracket transformed to the new coordinate system:

$$[\![f, g]\!]' = [\![f \circ T^{-1}, g \circ T^{-1}]\!] \circ T, \quad f, g \in C^\infty(\mathbb{R}^2).$$

The transformations from previous examples are simultaneously classical and quantum canonical transformations.

Canonical transformations of coordinates in phase space quantum mechanics

A transformation T of coordinates transforms the space of states $L^2(\mathbb{R}^2)$ into the Hilbert space $L^2(\mathbb{R}^2, \mu_T)$ with the standard scalar product, where $\mathrm{d}\mu_T(x', p') = |\det T'(x', p')| \, \mathrm{d}x' \, \mathrm{d}p'$. Of course, if T is also a classical canonical transformation then $\mathrm{d}\mu_T(x', p') = \mathrm{d}x' \, \mathrm{d}p'$, since the Jacobian of a classical canonical transformation is equal 1.

An important observation useful when passing to the ordinary description of quantum mechanics is the following. For a given quantum canonical transformation T the transformed star-product is equivalent with the Moyal product, i.e. there exist a unique vector space automorphism S_T of $C^\infty(\mathbb{R}^2)$ satisfying

- $S_T = \sum_{k=0}^{\infty} \hbar^k S_k$, $S_0 = 1$,
- $S_T(f \star' g) = (S_T f) \star'_T (S_T g)$, $f, g \in C^\infty(\mathbb{R}^2)$,
- $S_T x' = x'$, $S_T p' = p'$,
- $S_T(f^*) = (S_T f)^*$, $f \in C^\infty(\mathbb{R}^2)$,

where S_k are differential operators.

For a quantum canonical transformation T of coordinates

$$S_T \colon L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2, \mu_T)$$

and S_T is a Hilbert space isomorphism.

Canonical transformations of coordinates in phase space quantum mechanics

Transformation of observables treated as operators

Let T be a quantum canonical transformation of coordinates and $A \in C^\infty(\mathbb{R}^2)$. The transformed observable $A' = A \circ T$ can be treated as the following operator

$$\hat{A}' = A' \star'_T \; = A'_{M,S_T}(\hat{q}'_T, \hat{p}'_T) \equiv (S_T^{-1}A')_M(\hat{q}'_T, \hat{p}'_T),$$

where $\hat{q}'_T = x' \star'_T$, $\hat{p}'_T = p' \star'_T$.

Example: Linear transformations

For a linear transformation

$$(x,p) = T(x',p') = (dx' - bp', -cx' + ap')$$

an isomorphism $S_T = 1$.

Example: A class of nonlinear transformations

For a transformation

$$(x,p) = T(x',p') = (-ap' - a\phi'(x'), a^{-1}x')$$

an isomorphism S_T is equal

$$S_T = \exp\left(-\sum_{n=1}^{\infty} \frac{1}{(2n+1)!}(-1)^n \left(\frac{\hbar}{2}\right)^{2n} \phi^{(2n+1)}(x')\partial_{p'}^{2n+1}\right)$$
$$= \exp\left(\frac{i}{\hbar}\left(\phi\left(x' + \frac{1}{2}i\hbar\partial_{p'}\right) - \phi\left(x' - \frac{1}{2}i\hbar\partial_{p'}\right) - i\hbar\phi'(x')\partial_{p'}\right)\right).$$

Canonical transformations of coordinates in phase space quantum mechanics

Example: Nonlinear point transformations

For a point transformation

$$(x, p) = T(x', p') = (\phi(x'), (\phi'(x'))^{-1} p')$$

an isomorphism S_T is equal

$$S_T = 1 + \frac{1}{3!}\left(\frac{\hbar}{2}\right)^2 (\phi'(x'))^{-2}\Bigg(\Big(3(\phi''(x'))^2 - \phi'(x')\phi'''(x')\Big)p'\partial^3_{p'} + 3\phi'(x')\phi''(x')\partial_{x'}\partial^2_{p'} + 3(\phi''(x'))^2\partial^2_{p'}\Bigg) + o(\hbar^4).$$

Canonical transformations of coordinates in phase space quantum mechanics

Special case of the previous example

For a point transformation

$$(x,p) = T(x',p') = \begin{cases} (\sqrt{|2x'|}, p'\sqrt{|2x'|}), & x' > 0 \\ (-\sqrt{|2x'|}, p'\sqrt{|2x'|}), & x' < 0 \end{cases}$$

an isomorphism S_T is equal

$$S_T = \exp\left(\sum_{n=1}^{\infty}(-1)^n\left(\frac{\hbar}{2}\right)^{2n}\left(A_n \operatorname{sgn}(x')|2x'|^{-2n+1}\partial_{x'}\partial_{p'}^{2n} - B_n|2x'|^{-2n}\partial_{p'}^{2n}\right)\right)$$
$$= 1 - \frac{1}{8}\hbar^2 \operatorname{sgn}(x')|2x'|^{-1}\partial_{x'}\partial_{p'}^2 + \frac{1}{8}\hbar^2|2x'|^{-2}\partial_{p'}^2 + o(\hbar^4),$$

where A_n, B_n are some rational constants.

The End

of

Part 1