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Model of Hydrogen Atom Quantum Measurements on Rigged Hilbert Spaces

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The measurement procedure makes the isolated (closed) quantum system to be the open one. The operators of observables of rather simple explicit form are converted into pseudo-differential operators of more complex form. The author has proposed the method of establishing consistency between the theoretical data of conventional quantum mechanics of (isolated) quantum objects and experimental data on the measured values of the observables of corresponding open quantum objects. In this paper, the proposed correspondence is used for the construction of rigged Hilbert spaces, in which the operators of measured the observables of hydrogen-like atom admit spectral decomposition.

Key words and phrases: operator of measured quantum observable, rigged Hilbert space, spectral decomposition of unbounded self-adjoint operator.

1. Introduction

Let us recall the basic structures of quantum measurement model in Kuryshkin-Wodkiewicz and Kuryshkin-Weil representations.

The configuration space of an isolated physical object (for example, the Kepler problem - a hydrogen atom) $Q = \mathbb{R}^3$, the phase space $T^*Q = \mathbb{R}^3 \oplus \mathbb{R}^3$. Classical observables $A(q,p)$ are distributions on the phase space [1–3] of the object (system). According to the Weyl rule of quantization [4–7] quantum observables $O_W(A)$ are self-adjoint (unbounded) operators in rigged Hilbert space $\Phi \subset H = L_2(Q) \subset \Phi^*$.

The results of Shewell-Kuryshkin [8–10] on a one-to-one correspondence of quantization rules and quantum distribution functions (QDFs) puts the Weil rule into correspondence with Wigner QDF, so that

$$\langle A \rangle_\psi = (O_W(A)\psi, \psi) = \int A(q,p) W_\psi(q,p)\, dqdp \tag{1}$$

or, more generally,

$$\langle A \rangle_\rho = Tr\,(O_W(A)\rho) = \int A(q,p) W_\rho(q,p)\, dqdp. \tag{2}$$

In [11–13] on the basis of statistical correspondence, formulated by Blokhintsev and Terletsky, is developed the model of quantum mechanics with nonnegative QDF. Kuryshkin quantization rule to each $A(q,p)$ and some function $\phi \in H = L_2(Q)$ or density matrix ρ assigns the operator an explicit form of which is convenient to write with the help of auxiliary functions. Namely, to each function $\phi(q) \in L_2(Q)$, we assign its Fourier image $\tilde{\phi}(p) \in L_2(Q)$ and an auxiliary function

$$\Phi(q,p) = \frac{\exp\left\{\frac{i}{\hbar}(q,p)\right\}}{(2\pi\hbar)^{3/2}} \phi(q)\, \tilde{\phi}^*(p)$$

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on the phase space. To each mixed state $\rho = \sum_k c_k |\phi_k\rangle \langle\phi_k|$ we assign an auxiliary function

$$\Phi(q,p) = \frac{\exp\left\{\frac{i}{\hbar}\right\}}{(2\pi\hbar)^{3/2}} \sum_k \phi_k(q)\, \tilde{\phi}_k^*(p).$$

Then the rule for constructing operators of quantum mechanics with nonnegative QDF can be summarized as follows: the classical function $A(q,p)$ corresponds to a linear operator $O(A)$, whose action on an arbitrary function $\psi(q)$admitting the Fourier transform is defined by the equation:

$$O_{\phi,\rho}(A)\,\psi(q) = (2\pi\hbar)^{-3} \int \Phi_{\phi,\rho}(\xi - q, \eta - p)\, A(\xi,\eta)\, e^{\frac{i}{\hbar}((q-q')p)} \psi(q')\, d\xi d\eta dp dq. \tag{3}$$

The mean values of the operators (3) represented as

$$\langle A\rangle_\psi^\phi = (O_\phi(A)\,\psi, \psi) = \int A(q,p) F_\psi^\phi(q,p)\, dqdp, \tag{4}$$

where

$$F_\phi(q,p) = (2\pi\hbar)^{-3} \left| \int \phi^*(q-\xi)\,\psi(\xi)\, e^{-\frac{i}{\hbar}(\xi,p)} d\xi \right|^2$$

or, more generally,

$$\langle A\rangle_{\rho 1}^\rho = Tr\left(O_\rho(A)\,\rho_1\right) = \int A(q,p) F_{\rho 1}^\rho(q,p)\, dqdp, \tag{5}$$

where

$$F_{\rho 1}^\rho(q,p) = (2\pi\hbar)^{-3} \sum_k c_k \sum_j c_j \left| \int \phi_k^*(q-\xi)\,\psi_j(\xi)\, e^{-\frac{i}{\hbar}(\xi,p)} d\xi \right|^2$$

and

$$\rho_1 = \sum_j c_j |\psi_j\rangle \langle\psi_j|.$$

In [14–16] shown that the relation (5) may be written in an equivalent manner in the form proposed by Wodkiewicz [17, 18]. Namely

$$\langle A\rangle_{\rho 1}^\rho = \int A(q,p) P_{\rho 1}^\rho(q,p)\, dqdp, \tag{6}$$

where QDF of Wodkiewicz $P_{\rho 1}^\rho(q,p)$ is given by convolution of two Wigner functions

$$P_{\rho 1}^\rho(q,p) = (W_\rho * W_{\rho 1})(q,p). \tag{7}$$

One of them is QDF of a mixed state ρ_1 of a quantum object, the other is QDF of a mixed state ρ of the quantum filter instrument.

For pure state relations (6) and (7) retain the same form. These formulations allowed [19] to prove that the operator of the measured observable $O_\rho(A)$ is given by the Weyl quantization rule for the "measured" classical observable $O_W(A_\rho)$, where $A_\rho(q,p) = (A * W_\rho)(q,p)$ and $W_\rho(q,p)$ are Wigner's QDFs.

Theorem 1. *Quantization rule of Kuryshkin-Weil (3) to each of slowly increasing generalized functions $A(q,p)$ associates Weyl operator $O_W(A * W_\rho)$, where W_ρ is QDF Wigner of density matrix $\rho = \sum_k c_k |\phi_k\rangle \langle\phi_k|$ of the quantum filter.*

2. Kuryshkin-Wodkiewicz construction in Kuryshkin-Weil representation

This theorem makes it possible to build a rigged Hilbert space (RHS), provides spectral decomposition of the operator having mixed, discrete and continuous spectrum. In [20–22] and [23–25] conducted theoretical and mathematical studies of the structure of the RHS needed to describe the quantum system with the Hamiltonian $\hat{H} = O_W(H)$ and the Schrödinger equation $i\hbar\frac{\partial}{\partial t}\psi(t) = H\psi(t)$. Further, in [26] stated that the operator $O_W(A_\rho)$ satisfies the Schrödinger–Heisenberg equation,

$$\frac{dO_\rho(A)}{dt} = \left\{\left(\hat{L}^+_{\vec{p}}, \hat{L}^-_{\vec{q}}\right) - Ze^2\left(\hat{L}^+_{|\vec{q}|}\right)^{-3}\left(\hat{L}^+_{\vec{q}}, \hat{L}^-_{\vec{p}}\right)\right\} O_\rho(A) \tag{8}$$

that coincides with the Dirac equation

$$\frac{dO_\rho(A)}{dt} = \frac{1}{i\hbar}\left[O_\rho(A), O_W(H)\right] \tag{9}$$

on those operators for whom the latter relation is uniquely determined.

Let us recall briefly the arguments of [24] on the need to use the RHS to model quantum systems in order to justify in a similar manner the need for the RHS to model quantum measurements.

To find the eigenfunctions (classical and generalized) of the operator $O_\rho(H)$ first by von Neumann for bounded operators (with a discrete spectrum) in a Hilbert space, then by Gelfand and Vilenkin for unbounded operators (with mixed spectrum) in a rigged Hilbert space was justified spectral decomposition of essentially self-adjoint operators.

In addition to eigenfunctions of the operator's $O_\rho(H)$ the interpretation of the theory of quantum measurements needed in "observed average measured observable H (using quantum filter of measuring apparatus in the state ρ) in the state ψ"

$$\langle\psi, O_\rho(H)\,\psi\rangle \ \text{ or } Tr\left(O_\rho(H)\,\rho_1\right) \tag{10}$$

in the state $\rho_1 = \sum\limits_j c_j\,|\psi_j\rangle\langle\psi_j|$, and the dispersion of the measured values H in the state $\rho_1 = \sum\limits_j c_j\,|\psi_j\rangle\langle\psi_j|$.

From (10), (11) we see that we need such vectors $\psi \in L_2(Q)$ and their combination in mixed states which belong to the domains of $O_\rho(H)$ and of $O_\rho\left(H^2\right)$. It is possible by formal reasoning of the solution of the equation (8) or (9) in the form of the operator exponential, power series expansion of Taylor, to show that the state $\psi \in L_2(Q)$ on which these solutions are well defined, belongs to the domain of degrees of the measured observable $\psi \in D\left(O_\rho(H^n)\right)$.

Thus, the quantum mechanics of the measured values $O_\rho(H)$ is not functioning either in $H = L_2(Q)$and in $D\left(O_\rho(H)\right)$, but is functioning in the dense subspace Φ of infinitely differentiable functions on the configuration space Q, decreasing at infinity faster than any polynomial. By analogy with [20–25] let us postulate on the subspace $\Phi \subset H = L_2(Q)$ a countable system of norms.

3. Rigged Hilbert space with the system of norms, generated by operators of the measured observable of hydrogen-like atom

Let us consider the operators of the measured observables $O_\rho(\vec{q})$, $O_\rho(\vec{p})$ $O_\rho(H)$ and their degrees, which depend on the original quantum object (a hydrogen atom), on the state ρ of the quantum filter and maybe some other parameters of original

Hilbert space $\Phi \subset H = L_2(Q)$. Let us recall the marginal probability densities given by the integrals [27]

$$\alpha_0(\vec{q}) = \int \Phi(\vec{q}, \vec{p}) d\vec{p}$$

and

$$\beta_0(\vec{q}) = \int \Phi(\vec{q}, \vec{p}) d\vec{q}.$$

With their help, in [27] are built:

– operators $O_\rho(A(\vec{q})) = \int \alpha_0\left(\vec{\xi}\right) A\left(\vec{q} + \vec{\xi}\right) d\vec{\xi}$, in particular, the operators

$$O_\rho\left(\prod_{j=1}^{3} q_j^{nj}\right) = \prod_{j=1}^{3} \left\{ \sum_{kj=0}^{nj} C_{nj}^{kj} \left\langle q_j^{kj} \right\rangle_0 q_j^{nj-kj} \right\}, \tag{A1}$$

where $\langle A(\vec{q}) \rangle_0 = \int \alpha_0(\vec{q}) A(\vec{q})\, d\vec{q}$,

– operators $O_\rho(A(\vec{p})) = \int \beta_0(\vec{\eta}) A\left(\vec{\eta} - i\hbar\vec{\nabla}\right) d\vec{\eta}$, in particular, the operators

$$O_\rho\left(\prod_{j=1}^{3} p_j^{nj}\right) = \prod_{j=1}^{3} \left\{ \sum_{kj=0}^{nj} C_{nj}^{kj} \left\langle p_j^{kj} \right\rangle_0 \left(-i\hbar \frac{\partial}{\partial q_j}\right)_j^{nj-kj} \right\}, \tag{A2}$$

where $\langle A(\vec{p}) \rangle_0 = \int \beta_0(\vec{p}) A(\vec{p})\, d\vec{p}$.

For building an explicit form of the operator $O_\rho(H)$ one need more specific information on the construction, in particular in [28] is proposed a method of constructing the operators $O_\rho(H)$ of a hydrogen atom with the Hamiltonian function $H(\vec{q}, \vec{p}) = \frac{\vec{p}^2}{2\mu} - \frac{Ze^2}{|\vec{q}|}$ via the basis of Sturmian functions of the hydrogen atom. The results of calculation with a mixed states $\rho = \sum\limits_k c_k |\phi_k\rangle \langle\phi_k|$ and $\phi_k(\vec{q}) = St_{nl}\left({}^{q}\!/_{b_{nl}}\right) Y_{lm}(\vartheta, \phi)$, $k = (n, l, m)$ give

$$O_\rho\left(\frac{\vec{p}^2}{2\mu}\right) = O_W\left(\frac{\vec{p}^2}{2\mu}\right) + \frac{\hbar^2}{2\mu} \sum_k \frac{c_k}{b_k^2} \tag{A3}$$

and

$$O_\rho\left(-\frac{Ze^2}{|\vec{q}|}\right) = O_W\left(-\frac{Ze^2}{|\vec{q}|}\right) + \sum_k c_k V_k(q, \cos\theta; b_k). \tag{A4}$$

A notion of an abstract rigged Hilbert space and its classic implementation are given in [29,30]. It's Hilbert space $H = L_2(Q)$ and a subset S of infinitely differentiable functions $\psi \in H$ that decrease at infinity faster than any polynomial, so that the quantities $\|\psi\|_{n,l}$ are limited for each function $\psi \in S$:

$$\|\psi\|_{n,l} = \max_{\vec{q} \in Q} \left| \left(1 + |\vec{q}|^2\right)^n \frac{\partial^{l_1+l_2+l_3}\psi}{\partial q_1^{l_1} \partial q_2^{l_2} \partial q_3^{l_3}} (\vec{q}) \right|. \tag{11}$$

The values $\|\psi\|_{n,l}$ define a countable system of norms in the space S (Schwartz space). Three continuously embedded spaces

$$S \subset H = L_2(Q) \subset S', \quad S \subset H = L_2(Q) \subset S^*, \tag{12}$$

where S' (S^*) is a space conjugate (anti conjugate) to S, i.e. the space of linear (antilinear) functionals continuous in the topology defined by the system (11) of norms$\|\psi\|_{n,l}$ define a rigged Hilbert space.

In [23–25] is built a system of norms $\|\psi\|_{n,l,m}$, generated by observable operators of an isolated quantum system

$$\|\psi\|_{n,l,m} = \int \left|O_W\left(p^n\right)O_W\left(q^l\right)O_W\left(H^m\right)\psi\left(q\right)\right|dq. \tag{13}$$

In this case, the space Φ of infinitely differentiable rapidly decreasing functions continuously (with respect to all norms$\|\psi\|_{n,l,m}$) embedded in $H = L_2\left(Q\right)$, invariant with respect to the Schrödinger equation in the Heisenberg representation $i\hbar\frac{dO_W(A)}{dt} = \left[O_W\left(A\right), O_W\left(H\right)\right]$.

For the model of quantum measurements, i.e., for quantum mechanics with non-negative QDF, the system of norms (13) takes the form

$$\|\psi\|^{\rho}_{n,l,m} = \int \left|O_\rho\left(\vec{p}^{2n}\right)O_\rho\left(\vec{q}^{2l}\right)O_\rho\left(H^m\right)\psi\left(\vec{q}\right)\right|d\vec{q}. \tag{14}$$

The space Φ^ρ of infinitely differentiable rapidly decreasing functions continuously (with respect to all norms $\|\psi\|^{\rho}_{n,l,m}$) embedded in $H = L_2\left(Q\right)$, is invariant with respect to the Schrödinger equation in the Heisenberg representation of the form (8) and (9).

The system of norms (14) by virtue of (A1)–(A4) is equivalent to the system of norms

$$\|\psi\|^{\rho}_{n,l,m} = \int \left|\left(1+|\vec{q}^2|\right)^n\left(1+\Delta\right)^l O_\rho\left(H^m\right)\psi(\vec{q})\right|d\vec{q}.$$

Thus, the construction of nuclear rigged Hilbert spaces is modified for the model of quantum measurements. It should be noted that the explicit form of the operators $O_\rho\left(H^m\right)$, the moments of measured energy, is properly described in [31], but wrongly described in [32].

4. Conclusion

One of the important problems in the description of quantum-mechanical systems is to describe the characteristics of the measurement results, for example, spectral data of systems. After all the measured characteristics of quantum objects tell us the properties of these objects The author has proposed the method of establishing consistency between the theoretical data of conventional quantum mechanics of (isolated) quantum objects and experimental data on the measured values of the observables of corresponding open quantum objects. The measurement procedure makes the isolated (closed) quantum system to be the open one The operators of observables of rather simple explicit form are converted into pseudo-differential operators of more complex form. In this paper, the proposed correspondence is used for the construction of rigged Hilbert spaces, in which the operators of measured the observables of hydrogen-like atom admit spectral decomposition. Thus, the applicability of stable numerical method of investigation of discrete spectra of the measured quantum observables is proved.

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Модель квантовых измерений водородоподобного атома в оснащенном гильбертовом пространстве

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Процедура измерения превращает изолированную (замкнутую) квантовую систему в открытую. При этом операторы наблюдаемых достаточно простого явного вида преобразуются в псевдо-дифференциальные операторы более сложного вида. Ранее автором был предложен метод установления соответствия между теоретическими данными общепринятой квантовой механики (изолированных) квантовых объектов и экспериментальными данными об измеренных значениях наблюдаемых соответствующих открытых квантовых объектов. В настоящей работе предложенное соответствие использовано для построения оснащенного гильбертова пространства, в котором операторы измеренных наблюдаемых водородоподобного атома допускают спектральное разложение.

Ключевые слова: оператор измеренной квантовой наблюдаемой, оснащенное гильбертово пространство, спектральное разложение неограниченных самосопряженных операторов.

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