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

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1. The Operational Model of Quantum Measurements
2. Implication for the Hydrogen-like atoms
3. Model Verification
4. Summary

Quantum Measurements' and Quantum Estimation Models

- Standard Weyl–Berezin[1] quantization assigns pseudo-differential operators $O_w(A) : H \to H$ in the rigged Hilbert space $S(Q) \subset L_2(Q) \subset S'(Q)$ to the classical observable $A(p,q) \in S'(T * Q)$.
- 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 $\Phi(q,p) = \sum_k C_k \psi_k(q) F(\psi_k)(p)$) classical observable $(A * \Phi)(p,q) : O_\rho = O_w(A * \Phi)$

[1] Weyl, H.: Quantenmechanik und Gruppentheorie. Zeitschrift für Physik 46, 1–46 (1927); Berezin, F. A.: On a representation of operators with the help of functionals. Trans. Moscow Math. Soc. 17, 117–196 (1967)

[2] Holevo A. S. Statistical Structure of Quantum Theory. Lect. Notes Phys.,vol. m67. Springer, Berlin (2001)

[3] Ozawa, M.: Mathematical foundations of quantum information: Measurement and foundations. Sugaku, 61–2, pp. 113–132 (2009) (in Japanese)

[4] Sevastianov, L., Zorin, A., Gorbachev, A.: Pseudo-differential operators in the operational model of a quantum measurement of observables. Lecture Notes in Computer Science 7125, 174–181 (2012)

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”

Operates in

- 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 $\hat{\rho}_1 \otimes \hat{\rho}_2$

Quantization rule

The average value of the measured observable is equal to

$$\langle A\rangle_{\rho1\otimes\rho2} = \mathrm{Tr}\left\{\left(O_W(A)\otimes\hat{I}\right)(\hat{\rho}_1\otimes\hat{\rho}_2)\right\} = \mathrm{Tr}_1\left\{O_{\rho2}(A)\,\hat{\rho}_1\right\},$$

where Tr_1 is a partial trace over the space $L_2(Q_1)$ and

$$O_{\rho2}(A) = \mathrm{Tr}_2\left\{\left(O_W(A)\otimes\hat{I}\right)(\hat{\rho}_1\otimes\hat{\rho}_2)\right\}$$

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

$$\langle A\rangle_{\rho1\otimes\rho2} = \int A(q,p)\,(W_{\rho1} * W_{\rho2})(q,p)\,dqdp,$$

Theorem

Quantization rule of Kuryshkin-Wódkiewicz corresponds a continuous linear operator of the form $O_{\rho2}(A) = O_W(A * W_{\rho2}) : \ S(Q)\to S'(Q)$ to the distribution $A\in S'(T^*Q)$.

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 $\left\{\varphi_k = \sqrt{c_k}\psi_k\right\}_{k=1}^{\infty}$ with the integral relation:

$$(O_\rho(A)\Psi)(q) = (2\pi\hbar)^{-N}\int \Phi(\xi,\eta)\, A(q+\xi, p+\eta)\times$$
$$\times \exp\left\{\frac{i}{\hbar}\left\langle\left(q-q'\right)p\right\rangle\right\}\Psi\left(q'\right)dq'dpd\xi d\eta,$$

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 $\{\psi_k\}_{k=1}^{\infty}$.

Outline

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 $\hat{\rho}_2 = \sum C_k \left|\psi_k\right\rangle \left\langle\psi_k\right|$
- 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 $O_{\rho 2}(H)$:

$$[O_W(H * W_{\rho 2})\, u](q) = \int (H * W_{\rho 2})\left(\frac{q+\tilde{q}}{2}, p\right) \times \exp\left\{\frac{i}{\hbar} p\,(q-\tilde{q})\right\} u(\tilde{q})\, d\tilde{q}$$

Explicit form of the Hamiltonian

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

where:

- $\sum\limits_{j=1}^{n}C_j=1$
- Calculated kinetic energy operators:
  $O_i\left(\frac{\vec{p}^2}{2\mu}\right)=-\frac{\hbar^2}{2m}\Delta+\frac{\hbar^2}{2mb_i^2},\ \ i=1,...,\ n$
- First two calculated potential energy operators:
  $O_1(-\frac{Ze^2}{r})=-\frac{Ze^2}{r}+Ze^2e^{-\frac{2r}{b_1r_0}}\left(\frac{1}{r_0}+\frac{1}{br_0}\right),$
  $O_2(-\frac{Ze^2}{r})=-\frac{Ze^2}{r}+\frac{Ze^2}{b_2r_0}e^{-\frac{r}{b_2r_0}}\left(\frac{3}{4}+\frac{b_2r_0}{r}+\frac{1}{4}\frac{r}{b_2r_0}+\frac{1}{8}\left(\frac{r}{b_2r_0}\right)^2\right)$

Calculating Ritz matrix

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

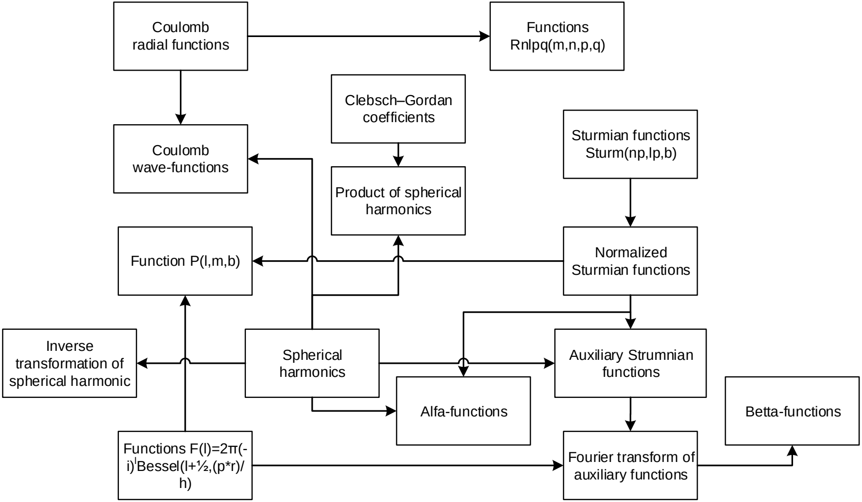
- M is a Ritz matrix of $O^M(H)$.
- B is an inner product of coordinate functions matrix.
- M is the number of dimensions corresponding to the operators $O_k(H)$
- First M basic functions $\psi_{nlm}^{E_0}(\vec{r}) = \tilde{S}_{nl}(k\vec{r})\, Y_{lm}(\theta, \phi)$ (Sturmian functions), where $k = \sqrt{-E_0}$.

Ritz matrix elements:

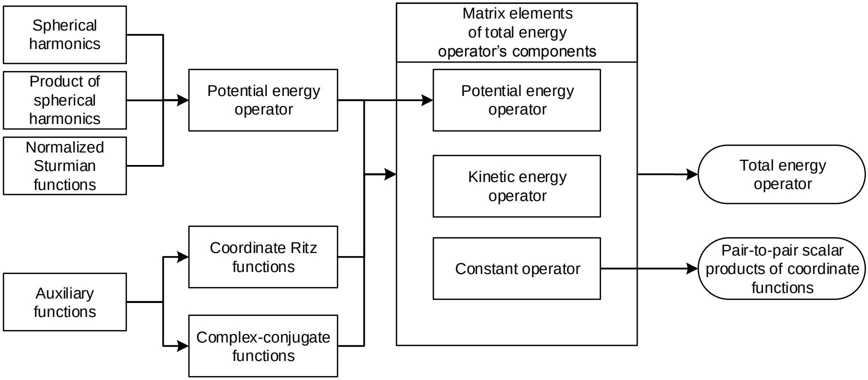
$$M_{kl}^{(j)} = \int \psi_k^{E_0}(\vec{r}) \left[O_j\left(\frac{\vec{p}^2}{2\mu}\right) + O_j(-\frac{Z_{eff}\, e^2}{r}) \right] \psi_l^{E_0}(\vec{r})\, d\vec{r}$$

Outline

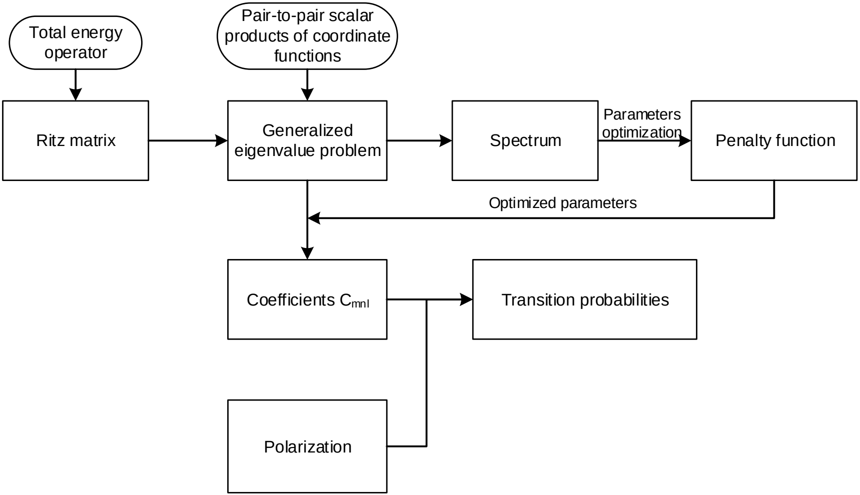
Source Functions



Matrix coefficients computations



Transition probabilities computations



Outline

Summary

- 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

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- Zorin A.V., Sevastianov L.A., Belomestny G.A. Numerical search for the states with minimal dispersion in quantum mechanics with non-negative quantum distribution function. Lect. Notes in Comp. Sci., vol. 3401, 613–621 (2005)
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- L. Sevastianov, A. Zorin, A. Gorbachev. Pseudo-Differential Operators in the Operational Model of a Quantum Measurement of Observables. Lecture Notes in Computer Science., vol. 7125, 174-181 (2012)
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Thank you!