Modeling of the Quantum System Spectral Characteristics

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Quantum Measurements and Quantum Estimation Models

- Wódkiewicz's phase-space representation of the quantum measurement's operational model
- Kuryshkin's model of the quantum mechanics with a non-negative quantum distribution function
- Ozawa prove of the operational model of quantum measurements and the quantum estimation model equivalence
- Universal model of the quantum measurements

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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"

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

$$\langle A \rangle_{\rho 1 \otimes \rho 2} = \mathrm{Tr}\left\{ \left(O_W(A) \otimes \hat{I} \right) (\hat{\rho}_1 \otimes \hat{\rho}_2) \right\} = \mathrm{Tr}_1 \left\{ O_{\rho 2}(A)\, \hat{\rho}_1 \right\},$$

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

$$O_{\rho 2}(A) = \mathrm{Tr}_2 \left\{ \left(O_W(A) \otimes \hat{I} \right) (\hat{\rho}_1 \otimes \hat{\rho}_2) \right\}$$

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

$$\langle A \rangle_{\rho 1 \otimes \rho 2} = \int A(q,p)\, (W_{\rho 1} * W_{\rho 2})(q,p)\, dq dp,$$

Theorem

Quantization rule of Kuryshkin-Wódkiewicz corresponds a continuous linear operator of the form $O_{\rho 2}(A) = O_W(A * W_{\rho 2}) : \; S(Q) \to S'(Q)$ *to the distribution* $A \in S'(T^* Q)$.

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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:

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

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

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

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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 $O_{\rho 2}(H)$:

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

Explicit form of the Hamiltonian

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

where:

- $\sum_{j=1}^{n} C_j = 1$
- Calculated kinetic energy operators:
  $O_i \left(\frac{\vec{p}^2}{2\mu} \right) = -\frac{\hbar^2}{2m}\Delta + \frac{\hbar^2}{2mb_i^2}, \quad i = 1, ..., n$
- First two calculated potential energy operators:
  $O_1(-\frac{Ze^2}{r}) = -\frac{Ze^2}{r} + Ze^2 e^{-\frac{2r}{b_1 r_0}} \left(\frac{1}{r_0} + \frac{1}{br_0} \right),$
  $O_2(-\frac{Ze^2}{r}) = -\frac{Ze^2}{r} + \frac{Ze^2}{b_2 r_0} e^{-\frac{r}{b_2 r_0}} \left(\frac{3}{4} + \frac{b_2 r_0}{r} + \frac{1}{4}\frac{r}{b_2 r_0} + \frac{1}{8}\left(\frac{r}{b_2 r_0} \right)^2 \right)$

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Arraying 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:

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

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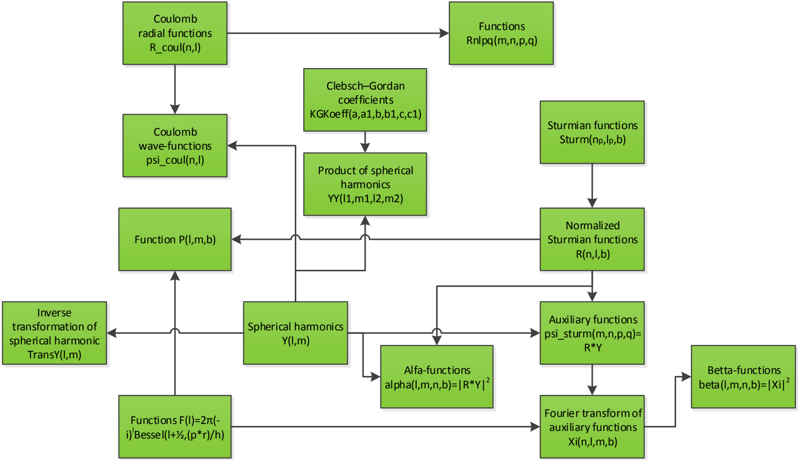
"SourceFunctions" library



Analytical calculations in Maple

Example (Calculation of spherical harmonics Y)

```
Phi:=(l,m)->(2*Pi)^(-1/2)*exp(I*m*phi);
### Internal Legendre polynomial(LegendreP) are complex-conjugated to the one used in calculations
Lej:=(l,x)->if l=0 then 1 else 1/(2^l*l!)*diff((1-x^2)^l,x$l) fi;
P1:=(l,m,x)->
  if m=0
    then Lej(l,x)
    else (1-x^2)^(m/2)*diff(Lej(l,x),x$m)
  fi;
Theta:=(d,l,m)->sqrt((2*l+1)*(l-m)!/(l+m)!/2)*subs(d=cos(theta),P1(l,m,d));
Y:=proc(l,m)
  description "";
  if (l>=0)and(abs(m)<=l) then
   if m<0
     then simplify((-1)^l*Theta(d,l,-m)*Phi(l,m),symbolic)
     else simplify((-1)^(l-m)*Theta(d,l,m)*Phi(l,m),symbolic)
   fi;
  fi;
end proc;
```

Analytical calculations in Maple

Example (Sturmian functions)

```
Sturm:=proc(np,lp,b)
local kk,alpha_nl,N_nl,altLaguerreL;
kk:=1/b:
alpha_nl:=kk*np:
N_nl:=-sqrt((np-lp-1)!/((np+lp)!)^3/2):
### Alternative notation of Laguerre polynomial instead of internal(LaguerreL) is used:
altLaguerreL := (n,a,x) -> (-1)^a*n!*LaguerreL(n-a,a,x):
N_nl*exp(-kk*r)*(2*kk*r)^(lp+1)
*simplify(altLaguerreL(np+lp,2*lp+1,2*kk*r)):
end proc;
```

Example (Normalization of sturmian functions)

```
R:=proc(n,l,b)
subs(r=r, Sturm(n,l,b) /r )
  /sqrt(int(subs(r=r,Sturm(n,l,b)^2/r^2)*r^2,r=0..infinity)) :
end proc;
```

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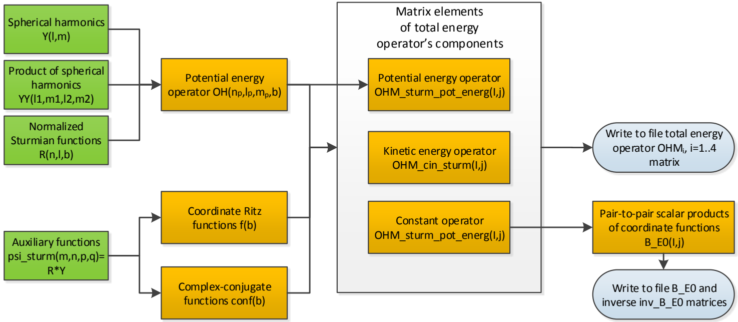
Matrix coefficients computations



Analytical calculations in Maple

Example (Calculations of potential energy operators)

```
OH:=proc(np,lp,mp,b)
local l,m,sumout,sumin,intr;
sumout:=0;
for l from 0 to 2*lp do
 sumin:=0;
intr:=int(r2^l/r^(l+1)*subs(r=r2,R(np,lp,b))^2*r2^2,r2=0..r)
+int(r^l/r2^(l+1)*subs(r=r2,R(np,lp,b))^2*r2^2,r2=r..infinity);
 for m from -l to l do
  sumin:=sumin+Y(l,m)*int(int(conjugate((-1)^l*Y(l,m))
   *YY(lp,mp,lp,mp,true)*sin(theta),theta=0..Pi),phi=0..2*Pi);
 od;
 sumout:=sumout+1/(2*l+1)*sumin*intr;
od;
expand(-4*Pi*Z*e^2*simplify(sumout));
end proc;
```

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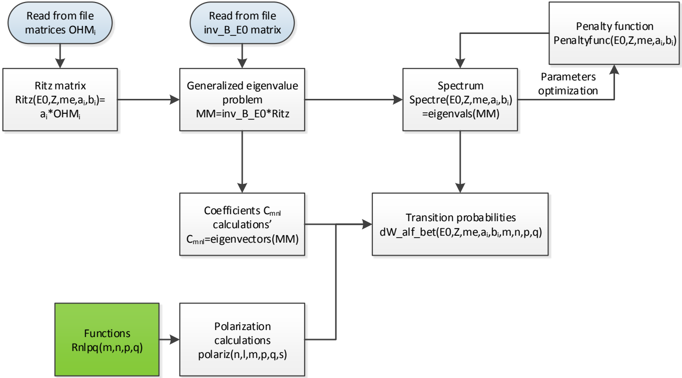
Transition probabilities computations



Analytical calculations in Maple

Example (penalty function H (first 30 levels))

```
penaltyfunc_H_30:=proc(E0q, b1qq,b2qq,b3qq,b4qq, a1qq,a2qq,a3qq, Z1q, meq, matrsize)
local i,j,MM,MM_,L1,L2,L;
MM:=matrix(matrsize,matrsize):
MM_:=matrix(matrsize,matrsize):
MM:=subs({a1q=a1qq,a2q=a2qq,a3q=a3qq,E0=E0q,Z=Z1q,me=meq,b1q=b1qq,b2q=b2qq,b3q=b3qq,b4q=b4qq},
evalm(matr_E0_)):
MM_:=evalm(inv_B_E0&*MM):
L1:=eigenvals(MM_):
L2:=[seq(L1[i],i=1..55)]:
L:=sort(L2):
(2*L[1]*(1-0.0)^2+1)^2+(2*L[2]*(2-0.0)^2+1)^2+sum((2*L[kkk_30]*(2-0.0)^2+1)^2,kkk_30=3..5)+
+sum((2*L[kk1_30]*(3-0.0)^2+1)^2,kk1_30=6..14)+ sum((2*L[kk2_30]*(4-0.0)^2+1)^2,kk2_30=15..30):
end proc;
```

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Summary

- Observable operators can be described in terms of Weyl-Kuryshkin quantization rule.
- Computer algebra methods of Maple allowed us to construct Ritz matrix of the hydrogen atom observables in the explicit form.
- Numeric studies in dedicated QDF package for Maple proved consistency of the Kuryshkin-Wódkiewicz model.

Thank you!