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Canonical transformations in quantum mechanics

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ABSTRACT

This paper presents the general theory of canonical transformations of coordinates in quantum mechanics. First, the theory is developed in the formalism of phase space quantum mechanics. It is shown that by transforming a star-product, when passing to a new coordinate system, observables and states transform as in classical mechanics, i.e., by composing them with a transformation of coordinates. Then the developed formalism of coordinate transformations is transferred to a standard formulation of quantum mechanics. In addition, the developed theory is illustrated on examples of particular classes of quantum canonical transformations.

1. Introduction

In classical Hamiltonian mechanics transformations of phase space coordinates (especially canonical transformations of coordinates) are an important part of the theory. Since quantum mechanics arises from Hamiltonian mechanics it is natural to ask if it is possible to introduce the concept of canonical transformations of coordinates in quantum mechanics. The importance of this problem was evident to scientists from the early days of quantum theory. The development of the theory of canonical transformations of coordinates in quantum mechanics is mainly contributed to Jordan, London and Dirac back in 1925 [1–7] and it is still an area of intense research.

In the usual approach to canonical transformations in quantum mechanics one identifies canonical transformations with unitary operators defined on a Hilbert space. Such an approach was used by Mario Moshinsky and his collaborators in a series of papers [8–12]. Also other researchers used such an approach [13–15]. Worth noting are also papers of [16,17] where an extension of canonical

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transformations to non-unitary operators is presented. Nevertheless, after so many years of effort, there is still a lack of a general theory of coordinate transformations in quantum mechanics, including a satisfactory complete theory of canonical transformations. With the following paper we are trying to fill this gap, at least to some extent.

A unitary operator $\hat{U}$ associated with some canonical change of coordinates transforms vector states from one coordinate system to the other: $\phi' = \hat{U}\phi$. Also observables, being operators on a Hilbert space of states, transform according to a prescription

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^{-1}, \tag{1}$$

where $\hat{A}$ is an initial operator and $\hat{A}'$ an operator after the change of coordinates. In particular, operators $\hat{q}, \hat{p}$ of position and momentum transform according to (1). Observe that the commutator of operators of position and momentum as well as their Hermitian property do not change after a unitary transformation. For this reason unitary operators are identified with canonical transformations.

To some unitary operators one can try to associate transformations defined on a classical phase space. It can be done using Weyl quantization rule. This rule formulated by Hermann Weyl [18,19] states that to every classical observable $A(x, p)$ (real-valued function defined on a phase space) written in a Cartesian coordinate system one can associate an operator on a Hilbert space by substituting for x and p operators of position and momentum $\hat{q}$, $\hat{p}$ and symmetrically ordering them. If one now considers a transformation of phase space coordinates (possibly depending on an evolution parameter t)

$$T = (Q, P): \mathbb{R}^2 \supset U \to W \subset \mathbb{R}^2,$$

then one can define operators

$$\hat{Q} = Q(\hat{q}, \hat{p}, t),$$
$$\hat{P} = P(\hat{q}, \hat{p}, t).$$

If $[\hat{Q}, \hat{P}] = i\hbar$ then the operators $\hat{Q}$, $\hat{P}$ can be thought of as operators of position and momentum associated to a new coordinate system, and T is then called a quantum canonical transformation. In some cases the operator $\hat{Q}$ can be written in a position representation, i.e., as an operator of multiplication by a coordinate variable. In fact, there exist a measure μ and a unitary operator $\hat{U}_T : \mathcal{H} \to L^2(\sigma(\hat{Q}), \mu)$ such that

$$\hat{U}_T\hat{Q}\hat{U}_T^{-1} = x',$$

where $\sigma(\hat{Q})$ is the spectrum of the operator $\hat{Q}$. The operator $\hat{U}_T$ is precisely the unitary operator corresponding to the quantum canonical transformation T.

At this point we arrive to a problem concerning Weyl quantization procedure. Namely, we could try to quantize a classical Hamiltonian system in some arbitrary canonical coordinate system using Weyl quantization rule. However, this way we would end up in non-equivalent quantum systems. As an example let us consider a classical harmonic oscillator which time evolution is governed by the Hamiltonian

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

In accordance with Weyl quantization rule to H corresponds the following operator

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

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

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