Invariant canonical quantization of classical mechanics

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Geometry of PDEs and Integrability,
14-18 October 2013, Teplice nad Bečvou

1. B. Podolsky, Phys. Rev. **32** (1928) 812
2. B.S. deWitt, Phys. Rev. **85** (1952) 653
3. B.S. deWitt, Rev. Mod. Phys. **29** (1957) 377
4. J.L. Gervais and A. Jevicki, Nucl. Phys. **B 110** (1976) 93
5. H. Essen, Am. J. Phys. **46** (1978) 983
6. H. Dekker, Physica **103 A** (1980) 586
7. Liu Zhang-Ju and Quian Min, Trans. AMS **331** (1992) 321
8. C. Duval and V. Ovsienko, Selecta Math. New Ser. **7** (2001) 271
9. C. Duval and G. Valent, J. Math. Phys. **46** (2005) 053516

Plan of presentation

1. Classical Liouville mechanics
2. Canonical quantization on a phase space
3. Quantum mechanics over configuration space
4. Quantization in curvilinear canonical coordinates
5. Covariant representation of Hamiltonian operators
6. Canonical quantization in Riemann space
7. Ambiguities in quantization process

Classical Liouville mechanics

Classical Hamiltonian system: $(M, \mathcal{P}, H)$

M - phase space: $M = T^*\mathcal{Q} = \mathcal{Q} \times \mathbb{R}^N$, $\mathcal{Q}$ - flat configuration space, $\dim \mathcal{Q} = N$
$\mathcal{P}$ - Poisson tensor
H - Hamiltonian function: smooth, real-valued function on M

Classical Poisson algebra: $\mathcal{A}_C = (C^\infty(M), \cdot, \{\ ,\ \}, ^-)$

$C^\infty(M) \ni F, H$: smooth complex-valued functions on M
$\cdot$: point-wise commutative dot product
$\{F, H\} := \mathcal{P}(\mathrm{d}F, \mathrm{d}H)$: Poisson bracket, i.e. Lie bracket induced by $\mathcal{P}$
$\bar{F} \in C^\infty(M)$: complex conjugation, being involution in $\mathcal{A}_C$

Classical observables: elements of $\mathcal{A}_C$ self-adjoint with respect to involution.

Classical Liouville mechanics

Classical states of Hamiltonian system: ϱ

ϱ - probability distribution:

1. $\varrho = \bar{\varrho}$ (self-conjugation),
2. $\int_M \varrho \, \mathrm{d}\Omega = 1$ (normalization),
3. $\int_M \bar{f} \cdot f \cdot \varrho \, \mathrm{d}\Omega \geq 0$ for $f \in C^\infty(M) \iff \varrho \geq 0$ (positivity).

Notice, that ϱ are closed with respect to commutative and associative multiplication being convolution:

$$\varrho_1(\xi) * \varrho_2(\xi) = \int \mathrm{d}\zeta \, \varrho_1(\zeta)\varrho_2(\xi - \zeta) = \varrho_3(\xi).$$

Pure states ϱ_{pure} are these ϱ which are idempotent

$$\varrho_{\text{pure}} * \varrho_{\text{pure}} = \varrho_{\text{pure}},$$

i.e. $\varrho_{\text{pure}} = \delta(\xi - \xi_0)$ are Dirac delta distributions (Hamiltonian mechanics).

Classical Liouville mechanics

Mixed states ϱ_{mix} can be characterized as convex linear combinations of pure states $\varrho_{\text{pure}}^{(\xi_0)}$

$$\varrho_{\text{mix}}(\xi) = \int_M \mathrm{d}\xi_0\, p(\xi_0)\varrho_{\text{pure}}^{(\xi_0)}(\xi) = \int_M \mathrm{d}\xi_0\, p(\xi_0)\delta(\xi - \xi_0) = p(\xi),$$

where $p(\xi_0) \geq 0$ and $\int_M \mathrm{d}\xi_0\, p(\xi_0) = 1$.

Quantities measured in experiment: $\langle A \rangle_\varrho$

$\langle A \rangle_\varrho$: expectation value of an observable A in a state ϱ:

$$\langle A \rangle_\varrho := \int_M (A \cdot \varrho)(\xi)\,\mathrm{d}\xi$$

For classical pure states $\varrho(\xi) = \delta(\xi - \xi_0)$

$$\langle A \rangle_{\delta(\xi-\xi_0)} := A(\xi_0).$$

Classical Hamiltonian mechanics case.

Classical Liouville mechanics

Time evolution of expectation value of any observable in arbitrary state for a given Hamiltonian system

Two equivalent descriptions:

1. Time evolution of observables (classical Heisenberg picture)

$$\frac{\mathrm{d}A}{\mathrm{d}t}(t) - \{A(t), H\} = 0$$

2. Time evolution of states (classical Schrödinger picture)

$$\frac{\mathrm{d}\varrho}{\mathrm{d}t}(t) - \{H, \varrho(t)\} = 0 \quad \text{(Liouville equation)}$$

Both descriptions yield equal predictions of measurements:

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

Classical Liouville mechanics

For pure state $\varrho(\xi) = \delta(\xi - \xi_0)$

$$\frac{\mathrm{d}\varrho}{\mathrm{d}t} - \{H, \varrho(t)\} = 0 \quad \Longrightarrow \quad \frac{\mathrm{d}\xi^i}{\mathrm{d}t} - \{\xi^i(t), H\} = 0$$

Schrödinger picture for $\delta(\xi - \xi_0)$ collapse onto Heisenberg picture for ξ^i.

Canonical (Darboux) coordinate chart: ξ

$$(\xi) = (q, p): \quad \{q^i, q^j\} = \{p_i, p_j\} = 0, \quad \{q^i, p_j\} = \delta^i_j$$

$$\mathcal{P} = \sum_i \frac{\partial}{\partial q^i} \wedge \frac{\partial}{\partial p_i}, \quad (\mathcal{P}^{ij}) = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

Time evolution of canonical coordinates

$$(q^i)_t = \{q^i, H\} = \frac{\partial H}{\partial p_i}, \quad (p_i)_t = \{p_i, H\} = -\frac{\partial H}{\partial q^i}.$$

Canonical quantization of Hamiltonian mechanics

Classical uncertainty relations for canonical coordinates in a given state ϱ

$$\triangle q^i \triangle p_j \geq 0, \quad \triangle A := \sqrt{\langle A^2 \rangle_\varrho - \langle A \rangle_\varrho^2}.$$

Equality occurs for classical coherent states. For example in a standard classical mechanics for pure states $\varrho(\xi) = \delta(\xi - \xi_0)$.

Quantization process

Classical canonical uncertainty relations are modified to quantum Heisenberg uncertainty relations

$$\triangle q^i \triangle p_j \geq 0 \quad \Longrightarrow \quad \triangle q^i \triangle p_j \geq \frac{1}{2}\hbar\delta^i_j$$

$\hbar$ — deformation parameter (Planck constant).

Realization: appropriate deformation of classical Liouville mechanics.

Canonical quantization of Hamiltonian mechanics

Deformation of classical Poisson algebra to $\mathcal{A}_Q = (C^\infty(M,\hbar), \star, [\![\,,\,]\!], *)$

$\star$: deformation of dot product to some noncommutative star product
$[\![\,,\,]\!]$: deformation of Poisson bracket to new Lie bracket (quantum Poisson bracket)
$*$: deformation of classical involution to new quantum involution

Desired properties of $\star$:

1. $F \star H = F \cdot H + \sum_{k=1}^{\infty} \hbar^k C_k(F,H)$, C_k — bilinear operators,
2. $F \star (G \star H) = (F \star G) \star H$ (associativity),
3. $[\![F,H]\!]_\star = \{F,H\} + o(\hbar)$
4. $(F \star H)^* = H^* \star F^*$
5. $F \star 1 = 1 \star F \equiv F, \quad F,G,H \in \mathcal{A}_Q$

Quantum observables: self adjoint functions with respect to quantum involution, $\hbar$ dependent and complex in general.

Canonical quantization of Hamiltonian mechanics

The existence of a global $\star$-product for a general Poisson manifold: Kontsevich (1997)

Invariant formulation of a $\star$-product on $M = Q \times \mathbb{R}^N$

Vector-field representation of a Poisson tensor:

$$\mathcal{P} = \sum_{j=1}^{N} X_j \wedge Y_j = \sum_{j=1}^{N} (X_j \otimes Y_j - Y_j \otimes X_j)$$

$$[X_i, Y_j] = [X_i, X_j] = [Y_i, Y_j] = 0 \quad \Rightarrow \quad \text{Jacobi identity}$$

Natural $\star$-product induced by X, Y:

$$\star = \exp\left(\frac{1}{2} i\hbar \sum_{j=1}^{N} \overleftarrow{X_j} \wedge \overrightarrow{Y_j}\right) = \exp\left(\frac{1}{2} i\hbar \sum_{j=1}^{N} (\overleftarrow{X_j}\overrightarrow{Y_j} - \overleftarrow{Y_j}\overrightarrow{X_j})\right).$$

Canonical quantization of Hamiltonian mechanics

Natural Lie bracket:

$$[\![F,H]\!]_\star=\frac{1}{i\hbar}[F,G]_\star=\frac{1}{i\hbar}(F\star H-H\star F)=\{F,H\}+o(\hbar).$$

Quantum involution coincides with the classical one:

$$\overline{F\star H}=\overline{H}\star\overline{F}.$$

Bad news: non uniqueness

There exist different vector fields X_i', Y_i' giving the same Poisson tensor. In consequence, the whole family of $\star$-products is related to the same Poisson tensor.

Good news: all these $\star$-products are equivalent.

Canonical quantization of Hamiltonian mechanics

Two star-products $\star$ and $\star'$ on a Poisson manifold $(M, \mathcal{P})$ are said to be equivalent if there exists a morphism

$$S = \mathrm{id} + \sum_{k=1}^{\infty} \hbar^k S_k$$

S_k — linear operators on $C^\infty(M)$, that

$$S(F \star H) = SF \star' SH.$$

In the case of $M = \mathcal{Q} \times \mathbb{R}^N$, if $\mathcal{P} = \sum X_j \wedge Y_j = \sum X'_j \wedge Y'_j$ and $(X, Y) \to \mathcal{A}_Q$, $(X', Y') \to \mathcal{A}'_Q$, then there exists an appropriate S making $\mathcal{A}_Q$ and $\mathcal{A}'_Q$ isomorphic.

Equivalent descriptions: $(A, \star) \Leftrightarrow (A' = SA, \star')$

Canonical quantization of Hamiltonian mechanics

Example.

For any Darboux coordinates (q,p) on $M=\mathbb{R}^2$ there is a natural choice

$$X=\partial_q, \quad Y=\partial_p$$

leading to Moyal product in that chart

$$\star_M=\exp\left(\frac{1}{2}i\hbar\overleftarrow{\partial}_q\overrightarrow{\partial}_p-\frac{1}{2}i\hbar\overleftarrow{\partial}_p\overrightarrow{\partial}_q\right)$$

There is also a family of equivalent products generated by classical canonical transformations T. For example

$$\star_T=\exp\left(\frac{1}{2}i\hbar\overleftarrow{D}_q\overrightarrow{D}_p-\frac{1}{2}i\hbar\overleftarrow{D}_p\overrightarrow{D}_q\right)$$

$$D_q=q^2\partial_q-2qp\partial_p, \quad D_p=q^{-2}\partial_p, \quad [D_q,D_p]=0$$

and

$$\mathcal{P}=\partial_q\wedge\partial_p=D_q\wedge D_p$$

Canonical quantization of Hamiltonian mechanics

Related canonical transformation T: $(q,p) \mapsto T(q,p) = (-q^{-1}, q^2 p)$

S_T morphism:

$$F \star_T H = S_T(S_T^{-1} F \star_M S_T^{-1} H)$$

$$S_T = \mathrm{id} + \frac{1}{4}\hbar^2(2q^{-2}\partial_p^2 + q^{-2}p\partial_p^3 - q^{-1}\partial_q\partial_p^2) + o(\hbar^4)$$

Both products lead to a canonical quantum brackets

$$[\![q,p]\!]_{\star_M} = 1, \quad [\![q,p]\!]_{\star_T} = 1$$

Infinite family of admissible quantization procedures.

Admissible choice of quantization, verified by experiment:
Moyal quantum algebra in Euclidean chart on $\mathcal{Q} = \mathbb{R}^N$ with quantum observables equal to classical ones.

Canonical quantization of Hamiltonian mechanics

Transformation of star-product

$$\star_M^{(x,p)} \quad \xrightarrow{T} \quad \star^{(x',p')} \qquad (A', \star^{(x',p')})$$

$$\uparrow S_T$$

$$\star_M^{(x',p')} \qquad (S_T^{-1}A', \star_M^{(x',p')})$$

The class of canonical point transformations

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

New coordinates on $\mathcal{Q}$ define flat metric g with respective connection.

$$S_T = \mathrm{id} + \frac{\hbar^2}{4!}\Big(3\Gamma^i_{rj}(x')\Gamma^r_{ik}(x')\partial_{p'_j}\partial_{p'_k} + 3\Gamma^i_{jk}(x')\partial_{x'^i}\partial_{p'_j}\partial_{p'_k}$$
$$+ \left(2\Gamma^i_{nr}(x')\Gamma^n_{jk}(x') - \partial_{x'^r}\Gamma^i_{jk}(x')\right) p'_i\partial_{p'_j}\partial_{p'_k}\partial_{p'_r}\Big) + o(\hbar^4)$$

Canonical quantization of Hamiltonian mechanics

Quantum states

For a phase space $M = \mathcal{Q} \times \mathbb{R}^N$ and a $\star$-product defined on it, states are real quasi-probabilistic distributions from $\mathcal{H} = L^2(M)$, defined by:

1. $\varrho = \bar{\varrho}$ (self-conjugation),
2. $\int_M \varrho \, \mathrm{d}\Omega = 1$ (normalization),
3. $\int_M \bar{f} \star f \star \varrho \, \mathrm{d}\Omega \geq 0$ for $f \in C^\infty(M; \hbar)$ (positive define).

Pure states $\varrho_{\text{pure}} \in \mathcal{H}$ are these ϱ which are idempotent

$$\varrho_{\text{pure}} \star \varrho_{\text{pure}} = \frac{1}{(2\pi\hbar)^N} \varrho_{\text{pure}}.$$

Mixed states $\varrho_{\text{mix}} \in \mathcal{H}$ can be characterized as convex linear combinations of pure states $\varrho_{\text{pure}}^{(\lambda)}$

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

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

Canonical quantization of Hamiltonian mechanics

Expectation value of quantum observable A in a state ϱ

$$\langle A \rangle_\varrho := \int_M (A \star \varrho)(\xi)\, \mathrm{d}\xi = \int_M (A \cdot \varrho)(\xi)\, \mathrm{d}\xi.$$

Time evolution of expectation value $\langle A \rangle_\varrho$

1. Time evolution of observables (quantum Heisenberg picture)

$$\frac{\mathrm{d}A}{\mathrm{d}t}(t) - [\![A(t), H]\!]_\star = 0$$

2. Time evolution of states (quantum Schrödinger picture)

$$\frac{\mathrm{d}\varrho}{\mathrm{d}t}(t) - [\![H, \varrho(t)]\!]_\star = 0$$

Both descriptions yield equal predictions of measurements:

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

Quantum mechanics over configuration space

Ordinary quantum mechanics: operator representation over configuration space $\mathcal{Q}$ (Błaszak, Domański 2012)

Consider Euclidean chart (x, p) with $\star_M$-product. The Hilbert space of states $\mathcal{H} = L^2(M)$ takes the form of a Hilbert space $L^2(\mathbb{R}^{2N})$ which can be written as the following tensor product of the Hilbert space $L^2(\mathbb{R}^N)$ and a space dual to it $(L^2(\mathbb{R}^N))^*$:

$$\mathcal{H} = \left(L^2(\mathbb{R}^N)\right)^* \otimes_M L^2(\mathbb{R}^N),$$

where the tensor product $\otimes_M$ is defined by

$$\mathcal{H} \ni \Psi(x,p) = (\varphi^* \otimes_M \psi)(x,p) = \frac{1}{(2\pi\hbar)^N} \int \mathrm{d}y\, e^{-\frac{i}{\hbar}py} \bar{\varphi}\left(x - \frac{1}{2}y\right) \psi\left(x + \frac{1}{2}y\right)$$

where $\varphi, \psi \in L^2(\mathbb{R}^N)$.

Pure states: $\varrho_{\text{pure}}(x,p) = (\varphi^* \otimes_M \varphi)(x,p)$ — Wigner functions

Quantum mechanics over configuration space

Quantum observables $A \in \mathcal{A}_Q$ treated as operators $\hat{A} = A \star_M$ take the form

$$A \star_M = \hat{1} \otimes_M A_W(\hat{q}, \hat{p}),$$

where $A_W(\hat{q}, \hat{p})$ is the function A of symmetrically ordered (Weyl ordered) operators of position and momentum: $\hat{q}^i = x^i$ and $\hat{p}_j = -i\hbar\partial_{x^j}$. In particular, from this it follows that

$$A \star_M \Psi = \varphi^* \otimes_M A_W(\hat{q}, \hat{p})\psi,$$

$$\Psi \star_M A = A_W^\dagger(\hat{q}, \hat{p})\varphi^* \otimes_M \psi,$$

for $\Psi = \varphi^* \otimes_M \psi$ and $\varphi, \psi \in L^2(\mathbb{R}^N)$.

Quantization in curvilinear canonical coordinates

Now, let us consider the $\star$-product in an arbitrary coordinate system (x, p). Let S denotes an isomorphism giving the equivalence with $\star_M$. Then the twisted tensor product, denoted by $\otimes_S$, can be defined by the formula

$$\varphi^* \otimes_S \psi := S(\varphi^* \otimes_M \psi),$$

and the new S-ordering by the formula

$$A_S(\hat{q}, \hat{p}) := (S^{-1}A)_W(\hat{q}, \hat{p}).$$

All previous formulas hold true provided that we replace the tensor product $\otimes_M$ with $\otimes_S$ and the Weyl ordering with S-ordering.

Quantization in curvilinear canonical coordinates

Transformation of states

$$(\varphi^* \otimes_M \psi) \circ T = (\hat{U}_T \varphi)^* \otimes_{S_T} \hat{U}_T \psi,$$

where

$$(\hat{U}_T \varphi)(x') = \varphi(\phi(x')) \in L^2(\mathcal{Q}, \mathrm{d}\mu), \quad \mathrm{d}\mu = |g|^{\frac{1}{2}}\, \mathrm{d}x'.$$

Transformation of operators

$$A'_{S_T}(\hat{q}', \hat{p}') \equiv (S_T^{-1}(A \circ T))_W(\hat{q}', \hat{p}') = \hat{U}_T A_W(\hat{q}, \hat{p}) \hat{U}_T^{-1},$$

where

$$\hat{q}'^i = \hat{U}_T Q^i(\hat{q}) \hat{U}_T^{-1} = x'^i,$$

$$\hat{p}'_i = \hat{U}_T (P_i)_W(\hat{q}, \hat{p}) \hat{U}_T^{-1} = -i\hbar \left(\partial_{x'^i} + \frac{1}{2} \Gamma^k_{ik}(x') \right),$$

and $T^{-1}(x, p) = (Q^1(x), \dots, P_N(x, p))$.

Quantization in curvilinear canonical coordinates

Example: Quantization in canonical spherical coordinates

Let us consider a canonical point transformation $T(r, \theta, \phi, p_r, p_\theta, p_\phi) = (x, y, z, p_x, p_y, p_z)$

$$\begin{aligned}
x &= r \sin\theta \cos\phi, \\
y &= r \sin\theta \sin\phi, \\
z &= r \cos\theta, \\
p_x &= \frac{r p_r \sin^2\theta \cos\phi + p_\theta \sin\theta \cos\theta \cos\phi - p_\phi \sin\phi}{r \sin\theta}, \\
p_y &= \frac{r p_r \sin^2\theta \sin\phi + p_\theta \sin\theta \cos\theta \sin\phi + p_\phi \cos\phi}{r \sin\theta}, \\
p_z &= \frac{r p_r \cos\theta - p_\theta \sin\theta}{r}.
\end{aligned}$$

and related isomorphism S_T:

$$
\begin{aligned}
S_T = \mathrm{id} + \frac{1}{4}\hbar^2 \Bigg[& \frac{1}{r^2}\partial_{p_r}^2 - \partial_{p_\phi}^2 + \frac{1}{2}\left(\frac{1}{\sin^2\theta} - 3\right)\partial_{p_\theta}^2 + \frac{1}{r\tan\theta}\partial_{p_r}\partial_{p_\theta} \\
& - \frac{1}{3}p_\phi\partial_{p_\phi}^3 - \frac{1}{3}p_\theta\partial_{p_\theta}^3 - \frac{1}{2}\sin\theta\cos\theta\partial_\theta\partial_{p_\phi}^2 + \frac{1}{\tan\theta}p_\phi\partial_{p_\theta}^2\partial_{p_\phi} \\
& - \frac{1}{2}p_\theta\partial_{p_\theta}\partial_{p_\phi}^2 + \frac{1}{\tan\theta}\partial_\phi\partial_{p_\theta}\partial_{p_\phi} - \frac{1}{2}r\sin^2\theta\partial_r\partial_{p_\phi}^2 - \frac{1}{2}r\partial_r\partial_{p_\theta}^2 \\
& + \frac{1}{r^2}p_\phi\partial_r^2\partial_{p_\phi} + \frac{1}{r^2}p_\theta\partial_{p_r}^2\partial_{p_\theta} - \sin\theta\left(\frac{1}{2}p_r\sin\theta - \frac{1}{r}p_\theta\cos\theta\right)\partial_{p_r}\partial_{p_\phi}^2 \\
& + \frac{1}{r}\partial_\phi\partial_{p_r}\partial_{p_\phi} - \frac{1}{2}p_r\partial_{p_r}\partial_{p_\theta}^2 + \frac{2}{r\tan\theta}p_\phi\partial_{p_r}\partial_{p_\theta}\partial_{p_\phi} + \frac{1}{r}\partial_\theta\partial_{p_r}\partial_{p_\theta}\Bigg] + o(\hbar^4).
\end{aligned}
$$

A quantum system after transformation to spherical coordinates will be described by a Hilbert space $L^2(V, \mathrm{d}\mu)$, where $V = (0,\infty)\times[0,\pi]\times[0,2\pi)$ and $\mathrm{d}\mu(r,\theta,\phi) = r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$.

Quantization in curvilinear canonical coordinates

The momentum operators associated to the spherical coordinate system take the form

$$\hat{p}_r = -i\hbar\left(\partial_r + \frac{1}{r}\right), \quad \hat{p}_\theta = -i\hbar\left(\partial_\theta + \frac{1}{2\tan\theta}\right), \quad \hat{p}_\phi = -i\hbar\partial_\phi.$$

Hydrogen atom

In the Cartesian coordinates, classical Hamiltonian H takes the form:

$$H(x,y,z,p_x,p_y,p_z) = \frac{p_x^2+p_y^2+p_z^2}{2m} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{\sqrt{x^2+y^2+z^2}}.$$

In the spherical coordinates it can be written in the form:

$$H'(r,\theta,\phi,p_r,p_\theta,p_\phi) = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2\sin^2\theta}\right) - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}.$$

Quantization in curvilinear canonical coordinates

The action of S_T on H' results in the following function

$$S_T^{-1}H' = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2\sin^2\theta}\right) - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} - \frac{\hbar^2}{8mr^2}\left(\frac{1}{\sin^2\theta} + 1\right).$$

From this it can be verified that to H' will correspond the following operator

$$H'_{S_T}(\hat{q},\hat{p}) = -\frac{\hbar^2}{2m}\left[\partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\left(\partial_\theta^2 + \frac{1}{\tan\theta}\partial_\theta + \frac{1}{\sin^2\theta}\partial_\phi^2\right)\right] - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}.$$

Note that the expression in square brackets is just the Laplace operator written in spherical coordinates.

Covariant representation of Hamiltonian operators

Classical Hamiltonians quadratic in momenta

Consider a Hamiltonian H in Euclidean coordinates

$$H(x,p) = \frac{1}{2}K^{ij}(x)p_i p_j + V(x),$$

where K^{ij} are components of some symmetric tensor K. In curvilinear coordinates (x', p') it takes a similar form

$$H'(x',p') = \frac{1}{2}K'^{ij}(x')p'_i p'_j + V(x').$$

Related quantum Hamiltonian

Using flatness property of the Levi-Civita connection of $g(x')$, we get

$$H'_{S_T}(\hat{q}', \hat{p}') = -\frac{\hbar^2}{2}\left(\nabla_i K'^{ij}\nabla_j + \frac{1}{4}K'^{ij}_{\ \ ;ij}\right) + V(x').$$

$\nabla_i K'^{ij}\nabla_j := \triangle_{K'}$: pseudo-Laplace operator.

Covariant representation of Hamiltonian operators

For a natural Hamiltonians, when $K'^{ij} = g^{ij}$:

$$H'_{S_T}(\hat{q}', \hat{p}') = -\frac{\hbar^2}{2} g^{ij} \nabla_i \nabla_j + V(x'),$$

$\nabla_i g^{ij} \nabla_j = g^{ij} \nabla_i \nabla_j \equiv \triangle$ — Laplace operator.

Consider a classical Hamiltonian H, which in curvilinear coordinates is

$$H'(x', p') = K'^{ijk}(x') p'_i p'_j p'_k,$$

where K'^{ijk} are components of some symmetric tensor K'.

Using flatness property of the Levi-Civita connection of $g(x')$, the related Hamiltonian operator takes the form

$$H'_{S_T}(\hat{q}', \hat{p}') = \frac{1}{2} i\hbar^3 \left(\nabla_i K'^{ijk} \nabla_j \nabla_k + \nabla_i \nabla_j K'^{ijk} \nabla_k + \frac{1}{4} \nabla_k K'^{ijk}{}_{;ij} + \frac{1}{4} K'^{ijk}{}_{;ij} \nabla_k \right).$$

Canonical quantization in Riemann space

Natural generalization: dropping flatness property of the connection + admissible generalization of S:

$$S = 1 + \frac{\hbar^2}{4!}\Big((3\Gamma^i_{rj}(x)\Gamma^r_{ik}(x) + \alpha R_{jk}(x))\partial_{p_j}\partial_{p_k} + 3\Gamma^i_{jk}(x)\partial_{x^i}\partial_{p_j}\partial_{p_k} \\ + \left(2\Gamma^i_{nr}(x)\Gamma^n_{jk}(x) - \partial_{x^r}\Gamma^i_{jk}(x)\right) p_i\partial_{p_j}\partial_{p_k}\partial_{p_r}\Big) + o(\hbar^4).$$

where R_{ij} is the Ricci tensor.

Canonical quantization in Riemann space

Quantization of Hamiltonians quadratic in momenta

$$H_S(\hat{q},\hat{p}) = -\frac{1}{2}\hbar^2\left(\nabla_i K^{ij}\nabla_j + \frac{1}{4}K^{ij}{}_{;ij} - \frac{1}{4}(1-\alpha)K^{ij}R_{ij}\right) + V.$$

In particular, when $K = g$

$$H_S(\hat{q},\hat{p}) = -\frac{1}{2}\hbar^2\left(\nabla_i g^{ij}\nabla_j - \frac{1}{4}(1-\alpha)R\right) + V,$$

where R is the scalar curvature.

Quantization of Hamiltonians cubic in momenta

$$H_S(\hat{q},\hat{p}) = \frac{1}{2}i\hbar^3\Big(\nabla_i K^{ijk}\nabla_j\nabla_k + \nabla_i\nabla_j K^{ijk}\nabla_k + \frac{1}{4}\nabla_k K^{ijk}{}_{;ij} + \frac{1}{4}K^{ijk}{}_{;ij}\nabla_k$$
$$- \frac{3}{4}(1-\alpha)\nabla_i K^{ijk}R_{jk} - \frac{3}{4}(1-\alpha)K^{ijk}R_{jk}\nabla_i\Big)$$

Ambiguities in quantization process

Alternative admissible quantization

Let us consider another invariant star product related to the decomposition of the classical Poisson tensor $\mathcal{P}$

$$f \star g = f \exp\left(\frac{1}{2} i\hbar \sum_k \overleftarrow{X}_k \overrightarrow{Y}_k - \frac{1}{2} i\hbar \sum_k \overleftarrow{Y}_k \overrightarrow{X}_k + P(\overleftarrow{X}_1 + \overrightarrow{X}_1, \ldots, \overleftarrow{Y}_N + \overrightarrow{Y}_N; \hbar) - P(\overleftarrow{X}_1, \ldots, \overleftarrow{Y}_N; \hbar) - P(\overrightarrow{X}_1, \ldots, \overrightarrow{Y}_N; \hbar)\right) g,$$

where P is some polynomial of $2N$ variables with coefficients dependent on $\hbar$, such that

$$\overline{P(X_1, \ldots, X_N, Y_1, \ldots, Y_N)} = P(Y_1, \ldots, Y_N, X_1, \ldots, X_N).$$

What is important, the complex-conjugation is the involution for this product as well.

Ambiguities in quantization process

An isomorphism S intertwining the previous star-product with the new one reads

$$S = \exp\big(P(X_1, \dots, Y_N; \hbar)\big).$$

Let us take $P(X_1, \dots, Y_N; \hbar) = -\frac{1}{8}\hbar^2 \sum_{k,j} X_k X_j Y_k Y_j$ and choose as the canonical star-product in a flat case the new product with $X_i = \partial_{x^i}$, $Y_i = \partial_{p_i}$ in a pseudo-Euclidean coordinates and choose the quantum observables $A_Q = A_C$. Such quantization is equivalent with the choice of standard Moyal star-product with another choice of quantum observables. Actually, for any curvilinear coordinates

$$A_Q = \exp\left(\frac{1}{4}\hbar^2 \sum_{k,j} \nabla_k \nabla_j \partial_{p_k} \partial_{p_j}\right) A_C.$$

Ambiguities in quantization process

Now, invariant quantization of a quadratic in momenta classical Hamiltonian gives the operator

$$H_S(\hat{q},\hat{p}) = -\frac{\hbar^2}{2}\nabla_i K^{ij}\nabla_j + V,$$

and for cubic in momenta term the related operator form

$$H_S(\hat{q},\hat{p}) = \frac{1}{2}i\hbar^3\left(\nabla_i K^{ijk}\nabla_j\nabla_k + \nabla_i\nabla_j K^{ijk}\nabla_k\right).$$

The extension onto non-flat case remains the same except the new form of quantum observable. So, with the particular choice $\alpha = 1$, Hamiltonian operators from previous slide are admissible quantum Hamiltonians for classical systems quadratic and cubic in momenta in any Riemann space. Such choice of quantization was called in a paper (Duval 2005) a "minimal" quantization, but was introduced ad'hoc without any justification from basic principles. Moreover, the same choice was done in by (Benenti 2002) in order to investigate quantum integrability and quantum separability of classical Stäckel systems.

1. Błaszak M. and Domański Z., *Phase space quantum mechanics*, Annals of Physics **327** (2012) 167
2. Błaszak M. and Domański Z., *Quantum trajectories*, Phys. Lett. **A 376** (2012) 3593
3. Błaszak M. and Domański Z., *Canonical transformations in quantum mechanics*, Annals of Physics **331** (2013) 70
4. Błaszak M. and Domański Z., *Canonical quantization of classical mechanics in curvilinear coordinates. Invariant quantization procedure.*, Annals of Physics **339** (2013) 89
5. Domański Z. and Błaszak M., *On equivalence of star-products in arbitrary canonical coordinates*, arXiv:1305.4026 [math-ph]
6. Błaszak M., Domański Z., Sergyeyev A. and Szablikowski B., *Integrable quantum Stäckel systems*, Phys. Lett. A **377** (2013) 2564