On the numerical and analytical analysis of the optical properties of hydrogen-like atoms in the operational model of quantum measurements

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Outline

1. The Operational Model of Quantum Measurements
2. Implication for the Hydrogen-like atoms
3. Model Verification
4. Summary
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Standard Weyl–Berezin\(^1\) quantization assigns pseudo-differential operators 
\( O_w (A) : H \rightarrow H \) in the rigged Hilbert space 
\( S (Q) \subset L_2 (Q) \subset S' (Q) \) to the classical observable 
\( A (p, q) \in S' (T \ast Q) \).

Measured values of the quantum observables equals to the spectral properties of the quantum measurements’ theory\(^2\) operators.

There is an operator \( O_\rho (A) \) assigned\(^3\) to all classical observables 
\( A (p, q) \) and all input states \( \hat{\rho} = \sum_k C_k |\psi_k\rangle \langle \psi_k| \) of the measurement instrument’s quantum filter.

It was shown\(^4\) that \( O_\rho (A) \) is the Weyl operator from the deformed (by the convolution with the function \( \Phi (q, p) = \sum_k C_k |\psi_k\rangle \langle \psi_k| F (\psi_k) (p) \)) classical observable 
\( (A \ast \Phi) (p, q) : O_\rho = O_w (A \ast \Phi) \)

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Isolated (classical) object

Described by

- Configuration space $Q = \mathbb{R}^n$
- Phase space $T^* Q = \mathbb{R}^n \oplus \mathbb{R}^n$
- Classical Hamiltonian function $H(q, p)$
- Class of the (real) functions $\{A(q, p)\}$ of the classical observables
Corresponding quantum object

Described by

- Rigged Hilbert space $S(Q) \subset L_2(Q) \subset S'(Q)$
- Algebra of the state operators (density matrices) $\{\hat{\rho}\}$
- Lie-Jordan algebra of quantum observables $\{O(A)\}$, derived from the classical observables $A(q, p)$ with the help of the quantization rule
Composite system “object + filter”

A space $L_2(Q_1 \oplus Q_2) = L_2(Q_1) \oplus L_2(Q_2)$

With the operators of the ”measured” observable $O_W(A) \otimes \hat{I}$

States before the measurement procedure are given by the operators $\hat{\rho}_1 \otimes \hat{\rho}_2$
The average value of the measured observable is equal to
\[ \langle A \rangle_{\rho_1 \otimes \rho_2} = \text{Tr} \left\{ \left( O_{\mathcal{W}} (A) \otimes \hat{I} \right) (\hat{\rho}_1 \otimes \hat{\rho}_2) \right\} = \text{Tr}_1 \{ O_{\rho_2} (A) \hat{\rho}_1 \}, \]
where \( \text{Tr}_1 \) is a partial trace over the space \( L_2 (Q_1) \) and
\[ O_{\rho_2} (A) = \text{Tr}_2 \left\{ \left( O_{\mathcal{W}} (A) \otimes \hat{I} \right) (\hat{\rho}_1 \otimes \hat{\rho}_2) \right\} \]
is a partial trace over the space \( L_2 (Q_2) \).
On the other hand, the average value of the measured observable is equal to
\[ \langle A \rangle_{\rho_1 \otimes \rho_2} = \int A(q, p) (\mathcal{W}_{\rho_1} \ast \mathcal{W}_{\rho_2})(q, p) dq dp, \]

**Theorem**

Quantization rule of Kuryshkin-Wódkiewicz corresponds a continuous linear operator of the form \( O_{\rho_2} (A) = O_{\mathcal{W}} (A \ast \mathcal{W}_{\rho_2}) : S \left( Q \right) \rightarrow S' \left( Q \right) \) to the distribution \( A \in S' \left( T^* Q \right) \).
Quantum measurements operator

In the Kuryshkin-Wódkiewicz model of the quantum measurements operator $O_{\rho^2} (A) \equiv O_{\{\varphi_k\}} (A)$ is defined with a set of unnormalized functions $\{\varphi_k = \sqrt{c_k} \psi_k\}_{k=1}^{\infty}$ with the integral relation:

$$(O_{\rho} (A) \Psi)(q) = (2\pi \hbar)^{-N} \int \Phi(\xi, \eta) A(q + \xi, p + \eta) \times$$

$$\times \exp \left\{ \frac{i}{\hbar} \langle (q - q') p \rangle \right\} \Psi(q') dq' dp d\xi d\eta,$$

where function $\Phi(q, p)$ is defined on the phase space with the equation

$$\Phi(q, p) = \frac{\exp \left\{ -\frac{i}{\hbar} \langle q, p \rangle \right\}}{(2\pi \hbar)^{N/2}} \sum_k \varphi_k(q) \bar{\varphi}_k(p).$$

Note

Analytical (approximate) definition of the $O_{\rho^2} (A)$ operator requires definition of the $O_{\{\varphi_k\}} (A)$ operators in a fixed basis $\{\psi_k\}_{k=1}^{\infty}$. 
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Hydrogen-like atoms

- Weyl operator of the observable: \( \hat{H} \equiv O_{W}(H) = -\frac{\hbar^2}{2} \Delta - \frac{2}{|q|} \).
- Quantum filter in a state \( \hat{\rho}_2 = \sum C_k |\psi_k\rangle \langle \psi_k| \)
- Sturm functions \( \Psi_{nlm}(r,\theta,\varphi) = S_{nl}(r) Y_{lm}(\theta,\varphi) \) as basis functions \( \{\psi_k(\vec{r})\}_{k=1}^{\infty} \)
- Observable of the measured value \( O_{\rho_2}(H) \):

\[
[O_{W}(H \ast W_{\rho_2}) u](q) = \int (H \ast W_{\rho_2}) \left( \frac{q + \tilde{q}}{2}, p \right) \times \exp \left\{ \frac{i}{\hbar} p \left( q - \tilde{q} \right) \right\} u(\tilde{q}) \, d\tilde{q}
\]
Explicit form of the Hamiltonian

Due to the linearity: \( O(H) = \sum_{j=1}^{n} C_j \left( O_j \left( \frac{\vec{p}^2}{2\mu} \right) + O_j(-\frac{Ze^2}{r}) \right) \),

where:

- \( \sum_{j=1}^{n} C_j = 1 \)

- Calculated kinetic energy operators:
  \( O_i\left( \frac{\vec{p}^2}{2\mu} \right) = -\frac{\hbar^2}{2m}\Delta + \frac{\hbar^2}{2mb_i^2} \), \( i = 1, \ldots, n \)

- First two calculated potential energy operators:
  \( O_1(-\frac{Ze^2}{r}) = -\frac{Ze^2}{r} + Ze^2 e^{\frac{-2r}{b_1r_0}} \left( \frac{1}{r_0} + \frac{1}{br_0} \right) \)
  \( O_2(-\frac{Ze^2}{r}) = -\frac{Ze^2}{r} + \frac{Ze^2}{b_2r_0} e^{\frac{-r}{b_2r_0}} \left( \frac{3}{4} + \frac{b_2r_0}{r} + \frac{r}{4b_2r_0} + \frac{1}{8} \left( \frac{r}{b_2r_0} \right)^2 \right) \)
Calculating Ritz matrix

Generalized eigenvalue problem $M\vec{x} = \lambda B\vec{x}$.

- $M$ is a Ritz matrix of $O^M(H)$.
- $B$ is an inner product of coordinate functions matrix.
- $M$ is the number of dimensions corresponding to the operators $O_k(H)$
- First $M$ basic functions $\psi_{nlm}^{E_0}(\vec{r}) = \tilde{S}_{nl}(k\vec{r}) Y_{lm}(\theta, \phi)$ (Sturmian functions), where $k = \sqrt{-E_0}$.

Ritz matrix elements:

$$M^{(j)}_{kl} = \int \psi_{E_0}^k(\vec{r}) \left[ O_j \left( \frac{\vec{p}^2}{2\mu} \right) + O_j(-Z_{\text{eff}} e^2 r) \right] \psi_{E_0}^l(\vec{r}) d\vec{r}$$
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Source Functions

- Spherical harmonics
- Inverse transformation of spherical harmonic
- Sturmian functions
  - Sturm functions
  - Normalized Sturmian functions
- Functions
  - $F(l) = 2\pi i^{-l} \text{Bessel}(l+\frac{1}{2}, (p^*r)/\hbar)$
  - $R_{nlpq}(m,n,p,q)$
  - Clebsch–Gordan coefficients
  - Product of spherical harmonics
  - Fourier transform of auxiliary functions
  - Auxiliary Sturmian functions
  - Alfa-functions
  - Beta-functions
  - Functions $P(l,m,b)$
Matrix coefficients computations

- Spherical harmonics
- Product of spherical harmonics
- Normalized Sturmian functions
- Auxiliary functions
- Complex-conjugate functions
- Potential energy operator
- Coordinate Ritz functions
- Potential energy operator
- Kinetic energy operator
- Constant operator
- Pair-to-pair scalar products of coordinate functions

Matrix elements of total energy operator's components

Total energy operator
Transition probabilities computations

- Total energy operator
- Pair-to-pair scalar products of coordinate functions
- Ritz matrix
- Generalized eigenvalue problem
- Spectrum
- Parameters optimization
- Penalty function
- Optimized parameters
- Coefficients $C_{mnl}$
- Transition probabilities
- Polarization

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The Operational model for Quantum Measurements with Weyl-Kuryshkin quantization rule was considered.

The explicit form of the expressions for the hydrogen and alkali atoms measured energy were obtained.

Justification of the numeric calculations for the optical transition probabilities of the hydrogen-like atoms was developed.

Verification of the proposed mathematical model for the quantum measurements was made based on comparison of calculated transition probabilities with corresponding experimentally obtained values.
Publications on the subject of the report


Thank you!