Numerical solution of the three body scattering problem

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Outline

Introduction

Introduction

- Expanding of the tree body wave function
- Basis of hyperspherical adiabatic harmonics
- The standard projection procedure leads to effective equations for the expansion coefficients
- How can be solved?
- Have to find out properties of the basis functions

Introduction

- Geometrical connections $A_{ij} = \langle \phi_i, \partial_\rho \phi_j \rangle$
- Develop a formalism to study different models

  - scattering of a particle off a two body bound state
  - scattering of a particle off a resonant state of a pair of particles
- Investigate eigenvalues λ_k, eigenfunctions ϕ_k, and geometrical connections A_{ij} of the operator

$$h(\rho) = -\rho^{-2}\partial_\theta + V(\rho \cos\theta).$$

Faddeev Equation in $\{\rho, \theta\}$ Coordinates

Faddeev equation in $\{\rho, \theta\}$ coordinates

The Faddeev s-wave equation in polar coordinates

$$\left(-\partial_\rho^2 - \frac{1}{4\rho^2}\right) U(\rho,\theta) + \left(-\frac{1}{\rho^2}\partial_\theta^2 + V(\rho\cos\theta)\right) U(\rho,\theta) - -EU(\rho,\theta) = -V(\rho\cos\theta)\frac{\sqrt{3}}{4}\int_{\theta_-(\theta)}^{\theta_+(\theta)} d\theta' \; U(\rho,\theta')$$

where $\theta_+(\theta) = \pi/2 - |\pi/6 - \theta|$ and $\theta_-(\theta) = |\pi/3 - \theta|$

Faddeev equation in $\{\rho, \theta\}$ coordinates

The boundary conditions should be imposed for the scattering solution:

- Regularity of the solution

$$U(0,\theta) = U(\rho,0) = U(\rho,\pi/2) = 0$$

- Asymptotics as $\rho \to \infty$

$$U(\rho,\theta) \sim \varphi(x)\rho^{1/2}\sin(qy)/q + \\ +a(q)\varphi(x)\rho^{1/2}\exp(iqy) + A(\theta,E)\exp(i\sqrt{E}\rho),$$

where $x = \rho\cos\theta$.

Faddeev equation in $\{\rho, \theta\}$ coordinates

- The bound-state wave function of the two body target system $\varphi(x)$ obeys the equation

$$\{-\partial_x^2 + V(x)\}\varphi(x) = \epsilon\varphi(x)$$

- It is assumed that the discrete spectrum of the Hamiltonian $-\partial_x^2 + V(x)$ consists of one negative eigenvalue ϵ at most

Basis functions

Expansion basis

- As basis we choose the eigenfunctions set of the operator $h(\rho)$

$$\left(-\rho^{-2}\partial_\theta^2 + V(\rho\cos\theta)\right)\phi_k(\theta|\rho) = \lambda_k(\rho)\phi_k(\theta|\rho)$$

- ρ is an external parameter for $h(\rho)$
- EV and EF of $h(\rho)$ inherit parametrical dependence on ρ

Spectral properties

- The main spectral properties of the operator $h(\rho)$ as $\rho \to \infty$ and of the two body Hamiltonian $-\partial_x^2 + V(x)$

$$\lambda = \lim_{\rho \to \infty} \lambda_0(\rho) = \epsilon,$$

$$\phi_0(\theta|\rho) = \sqrt{\rho}\,\varphi(\rho\cos\theta)(1 + O(\rho^{-\mu}))$$

- Excited states $\phi_k(\theta|\rho), k \geq 1$, when $\rho \to \infty$ the asymptotic behavior is given by the formulas

$$\lambda_k(\rho) \sim \left(\frac{2k}{\rho}\right)^2,$$

$$\phi_k(\theta|\rho) \sim \frac{2}{\sqrt{\pi}} \sin(2k\theta)$$

Perturbation Theory

Perturbation theory - introduction

- If the parameter ρ is large the support of the potential $V(\rho\cos\theta)$ is small on the interval $[0, \pi/2]$
- The estimates for EV and EF of the operator $h(\rho)$ can be obtained by the perturbation theory considering the potential $V(\rho\cos\theta)$ as a small perturbation

$$\begin{aligned} \lambda_k &\sim \lambda_k^0 + \lambda_k^1, \\ \phi_k(\theta|\rho) &\sim \phi_k^0(\theta|\rho) + \phi_k^1(\theta|\rho) \end{aligned}$$

- The leading terms λ_k^0 and ϕ_k^0 for $k \geq 1$ are given by

$$\lambda_k^0 = (2k)^2/\rho^2,$$
$$\phi_k^0(\theta|\rho) = \frac{2}{\sqrt{\pi}}\sin(2k\theta)$$

Correction terms

- The first order correction terms λ_k^1 and ϕ_k^1 are defined in terms of the matrix elements of the potential $V(\rho\cos\theta)$

$$V_{nk}(\rho) = \langle \phi_n^0 | \, V \, | \, \phi_k^0 \rangle = \int_0^{\pi/2} d\theta \, \phi_n^0(\theta|\rho) V(\rho\cos\theta) \phi_k^0(\theta|\rho)$$

- As the model situation, the function $V(x)$ is taken in the form of Yukawa potential

$$V(x) = C \frac{\exp(-\mu x)}{x}$$

where C and μ are some parameters.

Calculation of corrections

- As we set $\rho \to \infty$, we can approximately calculate integral

$$V_{nk}(\rho) \sim (-1)^{n+k} \frac{16nkC}{\pi} \frac{[1 - \exp(-\mu R)(1 + \mu R)]}{\mu^2} \frac{1}{\rho^3}.$$

- The first order correction term λ_k^1 is

$$\lambda_k^1 = V_{kk} \sim \rho^{-3}$$

- The second order correction term λ_k^2 is

$$\lambda_k^2 = \sum_{n \neq k} \frac{|V_{nk}|^2}{\lambda_k^{(0)} - \lambda_n^{(0)}},$$

$$\lambda_k^2 \sim \rho^{-4}$$

Calculation of corrections

- For eigenfunctions the first correction term is given by

$$\phi_k^1 = \sum_{n \neq k} \frac{V_{nk}}{\lambda_k^{(0)} - \lambda_n^{(0)}} \phi_n^0 \sim \rho^{-1}$$

- From equation

$$\left(-\frac{1}{\rho^2} \partial_\theta^2 + V(\rho \cos \theta) \right) \phi_k(\theta|\rho) = \lambda_k(\rho) \phi_k(\theta|\rho)$$

one can obtain formula for A_{ij}

$$A_{ij} = \frac{\langle \phi_i | \frac{\partial V}{\partial \rho} | \phi_j \rangle}{\lambda_i - \lambda_j}$$

A_{ij}

- Rough calculation of A_{ij} leads to dependence

$$A_{ij} \sim \rho^{-2},\ i,j \neq 0$$

$$A_{ij} \sim \rho^{-5/2},\ i = 0\ or\ j = 0$$

Solution Expansion

Solution expansion

- The operator $h(\rho)$ is Hermitian on $[0, \pi/2]$ interval and its eigenfunction set $\{\phi_k(\theta|\rho)\}_0^\infty$ is complete.

$$U(\rho, \theta) = \phi_0(\theta|\rho)F_0(\rho) + \sum_{k\geq 1} \phi_k(\theta|\rho)F_k(\rho)$$

- Substituting this expansion in Faddev equation and projecting on basis functions lead to the following system of equations for $F_k(\rho), k = 0, 1, ...$

$$\left(-\partial_\rho^2 - \frac{1}{4\rho^2} + \lambda_k(\rho) - E\right) F_k(\rho) =$$

$$\sum_{i=0}^{\infty} \left(2A_{ki}\frac{\partial F_i(\rho)}{\partial \rho} + B_{ki}(\rho)F_i(\rho) - W_{ki}(\rho)F_i(\rho)\right)$$

Solution expansion

- The nonadiabatical matrix elements $A_{ki}(\rho), B_{ki}(\rho)$ and potential coupling matrix $W_{ki}(\rho)$ are given by integrals

$$A_{ki}(\rho) = \langle \phi_k | \, \partial_\rho \phi_i \rangle = \int_0^{\pi/2} d\theta \phi_k^*(\theta|\rho) \frac{\partial \phi_i(\theta|\rho)}{\partial \rho},$$

$$B_{ki}(\rho) = \langle \phi_k | \, \partial_\rho^2 \phi_i \rangle = \int_0^{\pi/2} d\theta \phi_k^*(\theta|\rho) \frac{\partial^2 \phi_i(\theta|\rho)}{\partial \rho^2},$$

$$W_{ki}(\rho) = \frac{\sqrt{3}}{4} \int_0^{\pi/2} d\theta \phi_k^*(\theta|\rho) V(\rho \cos\theta) \int_{\theta_-(\theta)}^{\theta_+(\theta)} d\theta' \phi_i(\theta'|\rho)$$

Solution expansion

- Presence of first derivative $F_i'(\rho)$ in the right part of the expression
- Matrix form of equation

$$\left(-\partial_\rho^2 - \frac{1}{4\rho^2} + \Lambda(\rho) - E\right) F(\rho) = 2AF'(\rho) + (B - W)F(\rho)$$

Solution expansion

- Transform equation in form

$$F''(\rho) + PF'(\rho) + QF(\rho) = 0$$

where $P = 2A$ and $Q = \left(\frac{1}{4\rho^2} - \Lambda(\rho) + E + B - W\right)$ are two-dimensional infinite matrices

- Introduce

$$F = UG$$

and elements of G are new unknown quantities

Solution expansion

$$UG'' + \left(2U' + PU\right) G' + \left(U'' + PU' + QU\right) G = 0$$

- Equation for matrix U

$$U' = -\frac{1}{2}PU = -AU$$

- As $\rho \to \infty$

$$U(\rho) = I + \int_{\rho}^{\infty} AUd\rho$$

Solution expansion

- Form without first derivative

$$UG'' + \left(-\frac{1}{2}P' - \frac{1}{4}P^2 + Q\right)UG = 0$$

- Substitute expressions for P and Q

$$G'' + U^{-1}(-A'(\rho) - A^2(\rho) + \frac{1}{4\rho^2} - \\ -\Lambda(\rho) + E + B - W)UG = 0$$

Solution expansion

- As $\rho \to \infty$ asymptotic behavior $U(\rho) \sim I$

$$\left(-\partial_\rho^2 - \frac{1}{4\rho^2} I + \Lambda(\rho) - E\right) G = \\ = \left(-A'(\rho) - A^2(\rho) + B(\rho) - W(\rho)\right) G$$

- The right hand side terms vanish for large ρ faster than ρ^{-2}. Hence this terms can be neglected.

$$\left(-\partial_\rho^2 - \frac{1}{4\rho^2} + \lambda_k^{as}(\rho) - E\right) G_k(\rho) = 0$$

here $\lambda_0^{as}(\rho) = \epsilon$ and $\lambda_k^{as}(\rho) = (2k)^2/\rho^2, k \geq 1$

Solution expansion

- Solutions to these equations with appropriate asymptotics can be expressed in terms of the Bessel (Y, J) functions and the Hankel $(H^{(1)})$ functions of the first kind as following

$$G_0(\rho) \sim \sqrt{\frac{\pi q\rho}{2}} \frac{Y_0(q\rho) - J_0(q\rho)}{\sqrt{2}q} + a_0(q)\sqrt{\frac{\pi q\rho}{2}} H_0^{(1)}(q\rho) e^{i\pi/4}$$

$$G_k(\rho) \sim a_k(E)\sqrt{\frac{\pi\sqrt{E}\rho}{2}} H_{2k}^{(1)}(\sqrt{E}\rho) e^{i(\pi/4+k\pi)}$$

Malfliet-Tjon Potential

Malfliet-Tjon potential

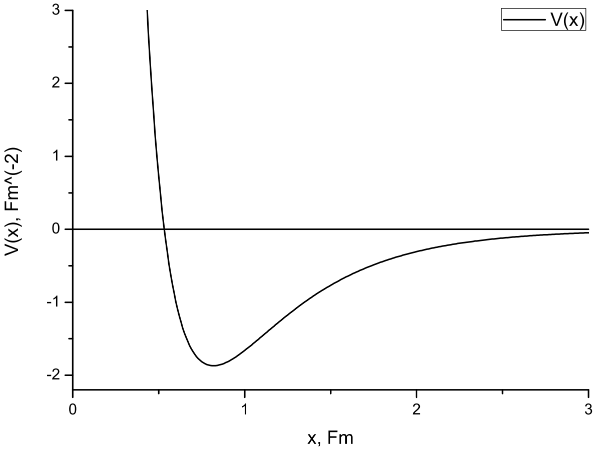
- A potential, which describes the modeling nucleon-nucleon interaction acting in the triplet state with the spin 3/2
- Form of the Yukawa terms superposition

$$V(x) = V_1 \frac{\exp(-\mu_1 x)}{x} + V_2 \frac{\exp(-\mu_2 x)}{x}$$

with parameters listed in the table

Coefficient	Value
V_1	$-626,885$MeV
V_2	$1438,72$MeV
μ_1	$1,55$ Fm^{-1}
μ_2	$3,11$ Fm^{-1}

Malfliet-Tjon potential



Unit system

- Proton-neutron interaction

$$\left(-\frac{\hbar^2}{2\mu}\partial_x^2 + V(x)\right)\psi(x) = E\psi(x),$$

- Reduced mass

$$\mu = \frac{m_p m_n}{m_p + m_n} \simeq \frac{m^2}{2m} = \frac{m}{2},\ m_p \simeq m_n = m$$

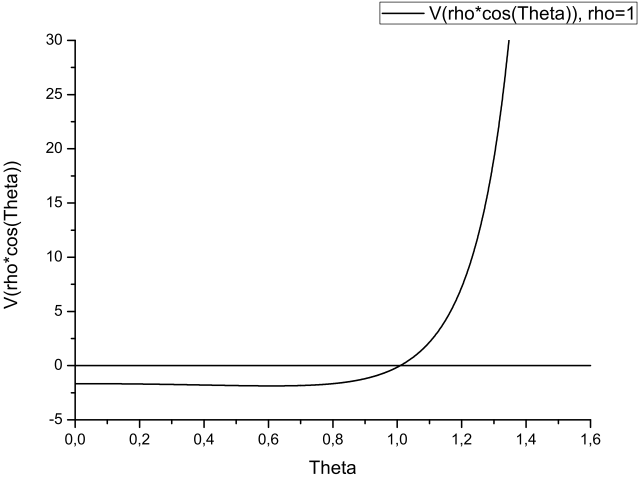
$$\left(-\partial_x^2 + \frac{m}{\hbar^2}V(x) - \frac{m}{\hbar^2}E\right)\psi(x) = 0$$

- $[V] = [E] = \text{MeV}$

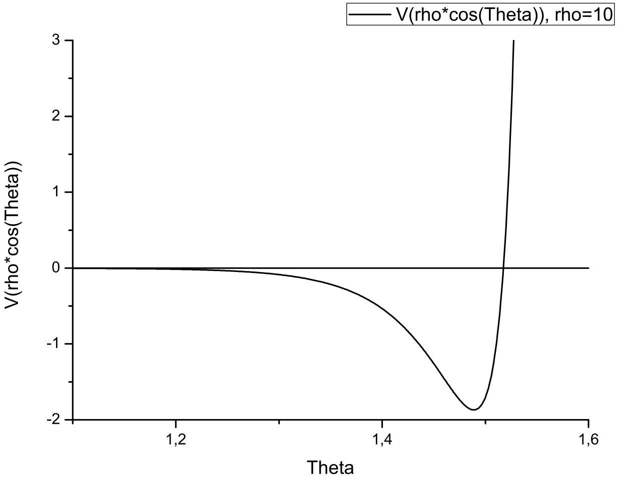
Unit system

- $$\frac{\hbar^2}{m} \simeq 41,47\,\mathrm{Fm}^2 * \mathrm{MeV}$$
- Obtain equation
$$\left(-\partial_x^2 + \widetilde{V}(x) - \widetilde{E}\right)\psi(x) = 0$$
where $[\widetilde{V}] = [\widetilde{E}] = \mathrm{Fm}^{-2}$
- Set $x = \rho\cos\theta$ in polar coordinates and ρ is parameter

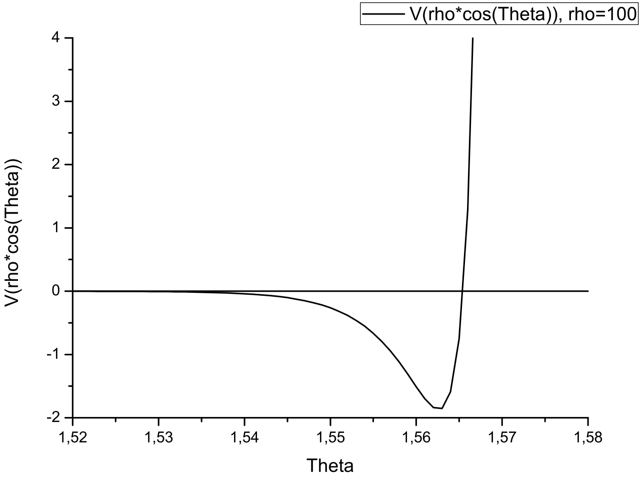
$\rho = 1$


V(rho*cos(Theta)), rho=1
V(rho*cos(Theta))
Theta
30
25
20
15
10
5
0
-5
0,0
0,2
0,4
0,6
0,8
1,0
1,2
1,4
1,6

$\rho = 10$



$\rho = 100$


V(rho*cos(Theta)), rho=100
4
3
2
1
0
-1
-2
1,52
1,53
1,54
1,55
1,56
1,57
1,58
Theta
V(rho*cos(Theta))

Numerical Calculations

Numerical calculations

- Finite-difference approach

$$\frac{-\phi_k(\theta - h) + 2\phi_k(\theta) - \phi_k(\theta + h)}{\rho^2 h^2} + \\ + V(\rho\cos\theta)\phi_k(\theta) = \lambda_k \phi_k(\theta)$$

where $h = \theta_{i+1} - \theta_i, i = 1, ..., N$ and $N \sim 100000$

- Boundary conditions

$$\phi_k(0) = \phi_k(\pi/2) = 0$$

Software

- CLAPACK
- Intel Math Kernel Library 10.0.1 for Unix
- 'DSTEVX': computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices.

Eigenvalues

Asymptotics

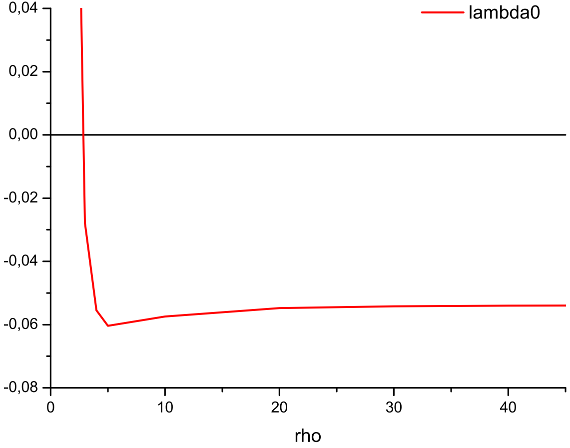
- $k = 0$

$$\lim_{\rho \to \infty} \lambda_0(\rho) = \epsilon$$

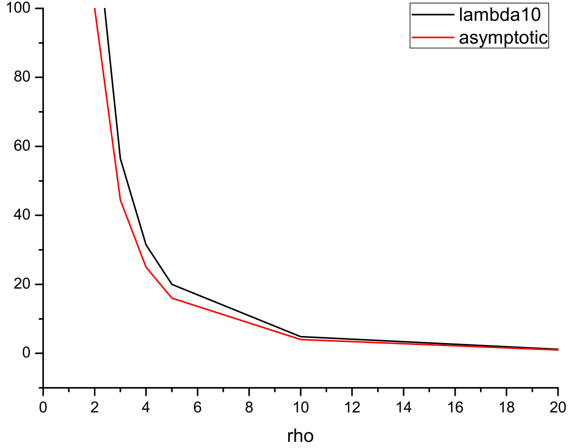
- $k \geq 1$

$$\lambda_k(\rho) \sim \left(\frac{2k}{\rho}\right)^2$$

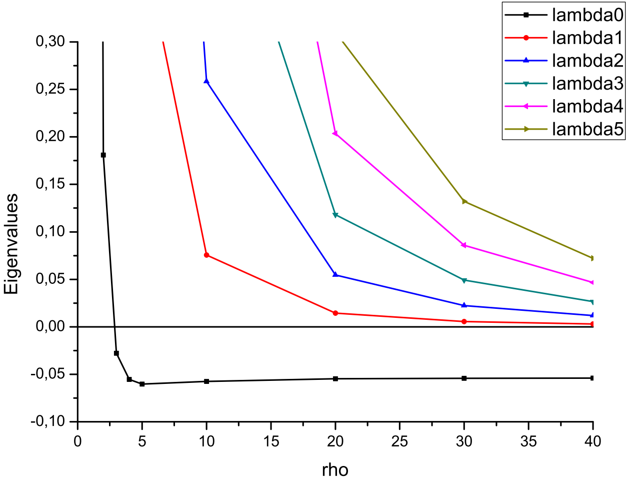
$\lambda_0(\rho)$



$\lambda_{10}(\rho)$



Eigenvalues

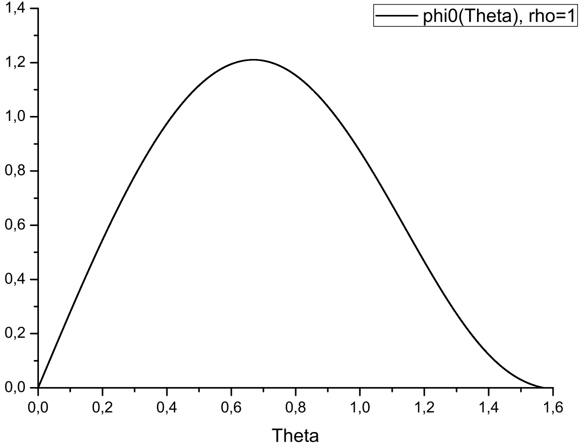


Deviation from asymptotics

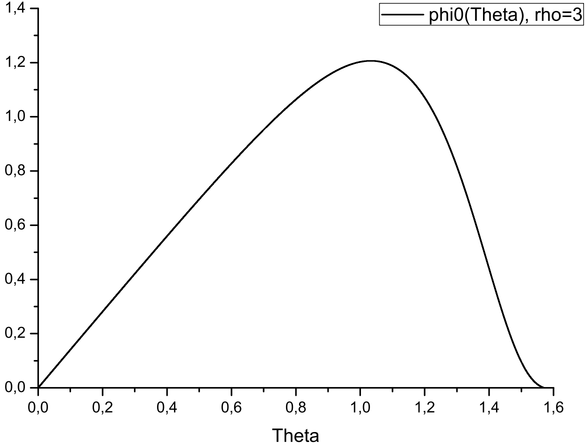
- $\rho \sim 10$ – deviation is big and varies from 10% up to 90%. For small k the absolute deviation is bigger than for big k.
- $\rho \sim 100$ – deviation is about $5 - 7\%$
- $\rho = 700$ – deviation is less than 1%
- $\rho \sim 1000$ – deviation is about $0,7\%$

Eigenfunctions

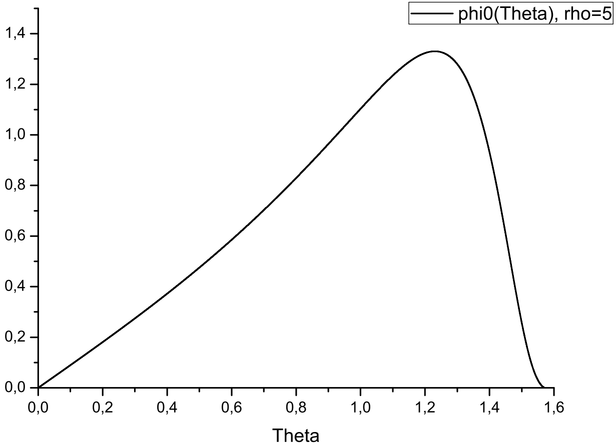
$\phi_0(\theta), \rho = 1$



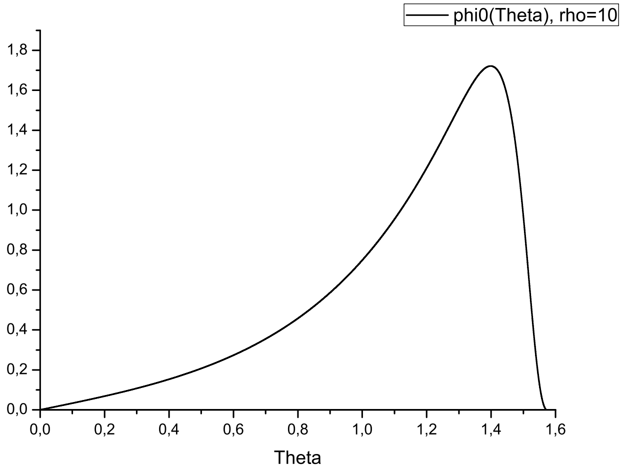
$\phi_0(\theta), \rho = 3$



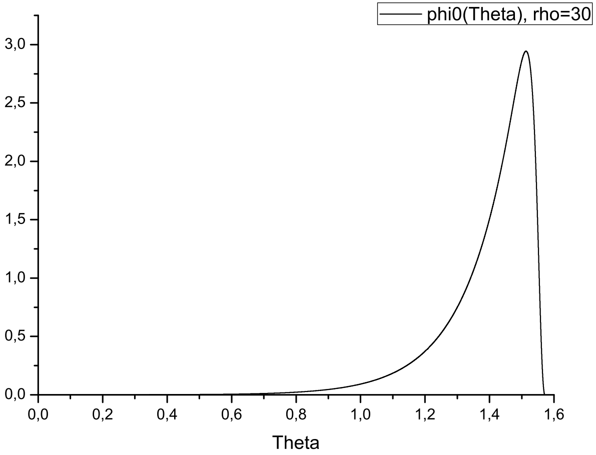
$\phi_0(\theta), \rho = 5$



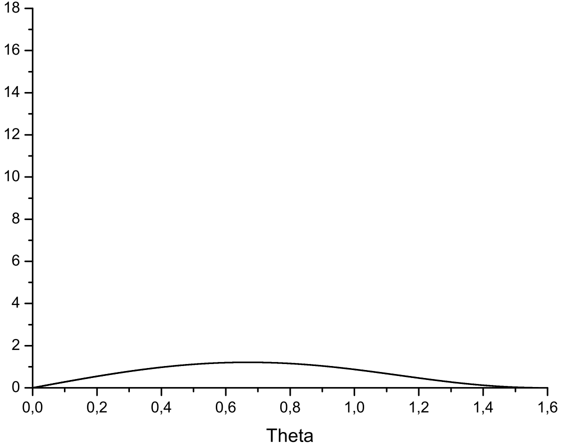
$\phi_0(\theta), \rho = 10$



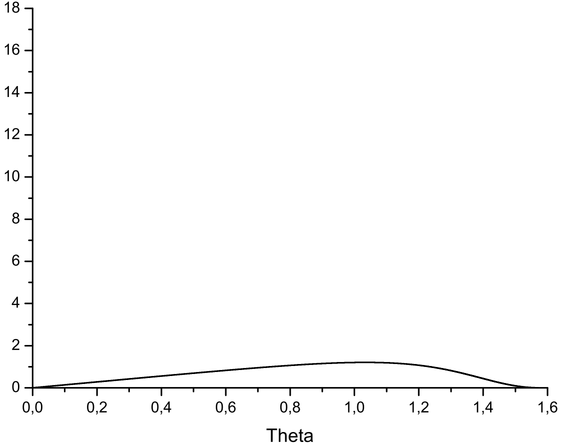
$\phi_0(\theta), \rho = 30$



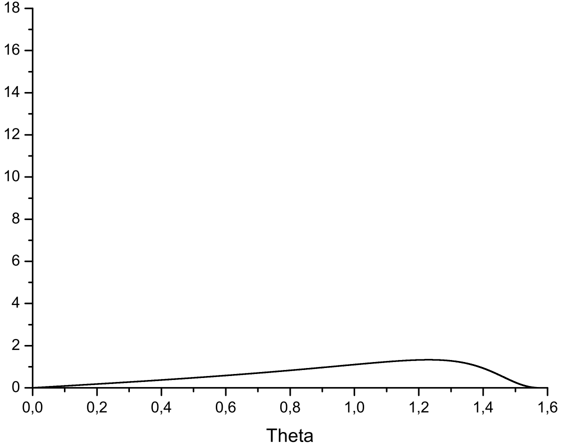
$\phi_0(\theta), \rho = 1$



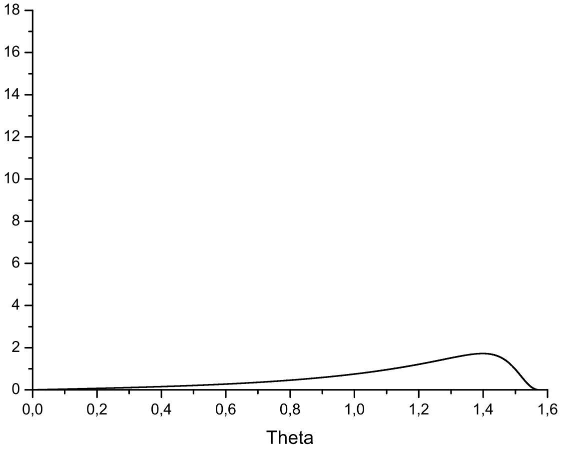
$\phi_0(\theta), \rho = 3$



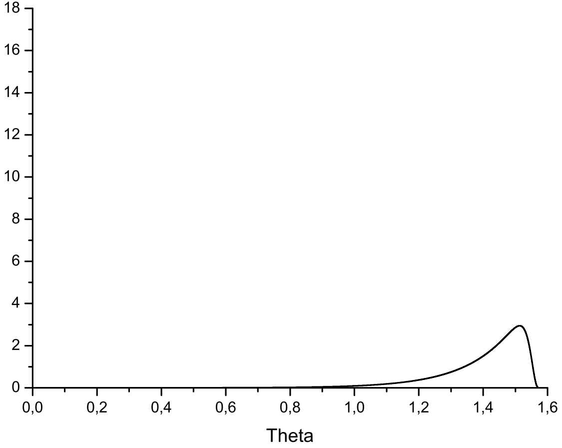
$\phi_0(\theta), \rho = 5$



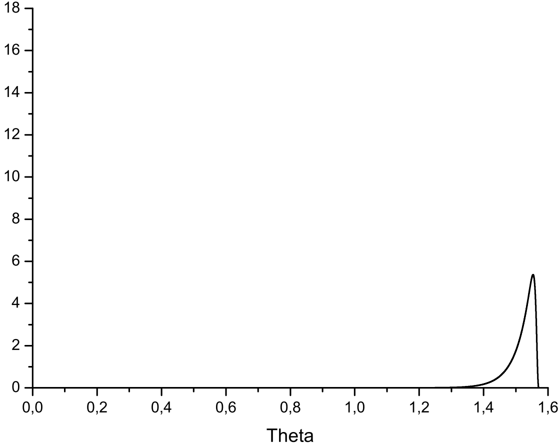
$\phi_0(\theta), \rho = 10$



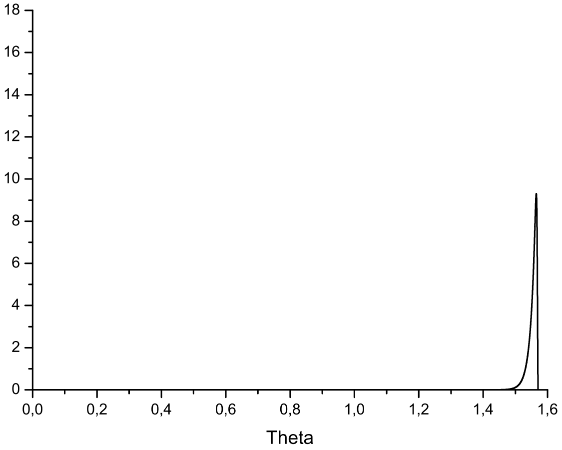
$\phi_0(\theta), \rho = 30$



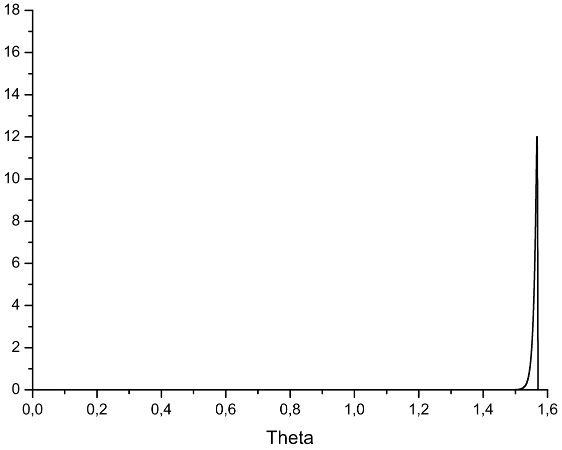
$\phi_0(\theta), \rho = 100$



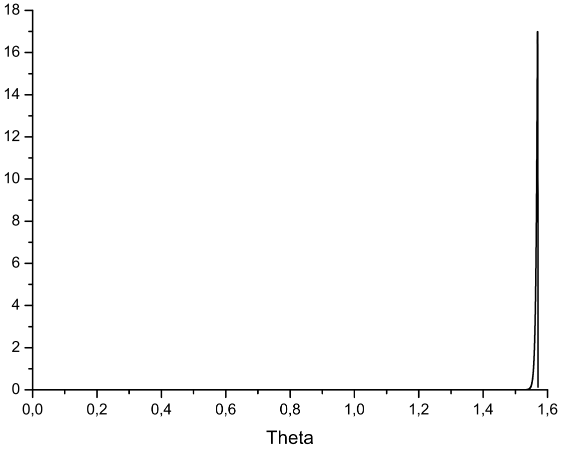
$\phi_0(\theta), \rho = 300$



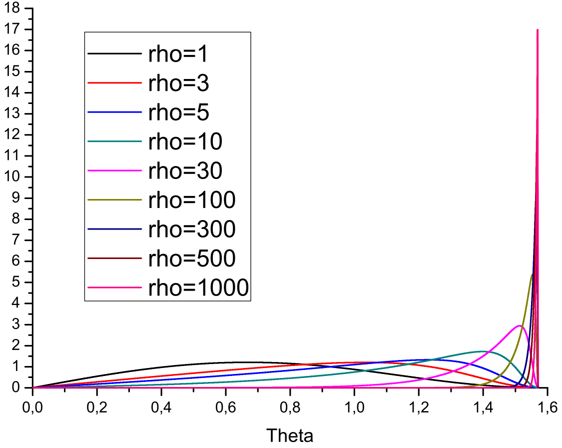
$\phi_0(\theta), \rho = 500$



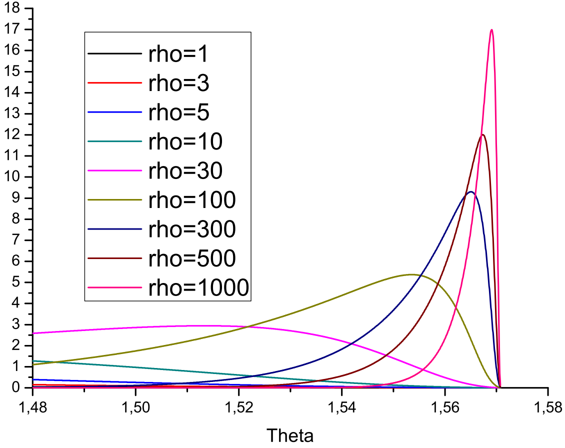
$\phi_0(\theta), \rho = 1000$



Step-by-step


rho=1
rho=3
rho=5
rho=10
rho=30
rho=100
rho=300
rho=500
rho=1000
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
0,0
0,2
0,4
0,6
0,8
1,0
1,2
1,4
1,6
Theta

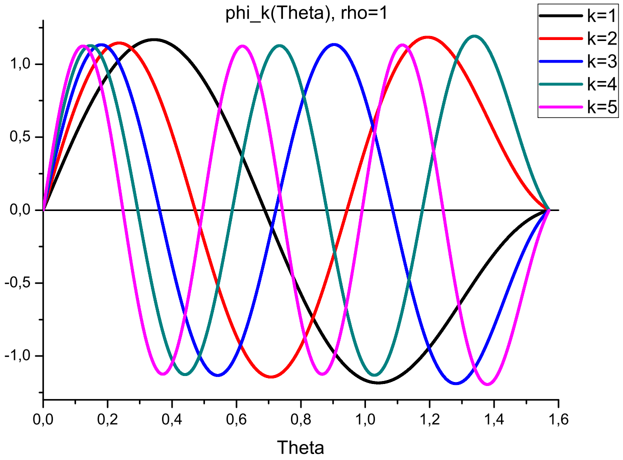
Step-by-step


rho=1
rho=3
rho=5
rho=10
rho=30
rho=100
rho=300
rho=500
rho=1000
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
1,48
1,50
1,52
1,54
1,56
1,58
Theta

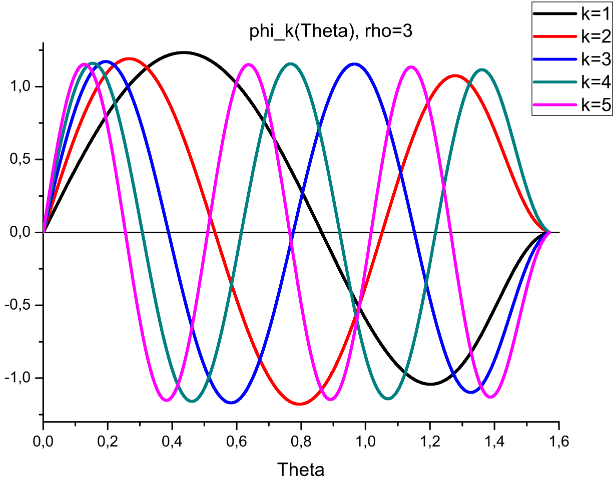
$\phi_0(\theta)$: conclusions

- As $\rho \to \infty$ eigenfunction ϕ_0 transforms into δ-function
- Computational problems: decreasing of spacing, time of computation, size of data, useless zero-area

$\phi_k(\theta), k \geq 1$



$\phi_k(\theta), k \geq 1$



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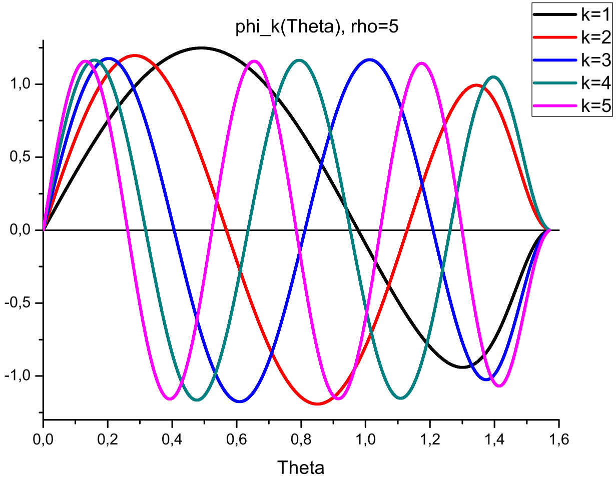
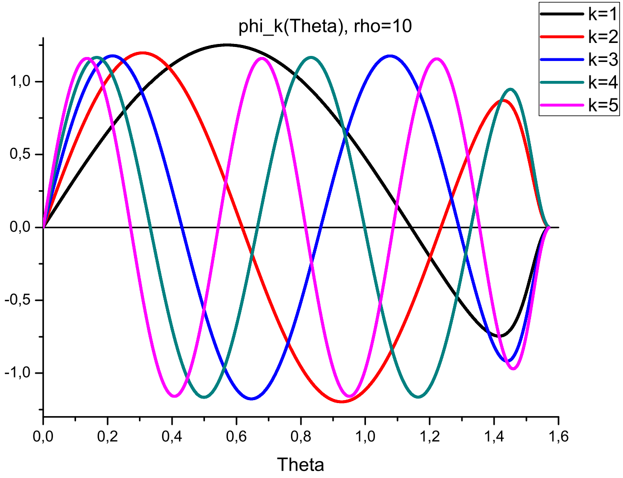
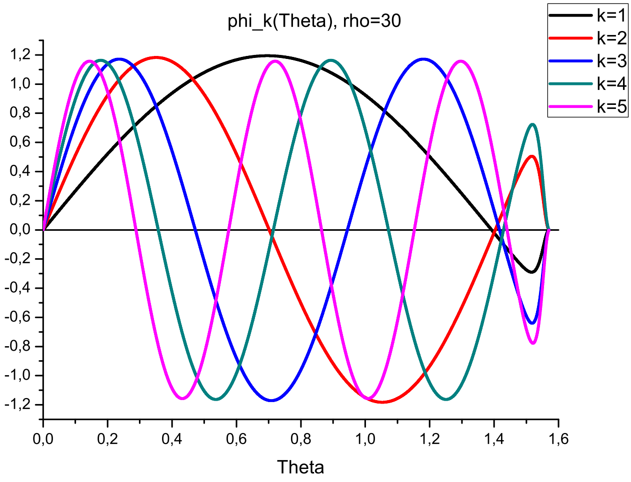


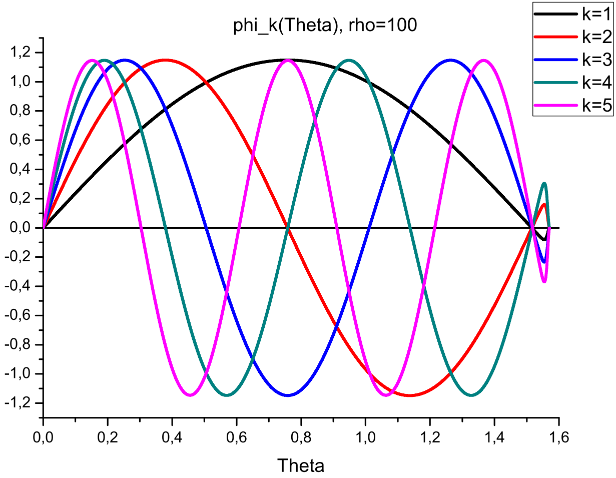
$\phi_k(\theta), k \geq 1$



$\phi_k(\theta), k \geq 1$



$\phi_k(\theta), k \geq 1$



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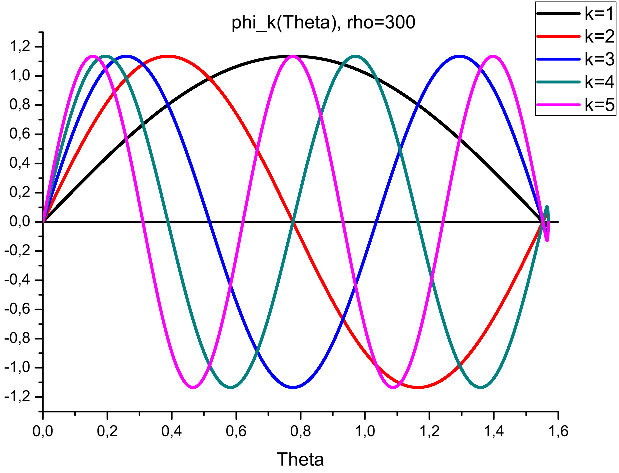
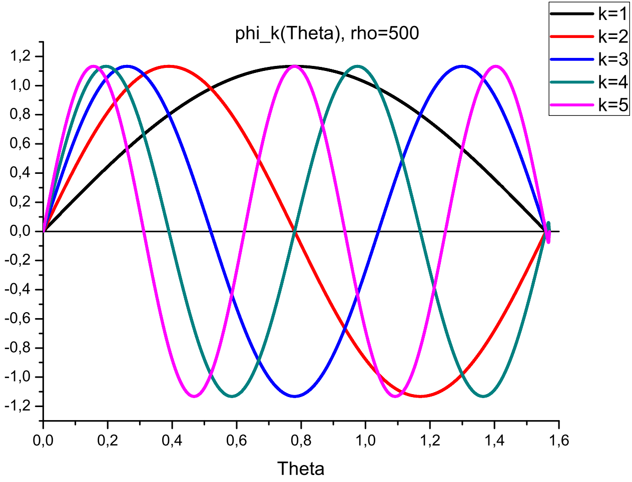
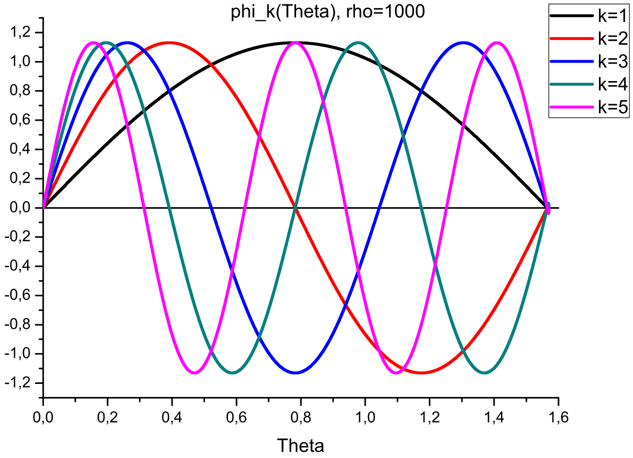


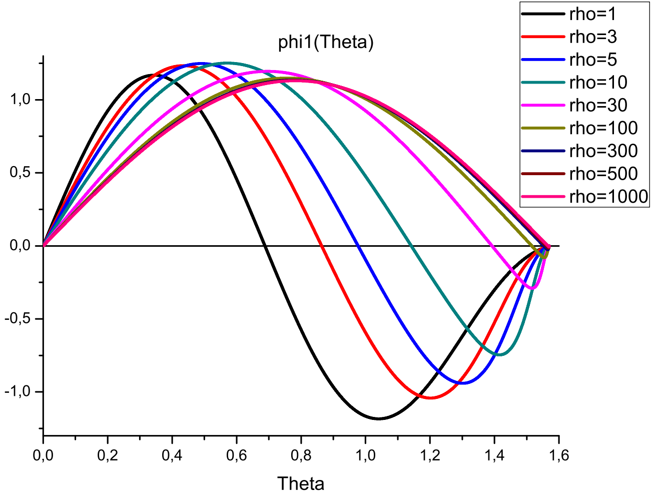
$\phi_k(\theta), k \geq 1$



$\phi_k(\theta), k \geq 1$



Step-by-step $\phi_1(\theta)$



Orthogonality and deviations

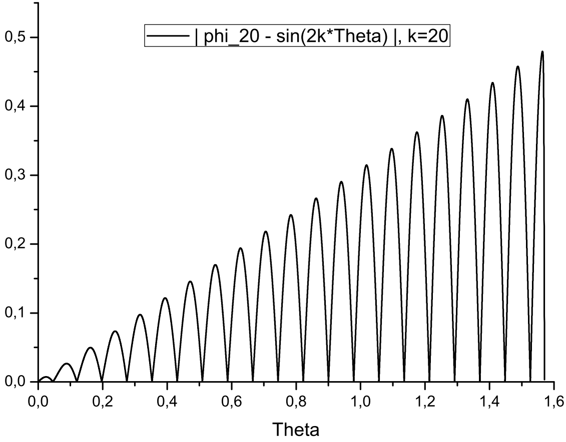
- Check orthogonality on each step
- When does eigenfunction reach its asymptotic behavior?

$$\max_{\theta} |\phi_{k,\rho}(\theta) - \sin(2k\theta)|$$

$\rho = 500$

k	max deviation
1	0,025055987697
2	0,050095937266
3	0,075103861927
4	0,100064122846
5	0,124961227783
6	0,149780111430
7	0,174506106355
...	...
14	0,343853748940
15	0,367366621881
16	0,390677267607
17	0,413776421157
18	0,436655434712
19	0,459306336123
20	0,481722165969

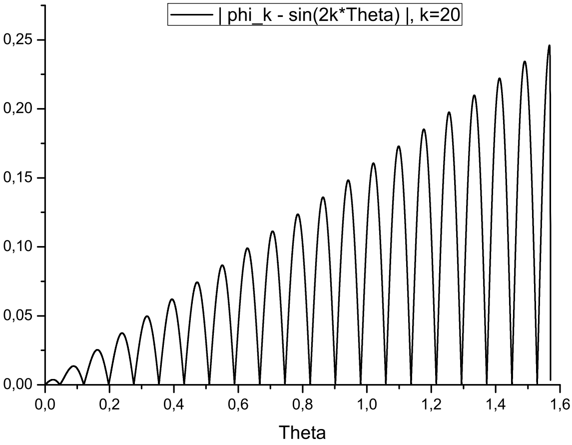
Deviation in case $k = 20$, $\rho = 500$



$\rho = 1000$

k	max deviation
1	0, 012548181991
2	0, 025094300382
3	0, 037636297454
4	0, 050172115034
5	0, 062699700358
6	0, 075217084552
7	0, 087722341482
...	...
14	0, 174758410342
15	0, 187098541399
16	0, 199410537020
17	0, 211691972534
18	0, 223941583831
19	0, 236157876824
20	0, 248338419864

Deviation in case $k = 20$, $\rho = 1000$



Geometrical connections

Geometrical connections

- Off-diagonal matrix of geometrical connections A with elements

$$A_{ki}(\rho) = \langle \phi_k | \phi_i' \rangle = \int_0^{\pi/2} d\theta \, \phi_k^*(\theta|\rho) \frac{\partial \phi_i(\theta|\rho)}{\partial \rho}$$

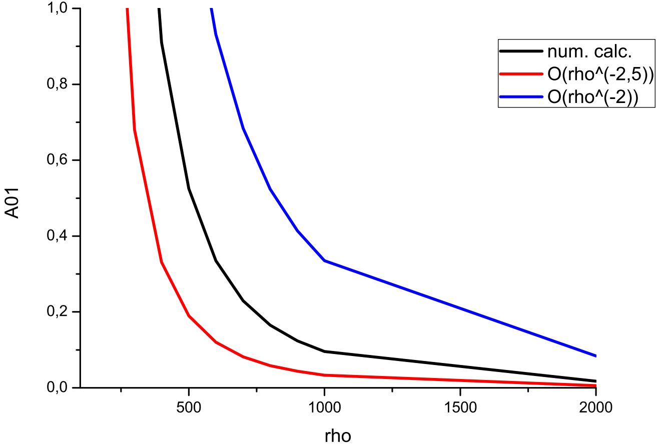
- Determines behavior of right part of equation

$$\left(-\partial_\rho^2 - \frac{1}{4\rho^2} I + \Lambda(\rho) - E \right) G =$$
$$= \left(-A'(\rho) - A^2(\rho) + B(\rho) - W(\rho) \right) G$$

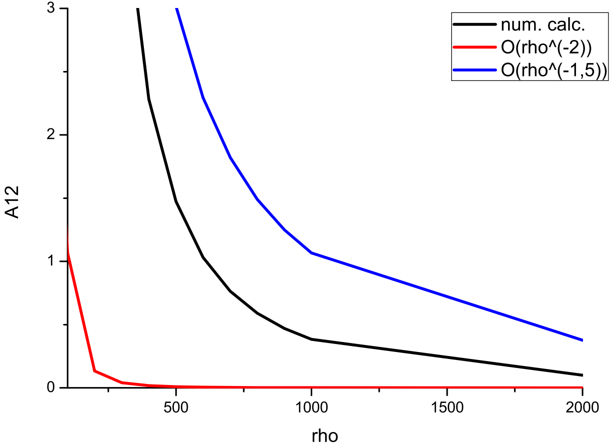
Geometrical connections

- $$A_{ki} = \frac{\langle \phi_k | \frac{\partial V}{\partial \rho} | \phi_i \rangle}{\lambda_k - \lambda_i}$$
- $A_{ki} = -A_{ik}$ and $A_{kk} = 0$

A_{ki}, $k = 0$ or $i = 0$


1,0
0,8
0,6
0,4
0,2
0,0
A01
500
1000
1500
2000
rho
num. calc.
O(rho^(-2,5))
O(rho^(-2))

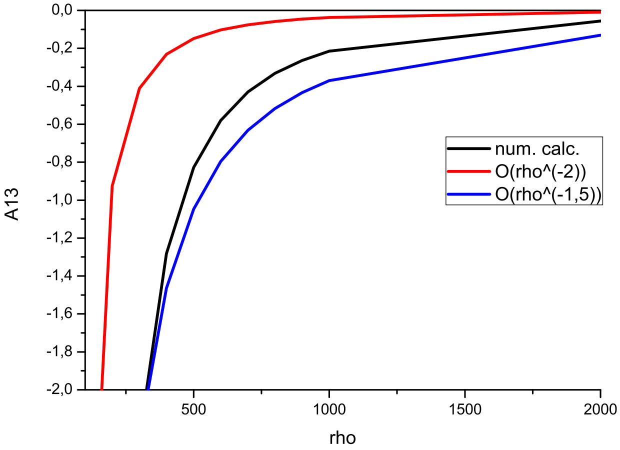
A_{ki}, $k \neq 0$ and $i \neq 0$



Numerical solution of the three body scattering problem

Leonid Rudenko

A_{ki}, $k \neq 0$ and $i \neq 0$



The last note about A_{ki}

- The behavior of geometrical connections A_{ki} is regular (no singularity or special points) in case of Malfliet-Tjon potential.

Thank you!