Quantization in arbitrary coordinate system and transformation of coordinates in quantum mechanics

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Replace x, y, z, p_x, p_y, p_z with operators of position and momentum:

$$\begin{aligned} x &\to \hat{q}_x = x, & p_x &\to \hat{p}_x = -i\hbar\partial_x, \\ y &\to \hat{q}_y = y, & p_y &\to \hat{p}_y = -i\hbar\partial_y, \\ z &\to \hat{q}_z = z, & p_z &\to \hat{p}_z = -i\hbar\partial_z. \end{aligned}$$

Note

Since operators of position and momentum do not commute they have to be appropriately ordered. We will use symmetric ordering of operators of position and momentum.

The result is an operator on the Hilbert space $L^2(\mathbb{R}^3)$:

$$\begin{aligned}\hat{H} &= -\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_z^2) + V(x, y, z) \\ &= -\frac{\hbar^2}{2m}\Delta + V(x, y, x).\end{aligned}$$

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Take a different coordinate system, e.g. spherical coordinate system:

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

Write the observable in new coordinates:

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

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Operators of position and momentum take the form:

$$\hat{q}_r = r, \qquad \hat{p}_r = -i\hbar\left(\partial_r + \frac{1}{r}\right),$$

$$\hat{q}_\theta = \theta, \qquad \hat{p}_\theta = -i\hbar\left(\partial_\theta + \frac{1}{2\tan\theta}\right),$$

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The resulting operator:

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

The operator $\hat{H}'$ is defined on the Hilbert space $L^2((0,\infty)\times[0,\pi)\times[0,2\pi),\mu)$, where $\mathrm{d}\mu(r,\theta,\phi) = r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$. Operators $\hat{H}$ and $\hat{H}'$ are not unitarily equivalent — they describe different quantum systems.

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The operator $\hat{H}'$ should have the following form:

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which we will receive by adding an appropriate correction term to the Hamiltonian $H'(r,\theta,\phi,p_r,p_\theta,p_\phi)$:

$$H'_\hbar(r,\theta,\phi,p_r,p_\theta,p_\phi) = H'(r,\theta,\phi,p_r,p_\theta,p_\phi) - \frac{\hbar^2}{8mr^2}\left(\frac{1}{\sin^2\theta}+1\right).$$

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To answer this question we have to move to deformation quantization approach to quantum mechanics.

Deformation quantization

It is possible to introduce a quantization of a classical Hamiltonian system (M, ω, H) by deforming the algebraic structure of the algebra of observables $C^\infty(M)$:

$$\cdot \quad \to \quad \star \quad \text{— noncommutative associative product}$$

$$\{\cdot, \cdot\} \quad \to \quad [\![\cdot, \cdot]\!] \quad \text{— deformed Poisson bracket}$$

where $[\![f, g]\!] = \frac{1}{i\hbar}(f \star g - g \star f)$.

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Note

In general it is possible to introduce a $\star$-product only on some pre-C^*-algebra $\mathcal{F}_\hbar(M) \subset C^\infty(M)$.

Example:
Introduce on M a flat torsionless symplectic connection ∇. Moreover, assume that M is almost geodesically simply connected: for every $x \in M$ there exists a neighborhood $U \subset M$ of x such that $M \setminus U$ is of measure zero, and every point in U can be connected with x by a unique geodesic. Then, we can define

$$(f \star g)(x) = \frac{1}{(\pi\hbar)^{2N}} \int_{T_x M} \int_{T_x M} f(\exp_x(u)) g(\exp_x(v)) e^{-\frac{2i}{\hbar}\omega_x(u,v)} \, \mathrm{d}u \, \mathrm{d}v$$

for $f, g \in C_c^\infty(M)$.

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for $f, g \in C_c^\infty(M)$.

Formal expansion in $\hbar$ of the $\star$-product:

$$f \star g = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i\hbar}{2}\right)^k \omega^{\mu_1\nu_1} \cdots \omega^{\mu_k\nu_k} (\underbrace{\nabla \cdots \nabla}_{k} f)_{\mu_1 \ldots \mu_k} (\underbrace{\nabla \cdots \nabla}_{k} g)_{\nu_1 \ldots \nu_k}.$$

We will focus on the case $M = T^*\mathcal{Q}$, where $\mathcal{Q}$ is an almost geodesically simply connected flat Riemannian manifold.

The Levi-Civita connection on $\mathcal{Q}$ can be lifted to a flat torsionless symplectic connection ∇ on M:

$$\mathbf{\Gamma}^{i}_{jk} = \Gamma^{i}_{jk}, \quad \mathbf{\Gamma}^{\bar{i}}_{\bar{j}k} = -\Gamma^{j}_{ik}, \quad \mathbf{\Gamma}^{\bar{i}}_{j\bar{k}} = -\Gamma^{k}_{ji},$$
$$\mathbf{\Gamma}^{\bar{i}}_{jk} = p_l(\Gamma^{r}_{jk}\Gamma^{l}_{ri} + \Gamma^{r}_{ik}\Gamma^{l}_{rj} - \Gamma^{l}_{ij,k}),$$

with the remaining components equal zero ($\bar{i} = N + i$).

In the special case $\mathcal{Q} = \mathbb{R}^N$ with the standard metric tensor and $M = T^*\mathbb{R}^N \cong \mathbb{R}^{2N}$ we arrive at the Moyal product

$$(f \star_M g)(x) = \frac{1}{(\pi\hbar)^{2N}} \int_{\mathbb{R}^{2N}} \int_{\mathbb{R}^{2N}} f(x+u)g(x+v)e^{-\frac{2i}{\hbar}\omega_{\mu\nu}u^\mu v^\nu} \, \mathrm{d}u \, \mathrm{d}v,$$

where

$$(\omega_{\mu\nu}) = \begin{pmatrix} 0_N & -I_N \\ I_N & 0_N \end{pmatrix}.$$

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Formal expansion in $\hbar$ of the $\star_M$-product:

$$\begin{aligned} f \star_M g &= f \exp\left(\frac{i\hbar}{2}\omega^{\mu\nu}\overleftarrow{\partial}_{x^\mu}\overrightarrow{\partial}_{x^\nu}\right) g \\ &= \sum_{k=0}^{\infty} \frac{1}{k!}\left(\frac{i\hbar}{2}\right)^k \omega^{\mu_1\nu_1}\cdots\omega^{\mu_k\nu_k}(\partial_{x^{\mu_1}}\cdots\partial_{x^{\mu_k}} f)(\partial_{x^{\nu_1}}\cdots\partial_{x^{\nu_k}} g). \end{aligned}$$

Coordinate systems

Let

$$M \supset U \ni x \mapsto (x^1(x), \dots, x^{2N}(x)) \in V \subset \mathbb{R}^{2N}$$

be a coordinate system on the phase space M. We will only consider coordinate systems which are almost global, i.e. $M \setminus U$ is of measure zero.

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The $\star$-product on M can be written in coordinates $(x^1, \ldots, x^{2N})$ resulting in a star-product on a subset $V \subset \mathbb{R}^{2N}$. We will denote such star-product by $\star^{(x)}$.

Coordinate system $(x^1, \dots, x^{2N})$ is called quantum canonical if there holds

$$[\![x^\alpha, x^\beta]\!] = \mathcal{J}^{\alpha\beta},$$

where

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Denote $(x^1, \dots, x^{2N})$ by $(q^1, \dots, q^N, p_1, \dots, p_N) \equiv (q^i, p_j)$. Then the quantum canonicity condition takes the form

$$[\![q^i, q^j]\!] = [\![p_i, p_j]\!] = 0, \quad [\![q^i, p_j]\!] = \delta^i_j.$$

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If $(q^1, \dots, q^N)$ is an almost global coordinate system on $\mathcal{Q}$ then the induced canonical coordinate system $(q^1, \dots, q^N, p_1, \dots, p_N)$ is classical and quantum canonical.

Main observation:
For any coordinate system $(x^1, \dots, x^{2N})$ on the symplectic manifold (M, ω), which is at the same time classical and quantum canonical, there exists a unique morphism S such that

$$S(f \star_M^{(x)} g) = Sf \star^{(x)} Sg,$$
$$Sx^\alpha = x^\alpha,$$
$$\overline{Sf} = S\bar{f}.$$

The morphism S gives an equivalence of the $\star$-product written in $(x^1, \dots, x^{2N})$ coordinates with the product $\star_M$ which in $(x^1, \dots, x^{2N})$ coordinates takes the form of the Moyal product.

The morphism S can be formally expanded into a power series

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

where

$$S_{2k} = \sum_{n=1}^{\infty} \frac{1}{n!} [x^{\alpha_1}, \ldots, [x^{\alpha_{n-1}}, F^{\alpha_n}]] \partial_{\alpha_1} \cdots \partial_{\alpha_n},$$
$$S_{2k-1} = 0,$$

for $k = 1, 2, \ldots$, $F^\alpha = \sum_{l=1}^{k} \left(-\frac{1}{4}\right)^l A^\alpha_{2l} S_{2(k-l)}$ and

$$A^\alpha_k f = \frac{1}{k!} \omega^{\mu_1 \nu_1} \ldots \omega^{\mu_k \nu_k} (\underbrace{\nabla \cdots \nabla}_{k} x^\alpha)_{\mu_1 \ldots \mu_k} (\underbrace{\nabla \cdots \nabla}_{k} f)_{\nu_1 \ldots \nu_k}.$$

From previous formulas:

$$S = \mathrm{id} + \hbar^2 \left(-\frac{1}{24} \mathbf{\Gamma}_{\alpha\beta\gamma} \partial^\alpha \partial^\beta \partial^\gamma + \frac{1}{16} \mathbf{\Gamma}^\mu_{\nu\alpha} \mathbf{\Gamma}^\nu_{\mu\beta} \partial^\alpha \partial^\beta \right) + O(\hbar^4),$$

where $\mathbf{\Gamma}_{\alpha\beta\gamma} = \omega_{\alpha\delta} \mathbf{\Gamma}^\delta_{\beta\gamma}$ and $\partial^\alpha = \omega^{\alpha\beta} \partial_{x^\beta}$.

Spherical coordinates:

$$S = \mathrm{id} + \hbar^2 \Bigg(-\frac{1}{12} p_\phi \partial_{p_\phi}^3 - \frac{1}{4}\partial_{p_\phi}^2 - \frac{1}{8}\sin\theta\cos\theta\partial_\theta\partial_{p_\phi}^2 - \frac{1}{12} p_\theta \partial_{p_\theta}^3 + \frac{1}{4\sin^2\theta} p_\phi \partial_{p_\theta}^2\partial_{p_\phi} - \frac{1}{4} p_\phi \partial_{p_\theta}^2 \partial_{p_\phi} + \frac{1}{8\sin^2\theta}\partial_{p_\theta}^2 - \frac{3}{8}\partial_{p_\theta}^2 - \frac{1}{8} p_\theta \partial_{p_\theta}\partial_{p_\phi}^2 + \frac{1}{4\tan\theta}\partial_\phi\partial_{p_\theta}\partial_{p_\phi} - \frac{1}{8} r\sin^2\theta\partial_r\partial_{p_\phi}^2 - \frac{1}{8} r\partial_r\partial_{p_\theta}^2 + \frac{1}{4r^2} p_\phi \partial_r^2 \partial_{p_\phi} + \frac{1}{4r^2} p_\theta \partial_{p_r}^2 \partial_{p_\theta} + \frac{1}{4r^2}\partial_{p_r}^2 - \frac{1}{8} p_r \sin^2\theta\partial_{p_r}\partial_{p_\phi}^2 - \frac{1}{4r} p_\theta \sin\theta\cos\theta\partial_{p_r}\partial_{p_\phi}^2 + \frac{1}{4r}\partial_\phi\partial_{p_r}\partial_{p_\phi} - \frac{1}{8} p_r \partial_{p_r}\partial_{p_\theta}^2 + \frac{1}{2r\tan\theta} p_\phi \partial_{p_r}\partial_{p_\theta}\partial_{p_\phi} + \frac{1}{4r}\partial_\theta\partial_{p_r}\partial_{p_\theta} + \frac{1}{4r\tan\theta}\partial_{p_r}\partial_{p_\theta} \Bigg) + O(\hbar^4).$$

To phase space functions f in Moyal quantization correspond symmetrically ordered functions $f(\hat{q}, \hat{p})$ of operators $\hat{q}^i = q^i$, $\hat{p}_j = -i\hbar \left(\partial_{q^j} + \frac{1}{2} \Gamma^k_{jk} \right)$.

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Using the fact that for a given coordinate system $(x^1,\dots,x^{2N})$ our quantization is equivalent with the Moyal quantization we can arrive at the formula for the operators corresponding to functions defined on M:

$$f \mapsto f_\hbar(\hat{q},\hat{p}),$$

where $f_\hbar = S^{-1}f = f - \hbar^2 S_2 f + O(\hbar^4)$ is a function f extended with appropriate correction terms.

Transformations of coordinates

Let $(q^1, \dots, q^N)$ and $(q'^1, \dots, q'^N)$ be two coordinate systems on $\mathcal{Q}$, wherease $(q^1, \dots, q^N, p_1, \dots, p_N)$ and $(q'^1, \dots, q'^N, p'_1, \dots, p'_N)$ induced canonical coordinate systems on M. Moreover, let

$$\phi\colon (q'^1, \dots, q'^N) \mapsto (q^1, \dots, q^N),$$
$$T\colon (q'^1, \dots, q'^N, p'_1, \dots, p'_N) \mapsto (q^1, \dots, q^N, p_1, \dots, p_N)$$

be corresponding transformations of coordinates. Then

$$f'_\hbar(\hat{q}', \hat{p}') = \hat{U}_T f_\hbar(\hat{q}, \hat{p}) \hat{U}_T^{-1},$$

where $f' = f \circ T$ and

$$(\hat{U}_T \psi)(q') = \psi(\phi(q')).$$

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If $T^{-1}(q,p) = (Q^1(q,p),\dots,Q^N(q,p),P_1(q,p),\dots,P_N(q,p))$ is a transformation to the coordinate system (q'^i,p'_j), then the maps Q^i,P_j are observables of position and momentum corresponding to the coordinate system (q'^i,p'_j). We get

$$\hat{q}'^i = \hat{U}_T Q^i(\hat{q},\hat{p})\hat{U}_T^{-1}, \quad \hat{p}'_j = \hat{U}_T P_j(\hat{q},\hat{p})\hat{U}_T^{-1}.$$

For a general symplectic manifold M with a flat torsionless symplectic connection ∇ and an almost global coordinate system

$$M \supset U \ni x \mapsto (q^1(x), \dots, q^N(x), p_1(x), \dots, p_N(x)) \in T^*V \cong V \times \mathbb{R}^N \subset \mathbb{R}^{2N},$$

which is classical and quantum canonical the whole procedure can be repeated: induced connection on T^*V can be projected to V and then we construct a metric tensor for which the projected connection is a Levi-Civita connection.

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The unitary operator corresponding to a transformation of coordinates:

$$(\hat{U}_T\psi)(q') = \frac{1}{(2\pi\hbar)^{N/2}} \int_V \psi(q) e^{-\frac{i}{\hbar}F(q,q')}\, \mathrm{d}\mu(q),$$

where $F(q, q')$ is a generating function of the coordinate transformation:

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

Literature

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Thank you!