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Kuryshkin-Wodkiewicz Model of Quantum Measurements for Atoms and Ions with One Valence Electron

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The structural form of the Kuryshkin-Wodkiewicz model of quantum measurement was developed in detail for quantum Kepler problem. For more complex objects such quantum structure is unknown. At the same time, a standard (non-structural) model of quantum measurement proposed by Holevo-Helstrom is suitable for any quantum object. The aim of this work is to spread the structural model of quantum measurement to a broader class of quantum objects — a model of quantum measurements of optical spectra of atoms and ions with one valence electron.

In this work the Kuryshkin-Wodkiewicz model with implementation of Weyl-Kuryshkin quantization rule is applied to the extended quantum Kepler problem of quantum systems with one valence electron, such as alkali metal atoms. The proof of the consistency of the model is based on two Kato theorems about compact perturbations of operators. In the proof process the explicit form of the discrete spectrum of the valence electron for various spectral series was achieved with dependence on the serial parameters of the disturbance spectrum of an isolated object in the process of quantum measurement.

Key words and phrases: quantum measurement models, quantization rule, a relatively compact perturbation of the observable operator, perturbation of the observable discrete spectrum

1. Introduction

The energy spectrum $E_n = -\frac{R}{2n^2}$ of the valence electron in a hydrogen atom is described by a discrete spectrum of the Hamiltonian operator $\hat{H} = -\frac{\Delta}{2} - \frac{1}{r}$ of the quantum Kepler problem with the Hamiltonian function $H(q,p) = \frac{\vec{p}^2}{2m} - \frac{e^2}{|\vec{r}|}$. The measured spectrum of the valence electron, except from the operator, is also dependent on the quantum state $\hat{\rho}$ of the probe of the measuring instrument, i.e. It is described by a discrete spectrum of the measured observable $O_\rho(H) = O_W(H * W_\rho.)$ [1, 2].

The constructive form of the Kuryshkin-Wodkiewicz model of quantum measurement is developed in detail for quantum Kepler problem [3] and quantum oscillator [4, 5]. For more complex objects such quantum construction is unknown. At the same time, a standard (non-constructive) model of quantum measurements of Holevo-Helstrom is suitable for any quantum object, any quantum system [6, 7].

The aim of this work is to spread the constructive model (of quantum measurements) of Kuryshkin-Wodkiewicz to a wider class of quantum objects, to construct a model of quantum measurements of optical spectra of atoms and ions with one valence electron. Hydrogen-like atoms - a hydrogen atom, muonic atoms, ions of different charges with a single electron. We are interested in the atoms of the alkali metals, consisting of a core (a nucleus together with all the filled electron shells) and the valence electron and ions with one valence electron.

2. Hydrogen-Like Atoms

Theory of the hydrogen atom in quantum mechanics is a theory of an electron in a hydrogen atom. Its energy spectrum under theoretical analysis where electron is treated

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as an isolated quantum object has a very simple form

$$E_n = -\frac{R}{2n^2} \tag{1}$$

The measurement process violates the isolated state of the quantum object, transferring it to an open state, forming a part of a complex system: "object+probe" [8–11].

The measured energy spectrum of an electron in a hydrogen atom is perturbed with respect to the spectrum (1):

$$\tilde{E}_n = E_n + \delta E_n \tag{2}$$

There is a description problem (of constructing a mathematical model) of the measured values of the optical spectrum of the hydrogen atom. This model is a Weyl–Kuryshkin quantization rule equipped with: a mixed quantum state $\{\varphi_k\}$ of the probe, smoothed (perturbed) classic observed $A * W_{\{\varphi_k\}}(q,p)$, applied to it the Weil quantization rule $O_{\{\varphi_k\}}(A) = O_W(A)$. Next step will be a theoretical study of the spectrum of this operator and the numerical calculation of parts of the discrete spectrum affiliated with $\{\varphi_k\}$ [12–15].

First remark. While the experimental data is obtained with respect to a valence electron spin, the model not considers the spin state. As a result, at the current stage the studied model can not fully describe quantum interaction. However, on the one hand, it is adequate for the averaged over spin experimental values, on the other hand a model can be generalized taking into account the electron spin by Stratonovich-Weyl quantization [16–18].

For the hydrogen atom model is verified with relative accuracy $\sim 10^{-16}$ (there is no special achievement in it). Before discussing the dependence of the perturbations δE_n of the hydrogen atom under the influence of the measuring device with a quantum probe in the state $\{\varphi_k\}$ let us recall what is known about the discrete energy spectrum of the valence electron in an isolated atom of an alkali metal with a serial number Z.

3. The Energy Spectrum of the Valence Electrons in the Atoms of the Alkali Metals

For atoms with more than one electron, even for the most simple, Schrodinger equation can not be solved immediately neither with analytical nor numerical methods. For this reason, the study of the spectra of many-electron atoms is based on an approximate model. The most appropriate approach turned out to be the one [19] that maintains an idea of the individual state of the electron in an atom, and the whole state of the atom is determined by a set of states of the electrons with respect to their interaction. This approach helps us obtain some general information about the system's possible energy levels for a given atom and their mutual arrangement.

General description of states of electrons in the atom is based on the assumption that each electron moves in an effective centrally symmetric field produced by the nucleus and all the other electrons. More detailed analysis focuses on the non-central part of the electrostatic and magnetic interaction of electrons. In the theory of atomic spectra these interactions are usually described as small corrections to the centrally symmetric field using methods of perturbation theory. Perturbation does not change the number of possible states of the system [19]. The calculation of the energy parameters can find practical use in various aspects of the atomic spectra theory. The key value of this calculations is determination of the wave functions. They are used in the calculation of the probabilities of radiative transitions, the effective excitation cross-sections and other characteristics of the atom. This is the main problem of the calculation of many-electron atoms, as energy levels can be obtained (and with high accuracy) from experiments.

In the approximation of a complete separation of the electronic variable the probability of radiative transitions $\kappa \to \kappa'$ between states κ and κ' can be expressed [19] through one-electron radial integrals

$$R_{\kappa\kappa'} = \int P_\kappa(r)\, r P_{\kappa'}(r)\, dr. \tag{3}$$

Therefore, the main task in the calculation of the transition probabilities is to find radial functions $P_\kappa(r)$, $P_{\kappa'}(r)$. For all of the atoms and ions, with the exception of those with a single electron, radial functions can be found only by approximate methods. Main methods of approximate calculation of the radial functions are different versions of variational methods and semi-empirical methods. All semi-empirical methods use of experimental values of energy levels.

Variational methods provide good approximation quality of functions $P_\kappa(r)$ in the area of values r, which is the most significant in the calculation of energy. For large values of r these functions can be very inaccurate. With the help of semi-empirical methods it is easier to get functions $P_\gamma(r)$, exact at large r, i.e. just in the region which is most important for the calculation of transition probabilities. Therefore, much more simple semi-empirical method gives a better agreement with experiment (the accuracy of calculation of the transition probabilities) than the method of self-consistent field [19].

In the method of self-consistent field wave functions are calculated simultaneously with eigenvalues of the system of differential equations, with energy parameters E_κ. Different approach is more preferable for calculating the radiation transition probabilities. We can pre-define values E_κ and lookup such single-electron radial functions $P_\kappa(r)$ that calculated values E_κ coincided with pre-defined. In this case the problem of self-consistent defined by the system of equations field is usually replaced by a single equation for the optical electron in an effective field. This equation has the form

$$\left\{ \frac{1}{r}\frac{d^2}{dr^2} - \frac{Z}{r} + \frac{l(l+1)}{2r^2} + V_\kappa(r) - E_\kappa \right\} P_\kappa(r) = 0. \tag{4}$$

The energy parameter E_κ is equal to the difference between the atom energy E_a and the "frozen" atomic core energy E_i [19]. Accuracy of functions $P_\kappa(r)$ largely depends on how close the selected value E_κ is to the true value of the difference $E_a - E_i$. In the semi-empirical method, the energy parameter E_κ is equal to the experimental value of the ionization potential I_κ. Even for the alkaline earth atoms, and even more so for the alkali, it is the most appropriate to apply the semi-empirical method of calculations [19]. When choosing an effective potential $V_\kappa(r)$ different approaches are available. However, in all cases, functions $P_\kappa(r)$ have good asymptotic because the behavior of these functions for large r is determined by pre-selection of E_κ.

One of approaches is to choose potential $V_\kappa(r)$ as a function of some fitted parameter whose value satisfies both boundary conditions. (In general case, the selected value E_γ does not belong to eigenvalue of the equation (4), an thus it does not necessary have to satisfy both of the boundary conditions: $P_\gamma(0) = 0$, $P_\gamma(r) \xrightarrow[r\to\infty]{} 0$).

4. Generalization of Kuryshkin-Wodkiewicz Model on the Valence Electrons of Alkali Metal Atoms

The spectral composition of terms (excluding spin interaction, relativistic corrections, etc.) of an isolated hydrogen atom can be easily calculated:

$$E_n = -\frac{R}{2n^2}. \tag{5}$$

Upon splitting of the terms, they acquire corrections δE_{nl} so that

$$E_{nl} = -\frac{R}{2n^2} + \delta E_{nl}. \tag{6}$$

In the measurement process (due to "interaction" with the quantum probe) the measured energy spectrum (after the projection on the original Hilbert space) becomes

$$E_{nl,\kappa} = -\frac{R}{2n^2} + \delta E_{nl} + \delta E_{\kappa}, \tag{7}$$

where κ is the multi-index of the quantum probe state. This is a standard approach for the hydrogen atom.

The spectral composition of terms of "hydrogen-like" alkali metals atoms is defined by the equation

$$E^Z_{nl} = -\frac{R}{2\left(n + \sigma^Z_l\right)^2}. \tag{8}$$

Upon splitting of the terms, they acquire corrections

$$E^Z_{nl,mm_s} = -\frac{R}{2\left(n + \sigma^Z_l\right)^2} + \delta E_{nl,mm_s}. \tag{9}$$

In the process of measuring the "measured" energy spectrum takes the form

$$E^Z_{nl,mm_s,\kappa} = -\frac{R}{2\left(n + \sigma^Z_l\right)^2} + \delta E_{nl,mm_s} + \delta E_{\kappa}. \tag{10}$$

There is no need to take into account the additional contributions of fine structure and hyperfine structure in the formula (6) and (9) of the measured values of observables – energy before generalization of the Weil–Kuryshkin quantization rules to the quantization rule of Kuryshkin-Stratonovich. Consequently, the measured values of the terms should be limited by the formulas

$$E^1_{n,\kappa} = -\frac{R}{2n^2} + \delta E^1_{\kappa} \tag{11}$$

and

$$E^Z_{nl,\kappa} = -\frac{R}{2\left(n + \sigma^Z_l\right)^2} + \delta E^Z_{\kappa}. \tag{12}$$

Moreover, contributions δE^1_{κ} and δE^Z_{κ} are obtained from the convolution $V(r) * W_{\{\varphi_k\}}(q,p)$, where

$$V^1(r) = -\frac{1}{r} \tag{13}$$

and

$$V^Z(r) = -\frac{1}{r} + \frac{\alpha^Z}{r^2}. \tag{14}$$

As a result the quantization rule of Weil-Kuryshkin is adequate for the alkali metals to the same extent as the potential $V_{\kappa}(r,\vartheta)$, with respect to the small corrections to the centrally symmetric field of core.

5. The Model of Quantum Measurements of Kuryshkin-Wodkiewicz for Atoms and Ions of Alkali Metals

Recall the form

$$O_\rho(H) = \hat{H} + \sum_j a_j \left(\frac{1}{2b_j} + V_j(r, \cos\vartheta) \right)$$

of the Hamiltonian of hydrogen atom perturbed by the probe measurement in a quantum state

$$\hat{\rho} = \sum_j a_j |\psi_j(b_j)\rangle \langle \psi_j(b_j)|.$$

Therefore, perturbation of the potential $V^1(r)$ measured by probe in the state $\hat{\rho}$ has a form $\delta V_\rho = \sum\limits_j a_j V_j(b_j, r, \cos\vartheta)$ that is

$$O_\rho\left(-\frac{1}{r}\right) = O_W\left(\left(-\frac{1}{r}\right) * W_\rho(\vec{r}, \vec{p})\right) = -\frac{1}{r} + \delta V_\rho(\vec{r}).$$

Ritz method makes it possible with the help of $\delta V_\rho(\vec{r})$ to calculate $\delta_\rho E_\kappa$ for the first spectral lines $\delta_\rho \lambda_\kappa^N = \left(\lambda_\kappa^\rho - \lambda_\kappa^1\right)^N$ through the calculations of eigenvalues of the Ritz matrix of dimension N. In the works [20–23] it is shown how to restore the state $\hat{\rho}$ by disturbances $\delta_\rho E_\kappa$. Thus, on the perturbation $\delta V_\rho(\vec{r})$ one can calculate $\hat{\rho} = \sum\limits_j a_j |\psi_j(b_j)\rangle \langle \psi_j(b_j)|$ such that

$$\left(-\frac{1}{r}\right) * W_\rho(\vec{r}, \vec{p}) = -\frac{1}{r} + \delta V_\rho(\vec{r}).$$

As a result, we get

Theorem 1. *For any mixed state* $\hat{\rho} = \sum\limits_j a_j |\psi_j(b_j)\rangle \langle \psi_j(b_j)|$ *of a quantum probe there exists a unique perturbation* $\delta V_\rho(\vec{r})$ *of potential* $V^1(\vec{r}) = -\frac{1}{r}$ *being* $V^1(r)$*-compact and equal to zero at infinity. And vice versa, to any* $V^1(r)$*-compact and equal to zero at infinity disturbance* $\delta V_\rho(\vec{r})$ *of potential* $V^1(r)$ *corresponds the state* $\hat{\rho} = \sum\limits_j c_j |\psi_j\rangle \langle \psi_j|$ *uniquely defined in a subspace* $H^N = \left\{ \sum\limits_{j=1}^N c_j \psi_j \right\}$ *of minimal dimension* N *in the Hilbert space* $L_2\left(\mathbb{R}^3\right)$.

Let us use the result of Kato's theorem [24]: If the operator $O(H) = \hat{H} + V(\vec{r})$ of the potential V can be written as the sum of two functions, one of which is continuous and bounded, and the other is the square-integrable on $\mathbb{R}^3$, while $V(\vec{r}) \xrightarrow[|\vec{r}|\to\infty]{} 0$, then V is $\hat{H}$-compact. Any perturbation $V_\kappa(r, cos\vartheta)$ of the centrally symmetric field $V^Z(r)$ in (14) in the problem (4) decreases at infinity, and thus according to Kato theorem $V^Z + V_\kappa$ is $\hat{H}$-compact, vanishing at infinity. According to the Statement 1 for $V_\kappa^Z(\vec{r}) = V^Z(r) + V_\kappa(r, \cos\vartheta)$ there is a state $\hat{\rho}_\kappa^Z = \sum c_j |\psi_j\rangle \langle \psi_j|$ defined uniquely in a subspace $H^N = \left\{ \sum\limits_{j=1}^N c_j \psi_j \right\}$ of minimal dimension N in the Hilbert space $L_2\left(\mathbb{R}^3\right)$ such that

$\left(V^1 * W_{\rho_\kappa^Z}\right)(\vec{r},\vec{p}) = V_\kappa^Z(\vec{r})$. Thus, for the measured Hamilton operator of a valence electron in the alkali metal atom the measured potential is:

$$V_{\kappa,\rho}^Z(\vec{r}) = \left(V_\kappa^Z * W_\rho\right)(\vec{r},\vec{p}) = \left\{\left(V^1 * W_{\rho_\kappa^Z}\right) * W_\rho\right\}(\vec{r},\vec{p}).$$

Hence, is valid

Theorem 2. *The quantization rule of Kuryshkin-Wodkiewicz applied to the valence electron in the alkali metal atom with an approximate pseudopotential $V_\kappa^Z(\vec{r})$ been measured by the quantum probe in the state $\hat{\rho} = \sum c_j |\psi_j\rangle \langle\psi_j|$ take the form of quantization rule of Kuryshkin-Weyl with the potential $\left(V_\kappa^Z * W_\rho\right)(\vec{r})$.*

Corollary 1. Quantum measurement by the quantum probe in the state $\hat{\rho}$ of the energy spectrum of the valence electron in the alkali metal atom with state values

$$E_{nl}^Z = -\frac{R}{2\left(n+\sigma_l^Z\right)^2}$$

of (8), will result in measured value

$$E_{nl,\rho}^Z = -\frac{R}{2\left(n+\sigma_l^Z\right)^2} + \delta E_\rho^Z$$

of (12).

6. Conclusion

In [2, 3, 25, 26] of quantum measurements applied to the quantum problem of Kepler has been implemented. In previous works a particular modification the model of quantum measurement has been applied to the problem of quantum oscillator [4, 5]. In this paper the Kuryshkin-Wodkiewicz model with implementation of Weyl-Kuryshkin quantization rule [3,25,26] is applied to the quantum systems with one valence electron like alkali metal atoms Kuryshkin-Wodkiewicz model implementing quantization rule Weil-Kuryshkin, extended to the quantum system with one valence electron, such as alkali metal atoms. The proof of the consistency of the model is based on two Kato theorems [24]. The explicit form of the discrete spectrum of the valence electron for various spectral series, depending on the serial parameters of the disturbance spectrum of an isolated object in the process of quantum measurement was achieved.

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Модель квантовых измерений Курышкина-Вудкевича для атомов и ионов с одним валентным электроном

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Конструктивная форма модели квантовых измерений Курышкина-Вудкевича детально разработана для квантовой задачи Кеплера. Для более сложных квантовых объектов такая конструкция неизвестна. В то же время стандартная (не конструктивная) модель квантовых измерений Холево–Хелстрома годится для любого квантового объекта. Целью данной работы является распространение конструктивной модели квантовых измерений на более широкий класс квантовых объектов — модель квантовых измерений оптического спектра атомов и ионов с одним валентным электроном.

В работе модель Курышкина–Вудкевича, реализующая правило квантования Вейля–Курышкина в приложении к квантовой задаче Кеплера, распространена на квантовые системы с одним валентным электроном, например, на атомы щелочных металлов. В основу доказательства состоятельности модели положены две теоремы Като о компактных возмущениях операторов. В ходе доказательства получены явные формулы дискретного спектра валентного электрона для различных спектральных серий, зависящие от сериальных параметров возмущения спектра изолированного объекта в процессе квантовых измерений.

Ключевые слова: квантовые модели измерения, правила квантования, относительно компактное возмущение наблюдаемого оператора, возмущение наблюдаемого дискретного спектра

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