Spectral computational Methods

Phys. 2016 conference, New Orleans

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by

George Rawitscher

Two basic computational methods:

a) Use Taylor series expansion (finite difference meth.)

b) Expand into a series of basis functions (Spectral meth.)

Finite Difference

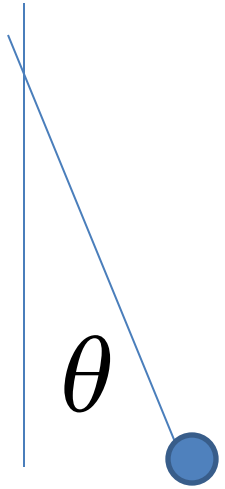


Equi-spaced points

$$f(x_n + h) = f(x_n) + hf'(x_n) + \frac{h^2}{2}f''(x_n) + \frac{h^3}{6}f'''(x_n) + O(h^4)$$
$$f(x_n - h) = f(x_n) - hf'(x_n) + \frac{h^2}{2}f''(x_n) - \frac{h^3}{6}f'''(x_n) + O(h^4)$$

$$\frac{1}{2}(f_{n+1} + f_{n-1}) = f_n + \frac{h^2}{2}f''_n + O(h^4)$$

Pendulum



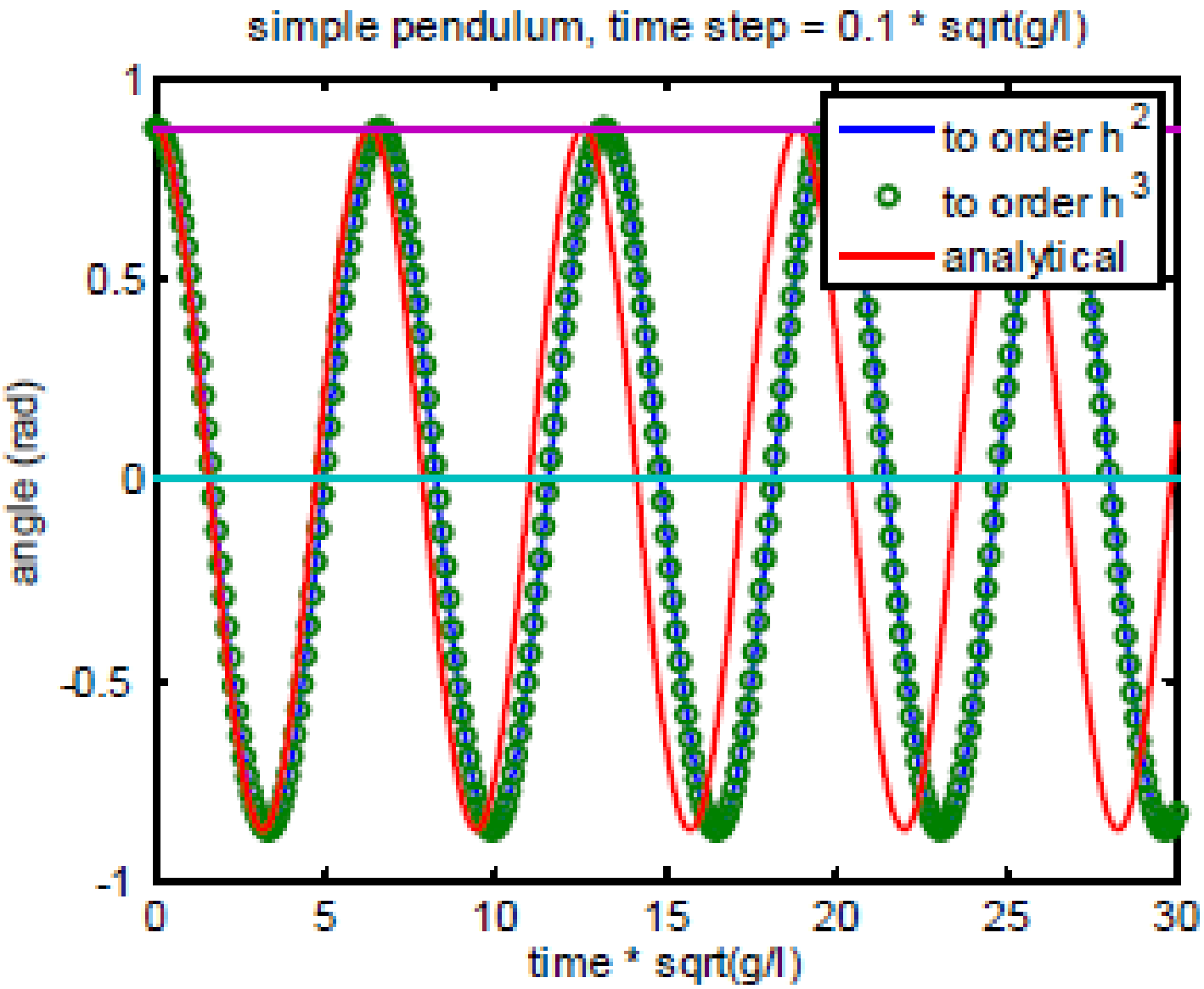
$$\frac{d^2}{dt^2}\theta = -\frac{g}{\ell}\sin(\theta)$$

Non-linear

$$\frac{d^2}{dt^2}\theta = -\frac{g}{\ell}\theta$$

"*Analytical* "

Linear

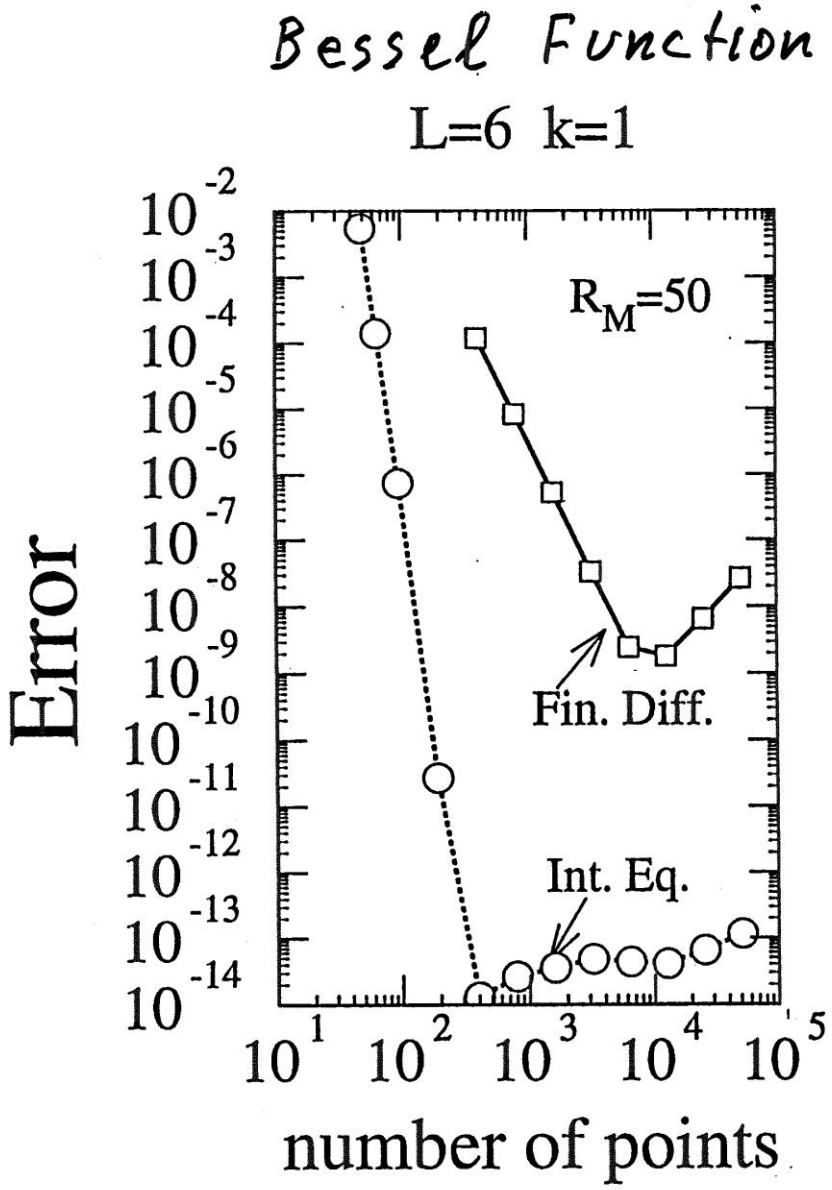

simple pendulum, time step = 0.1 * sqrt(g/l)
angle (rad)
time * sqrt(g/l)
to order h 2
to order h 3
analytical
1
0.5
0
-0.5
-1
0
5
10
15
20
25
30

Spectral Method

Galerkin

Collocation

$$(d^2/dr^2 - L(L+1)/r^2 + k^2)F_L(r) = 0$$



Numerov, Finite Diff. method

Spectral Method

Spectral Methods

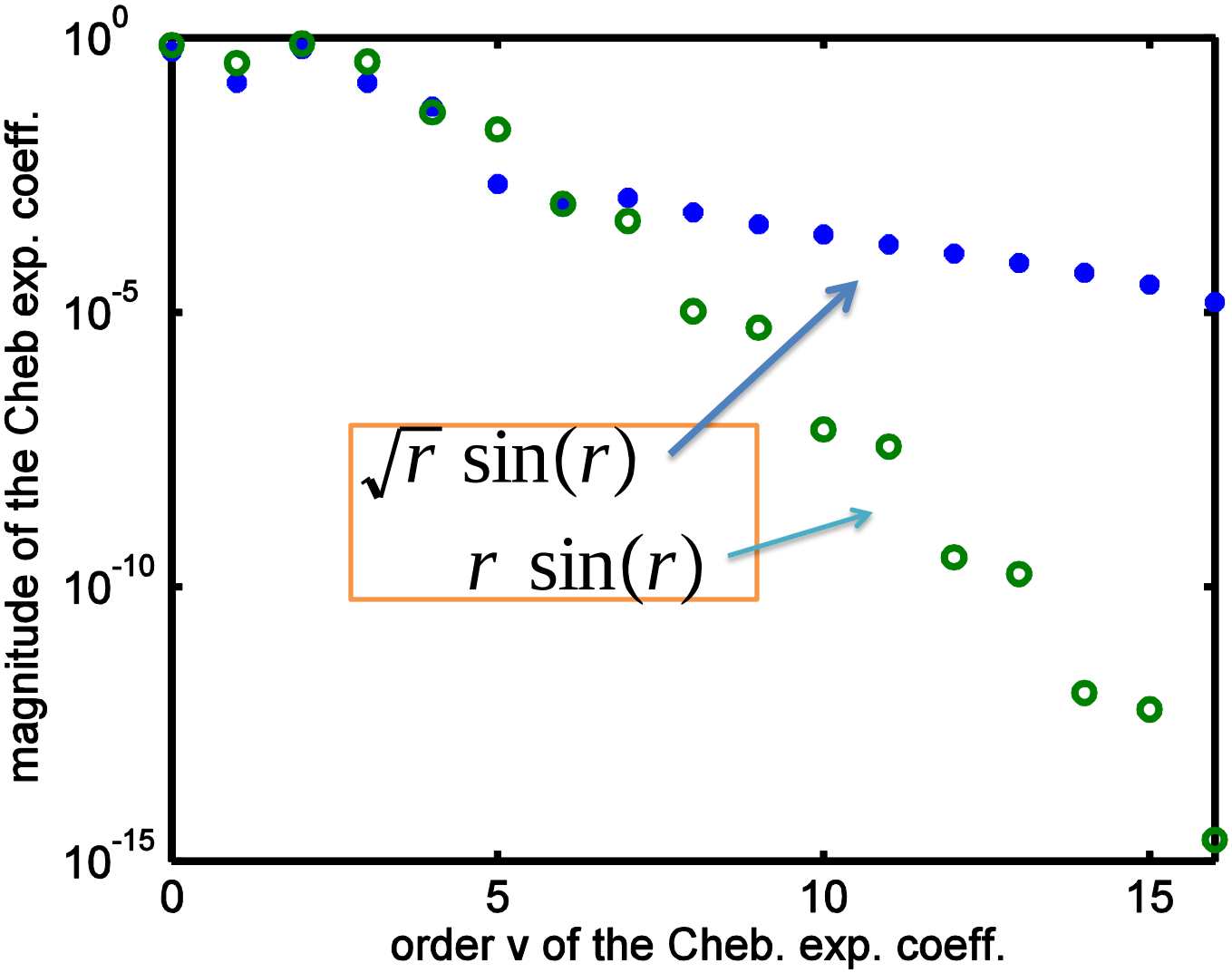
a) Expand the functions into a set of basis functions $\phi_n(x)$

$$f(x) = a_1\phi_0(x) + a_2\phi_1(x) + a_3\phi_2(x)\ldots\infty$$

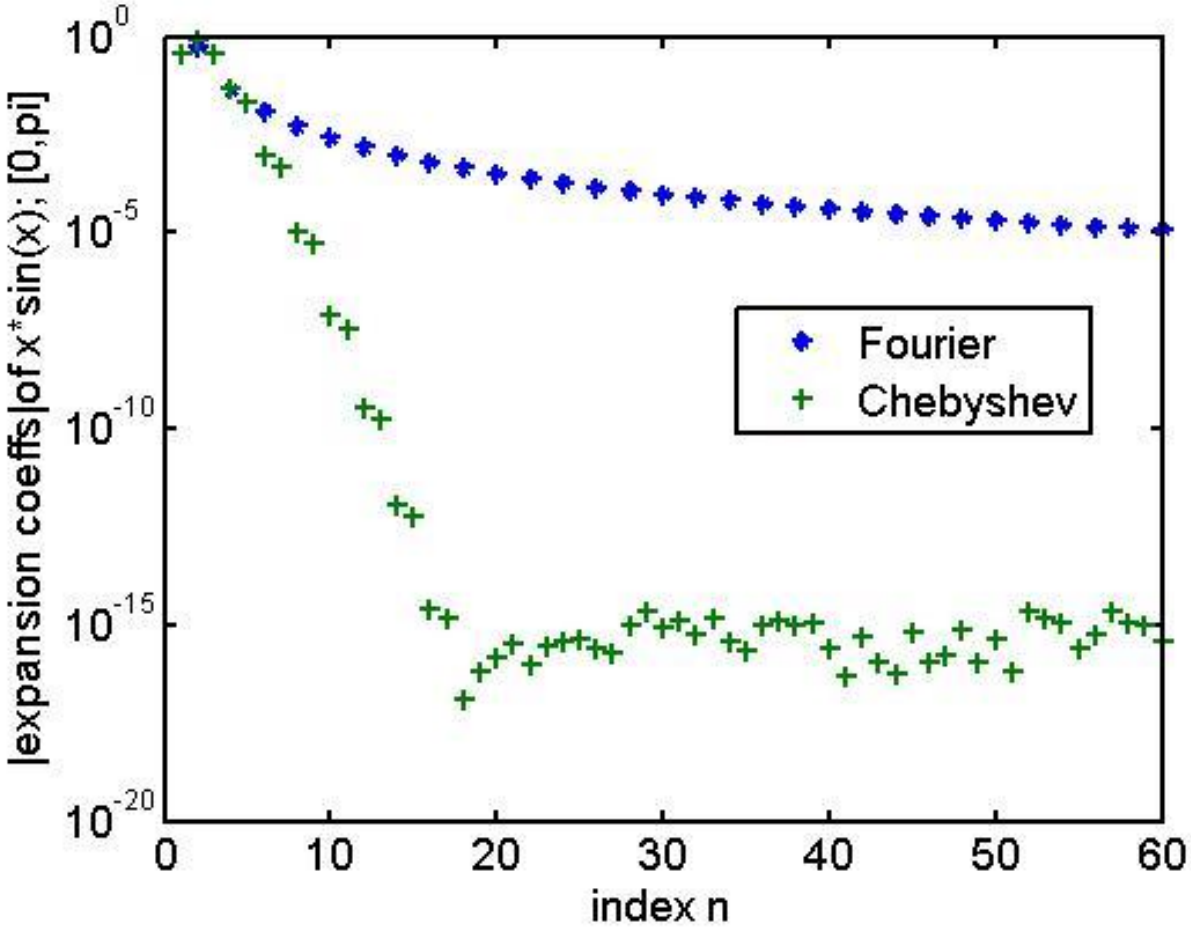
$$f^{(N)}(x) = \sum_{n=1}^{N+1} a_n\, \phi_{n-1}(x), \quad \textit{Truncated}$$

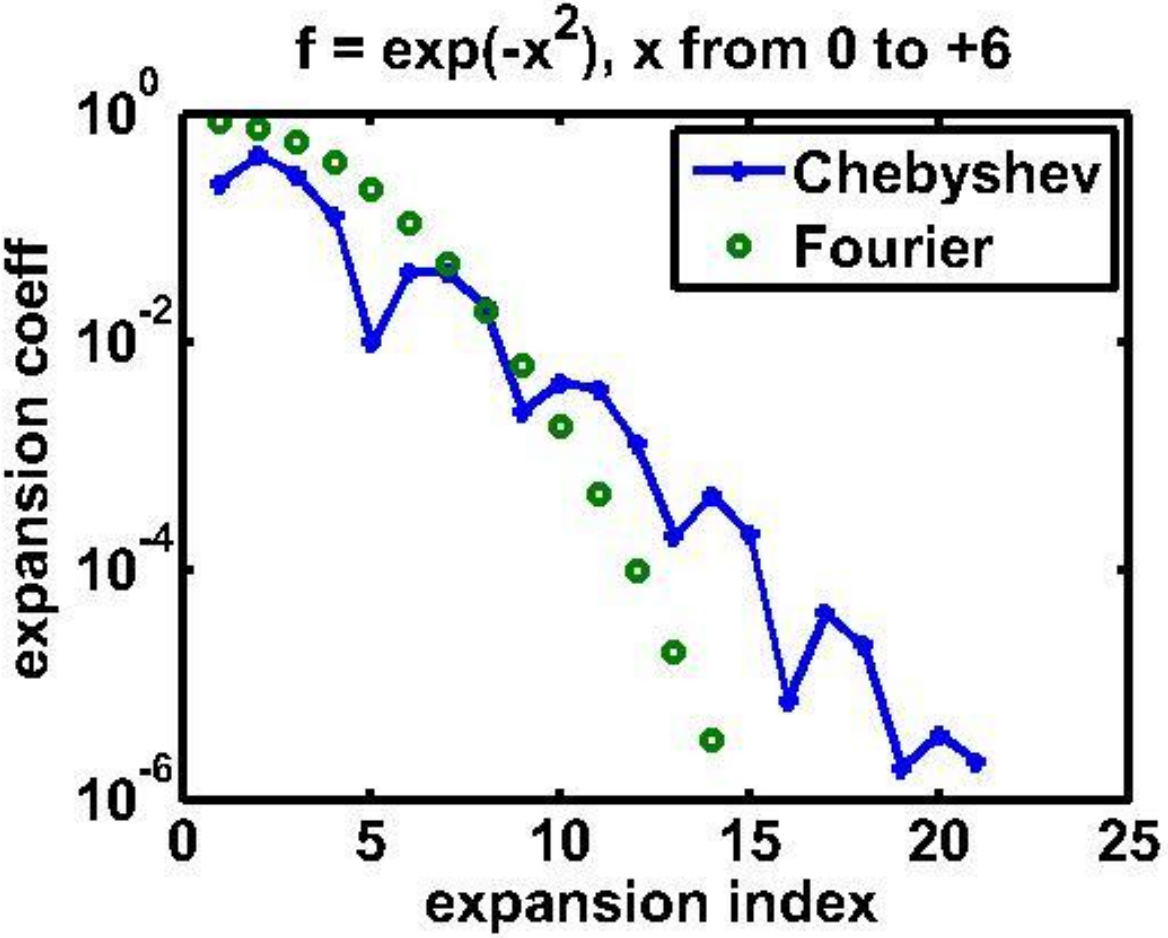
$$\text{Error} \quad \mathcal{R}(x) = f^{(N)}(x) - f(x)$$

Expansion into Chebyshevs



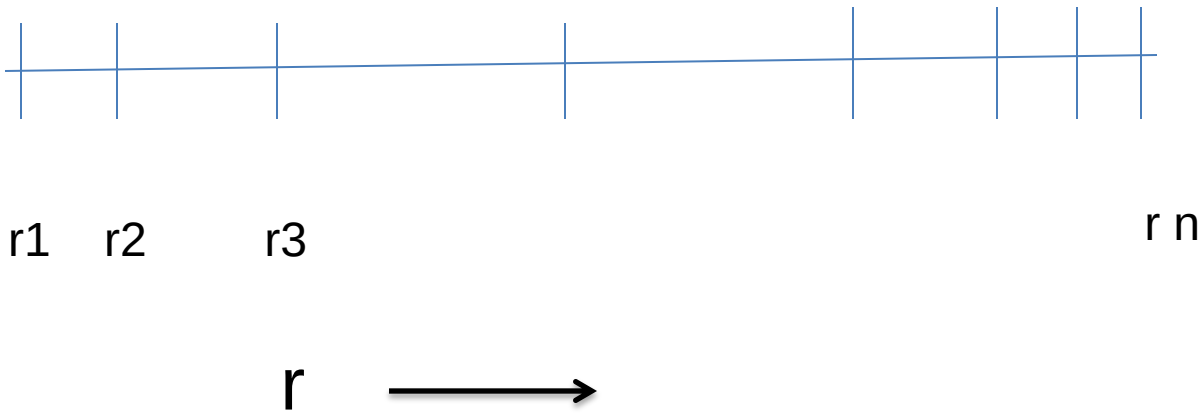
Expansion Coeffs of xsin(x) [0,pi]




f = exp(-x^2), x from 0 to +6
Chebyshev
Fourier
expansion coeff
10^0
10^-2
10^-4
10^-6
0
5
10
15
20
25
expansion index

Spectral Methods

b) Take all the support points into account simultaneously



Galerkin

$\hat{L}$ ← Linear operator

$$\hat{L}u(x) = f(x), \quad x \in [a,b]$$ ← Eq. to be solved for u
f is a known function

$$u^{(N)}(x) = \sum_{i=1}^{N+1} a_i \, \phi_i(x), \quad a \le x \le b$$ ← Basis functions

$$\hat{L}\, u^{(N)}(x) - f(x) = \mathcal{R}^{(N)}(x)$$ ← Residue to be minimized

Galerkin,

$$\langle \chi_i | \mathcal{R} \rangle = \int_a^b \chi_i(x) \rho(x) \mathcal{R}(x)\, dx$$

$$\sum_{i=1}^{N+1} L_{ji}\, a_i - F_j = \langle \chi_j | \mathcal{R} \rangle = 0, \quad j = 1, 2, \ldots, N+1$$

where

$$(\mathbf{L})_{j\,i} = L_{ji} = \langle \chi_j | \hat{L} \phi_i \rangle, \quad \text{and } F_j = \langle \chi_j | f \rangle$$

$$\mathbf{L} * (a) = (F)$$

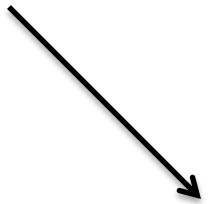


Matrix Eq. for the coefficients a

Collocation

$$\hat{L}\, u^{(N)}(x) = \sum_{i=1}^{N+1} a_i \, (\hat{L}\phi_i)_x = f(x)$$

How to avoid the overlap integrals



$$u^{(N)}(x) = \sum_{i=1}^{N+1} a_i \, \phi_i(x)$$

Curtis-Clenshaw matrix method to obtain the expansion coeffs. “a”

$$(f) \equiv \begin{pmatrix} f(r_1) \\ f(r_2) \\ \vdots \\ f(r_N) \end{pmatrix}; \quad (a) \equiv \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

$$(a) = C^{-1}(f)$$

N x N Matrix

$$(C^{-1})_{si} = \phi_i(r_s)$$

$$\sum_{i=1}^{N+1} a_i \, (\hat{L}\phi_i)_{r_s} = f(r_s); \quad s = 1, 2, \ldots, N+1$$

For all the mesh points s

$$\sum_{i=1}^{N+1} a_i \, (\hat{L}\phi_i)_{r_s} = f(r_s); \quad s = 1, 2, \ldots, N+1$$

$$(\mathbf{M})_{s\,i} = (\hat{L}\phi_i)_{r_s}$$

$$\sum_{i=1}^{N+1} (\mathbf{M})_{s\,i} \, a_i = f(r_s)$$

Basic matrix eq. for the a's

$$u^{(N)}(x) = \sum_{i=1}^{N+1} a_i \, \phi_i(x)$$

Curtis-Clenshaw matrix method to obtain the expansion coeffs. “a”

$$(f) \equiv \begin{pmatrix} f(r_1) \\ f(r_2) \\ \vdots \\ f(r_N) \end{pmatrix}; \quad (a) \equiv \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

r’s are mesh-points

that have to be chosen

carefully

$$(a) = C^{-1}(f)$$

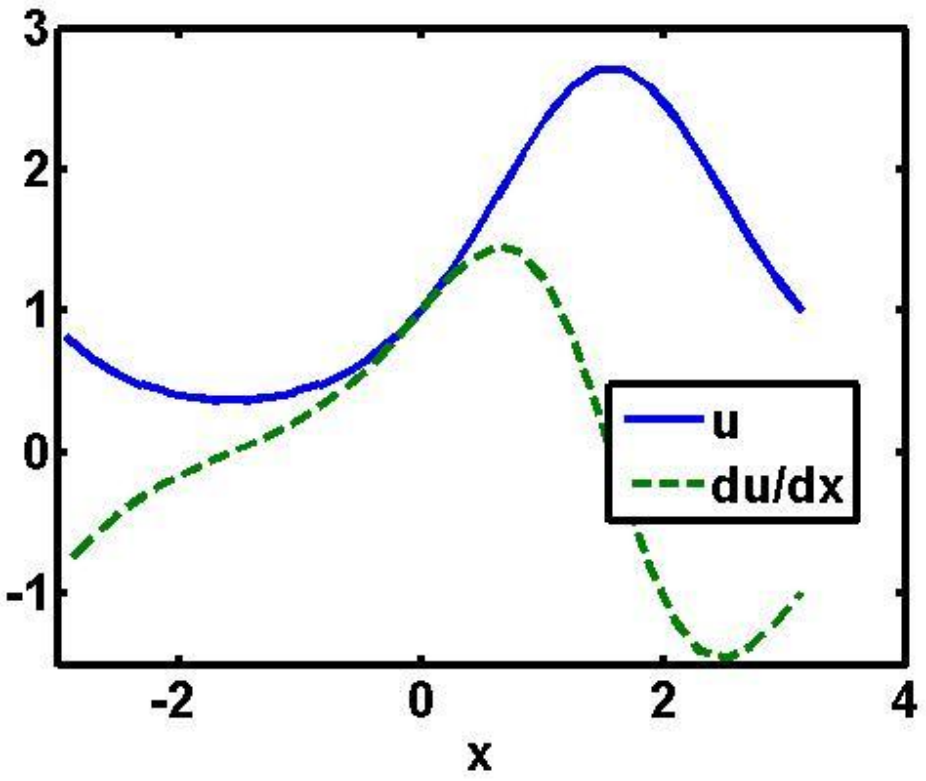
N x N Matrix

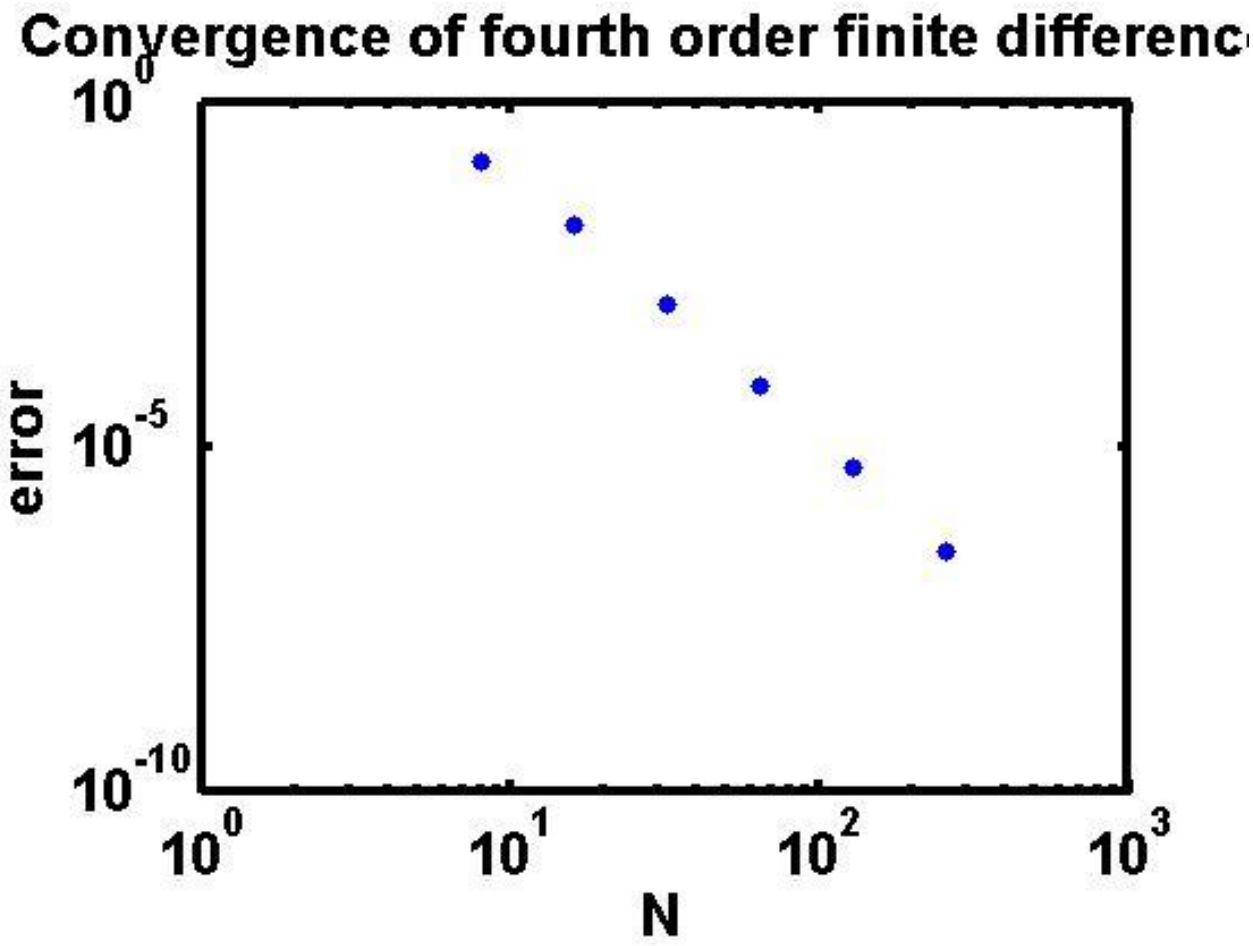
Derivative Example

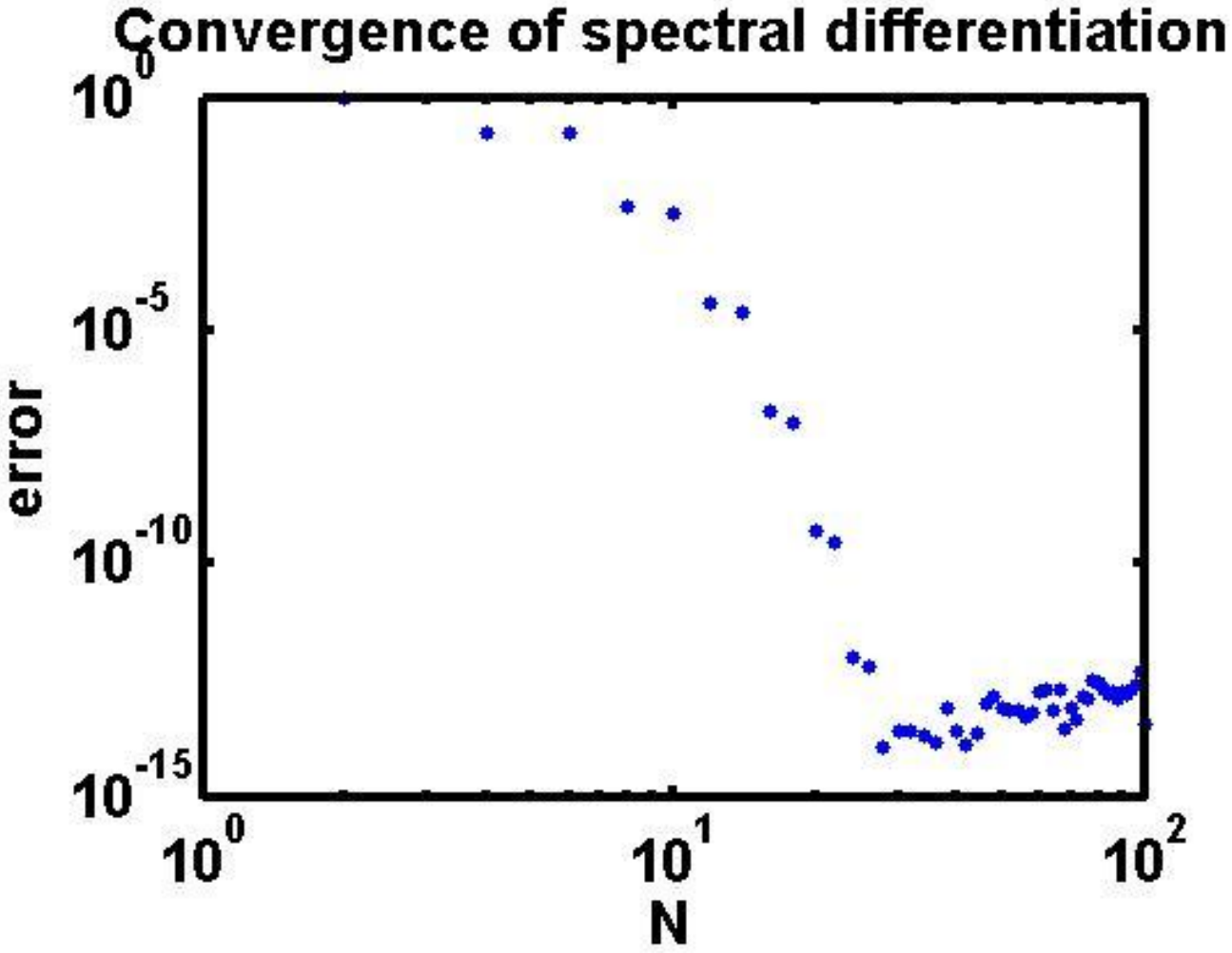
$$\hat{L} = \frac{d}{dx}$$

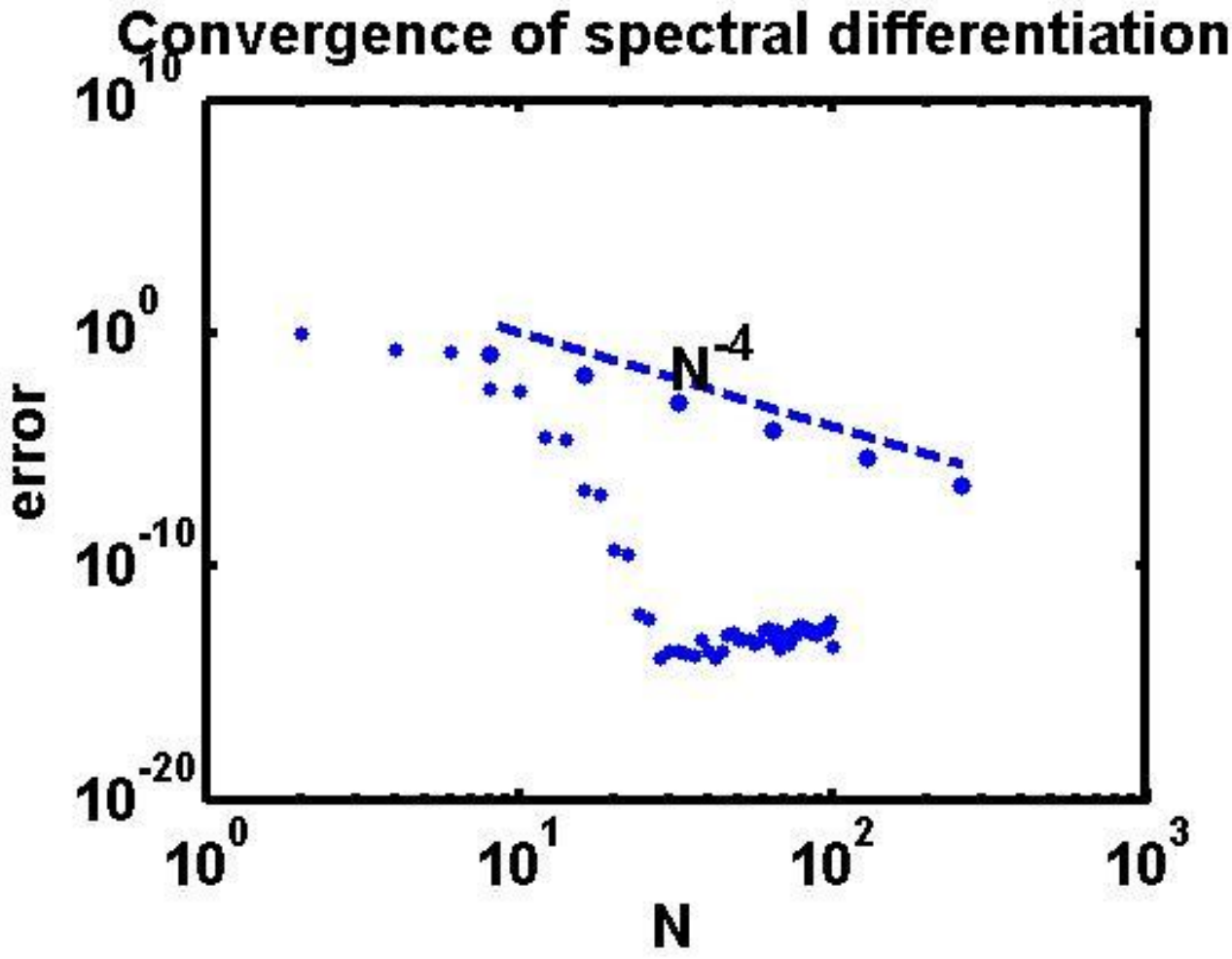
$$u(x) = e^{\sin(x)} \qquad u'(x) = \cos(x) \cdot u(x)$$

$$-\pi \leq x \leq \pi$$




Convergence of fourth order finite differenc
10^0
10^-5
10^-10
error
10^0
10^1
10^2
10^3
N


Convergence of spectral differentiation
error
N
10^{0}
10^{-5}
10^{-10}
10^{-15}
10^{0}
10^{1}
10^{2}

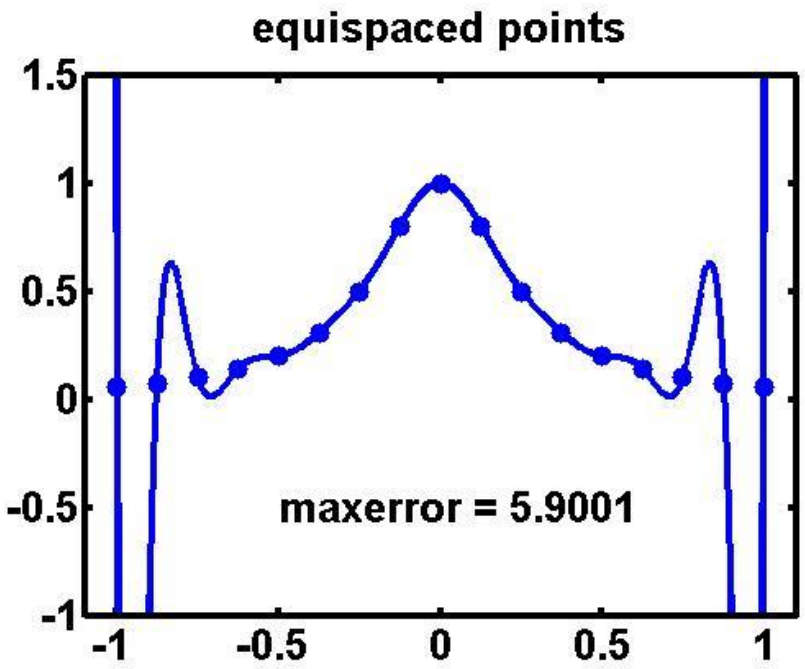

Convergence of spectral differentiation
10^10
10^0
10^-10
10^-20
error
N^-4
10^0
10^1
10^2
10^3
N

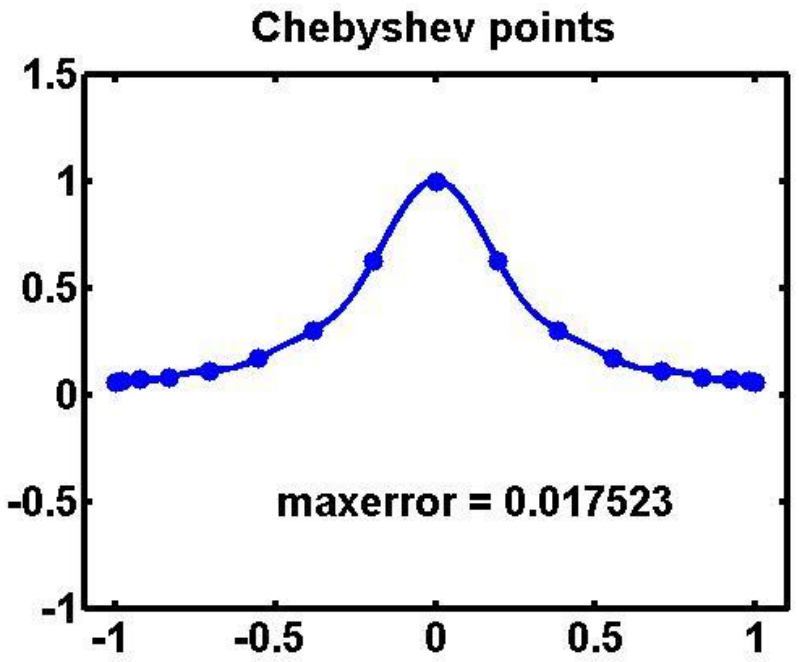
Interpolation Example

$$f(x) = 1/(1 + 16\,x^2)$$

N = 16

-1 < x <1





Chebyshev Polynomials

$-1 < x < 1$

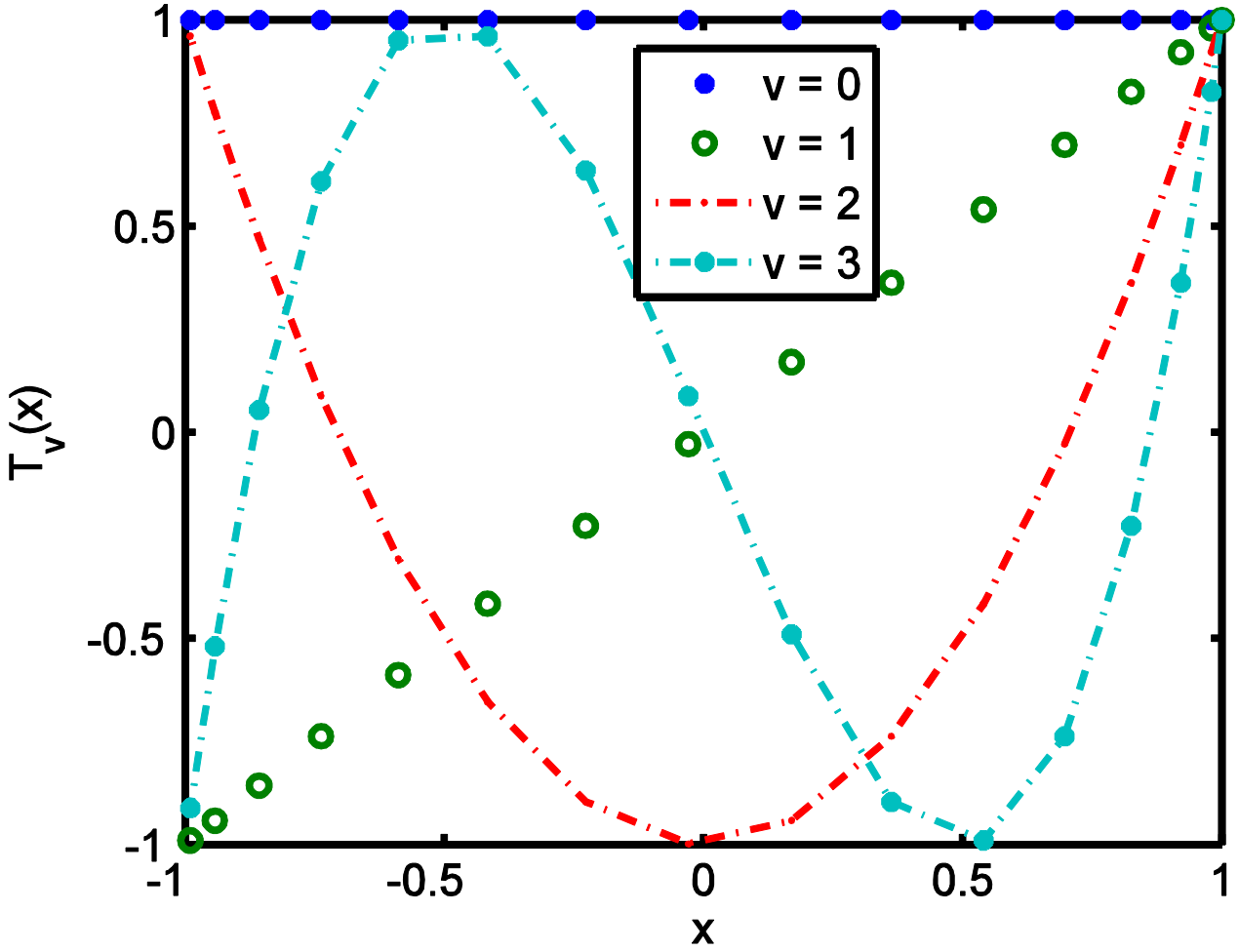
$$T_0 = 1$$

$$T_1 = x$$

$$T_2 = 2x^2 - 1$$

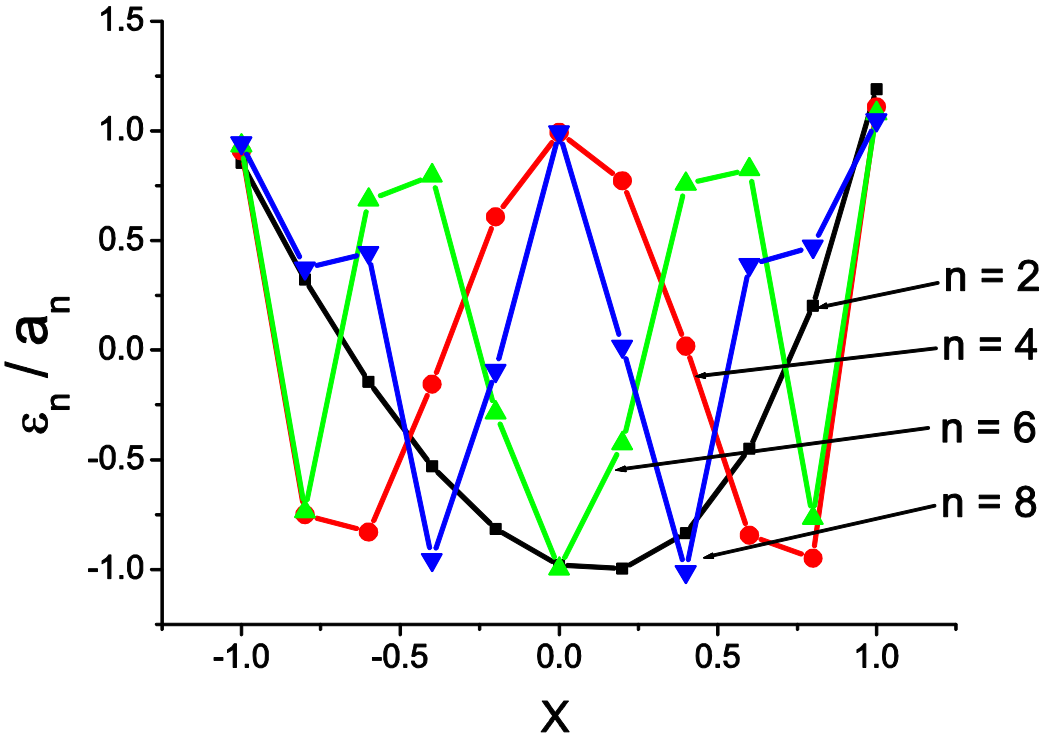
$$T_{n+1} = 2xT_n - T_{n-1}$$

Chebyshev Polynomials



Expand exp(x)

Expansion error is uniform. Truncate the expansion at “n”



Integral Properties

$$I_L(y) = \int_{-1}^{y} \bar{f}(x')dx'$$

$$I_L^{(N)}(y) = \sum_{n=0}^{N} b_n T_n(y),$$

$$\bar{f}^{(N)}(x) = \sum_{n=0}^{N} a_n T_n(y),$$

$$\begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_N \end{pmatrix} = S_L \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{pmatrix}$$

Diff. eq. $\longrightarrow$ Integral eq.

$$\left[\frac{d^2}{dr^2} + k^2 \right] \psi(r) = V(r)\psi(r)$$

$$\psi(r) = f(r) + \int \mathcal{G}(k; r, r')V(r')\psi(r')\, dr'$$

For the Chebyshev Spectral method need:

Four basic Matrices $C,\ C^{-1},\ S_L,\ S_R$

$(N+1)\times(N+1)$

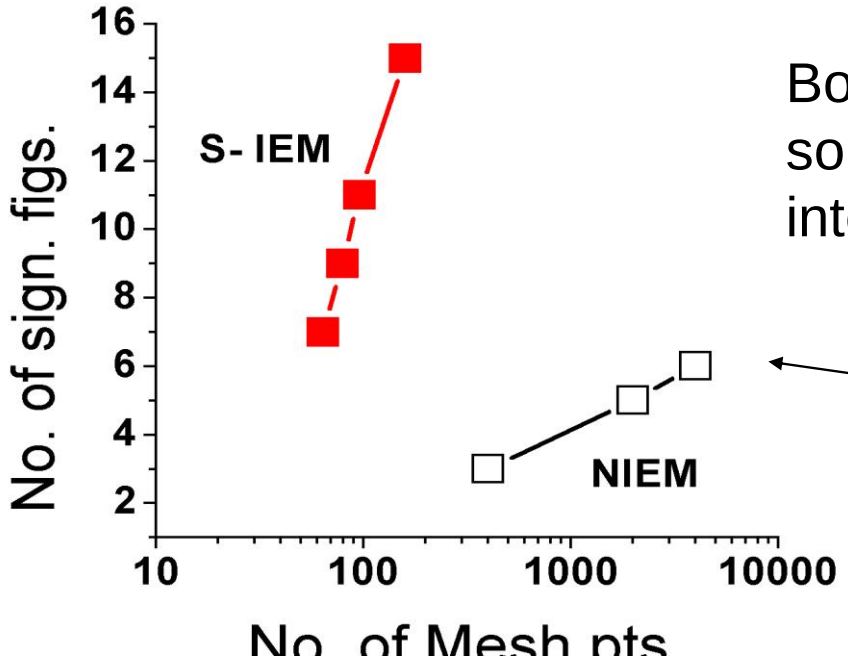
Plus : *Given N, find a list of the zeros of the Cheb.Pol.* T_{N+1}

$$\xi_i = \cos\left[\frac{(2i+1)}{2N+2}\pi\right] \quad (i = 0, 1, 2, \ldots N).$$

8 papers with I. Koltracht from 1996 to 2006

Examples

e-H scattering with exchange; Error in the singlet phase-shift

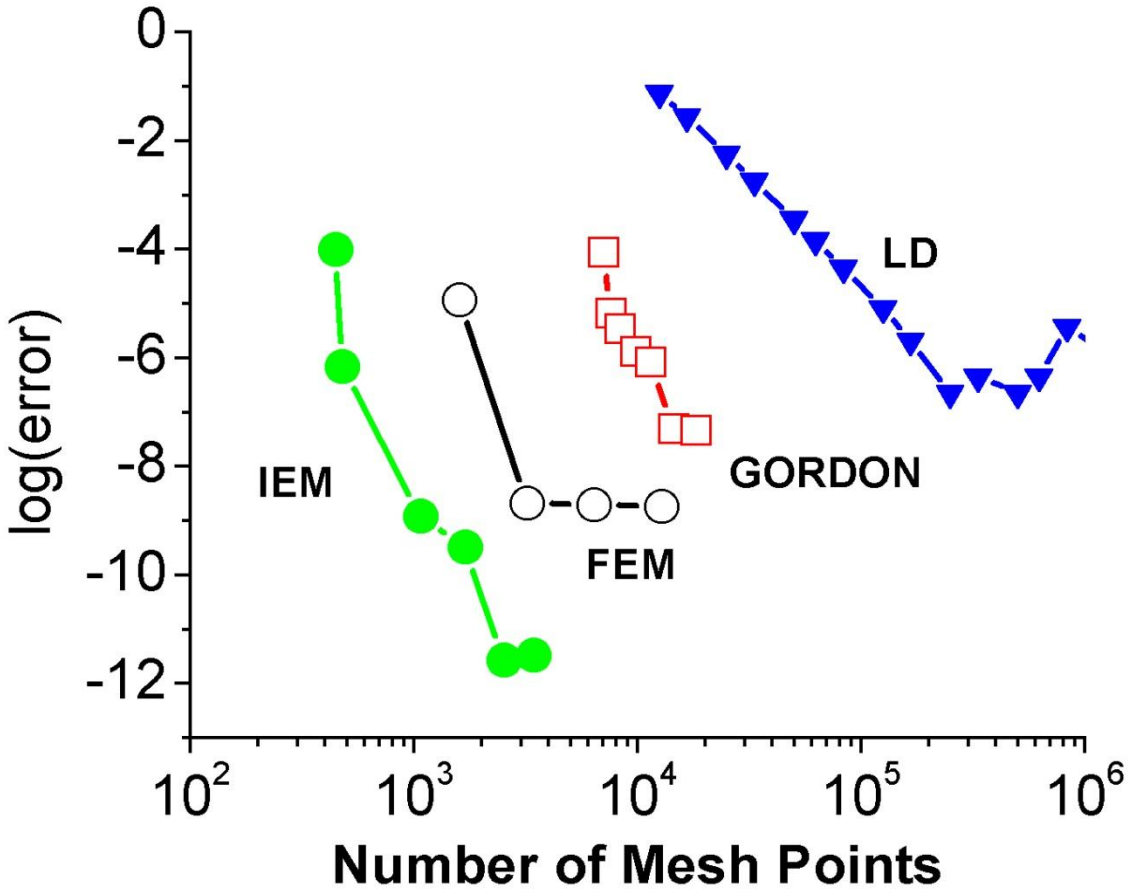


Both methods solve the same integral eqn.

Sams & Kouri
J. Ch. Phys (69)

Kang, Koltracht, Rawitscher, J. Chem. Phys., **118,** 9145 (2003)

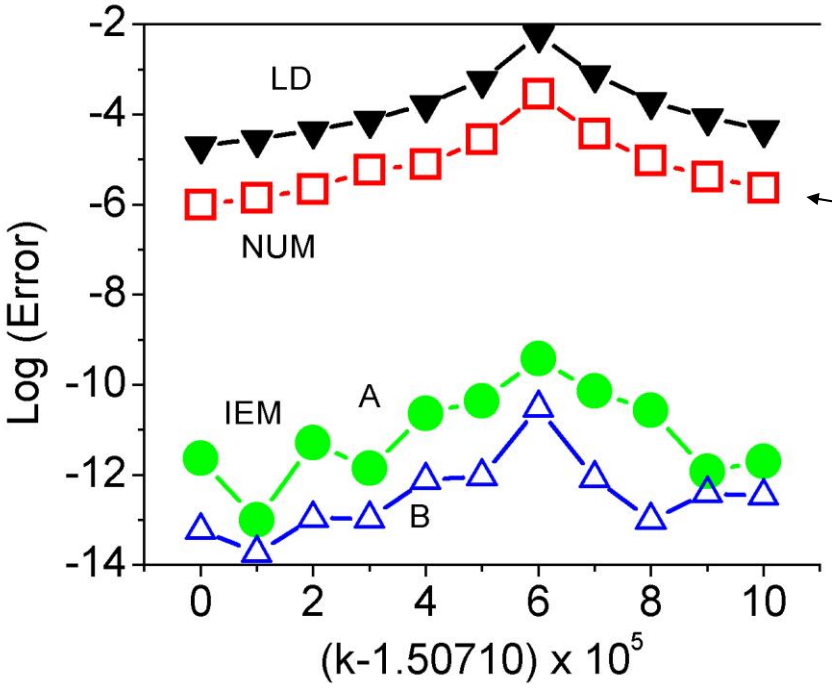
Scattering of two atoms, including an open and a bound Channel



Rawitscher,
Esry, Tiesinga
Burke, Koltracht

J. Chem Phys.
111, 10418 (1999)

Error of the resonant phase shift in a Morse Pot'l



Molscat, Balakrishnan

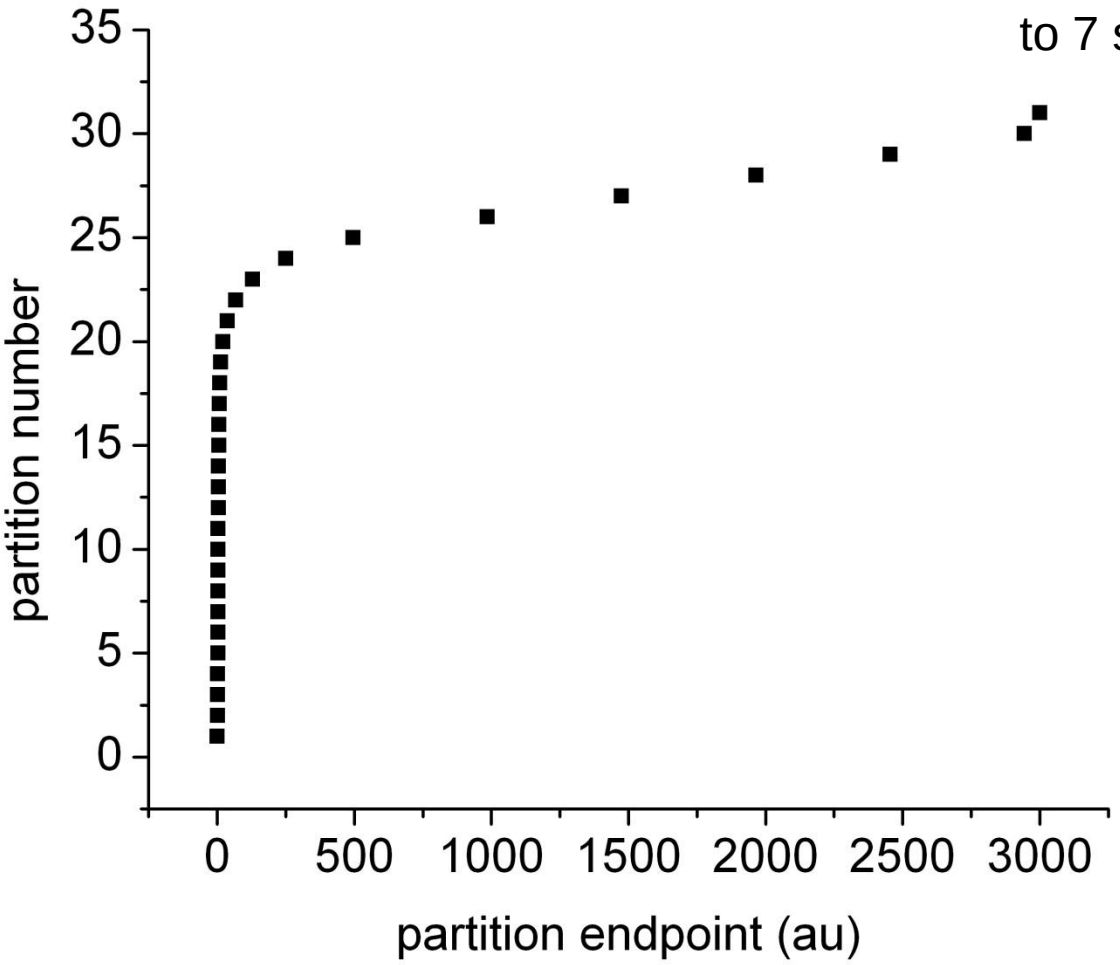
Zerrad

Rawitscher & Koltracht
CiSE **7**, 58 (2005)

Calculation of the He-He binding energy

Rawitscher and Koltracht,
Eur. J. Phys **27**, 1179 (2006)

E = -1.1 x 10^(-7) eV
to 7 significant figures



Phase-Amplitude description of a wave function

The Schroedinger partial wave equation

$$d^2\psi/dr^2 + k^2\psi = V_T\,\psi$$

$$V_T(r) = L(L+1)/r^2 + V(r)$$

Milne's eqs. (1930)

For the amplitude and phase, E > V

$$\psi(r) = y(r)\sin[\phi(r)]$$

$$d^2y/dr^2 + k^2y = V_T\, y + k^2/y^3$$

$$\phi(r) = \phi(r_0) + k\int_{r_0}^{r} [y(r')]^{-2}\, dr'$$

Solution of the amplitude Eq.

Spectral expansion

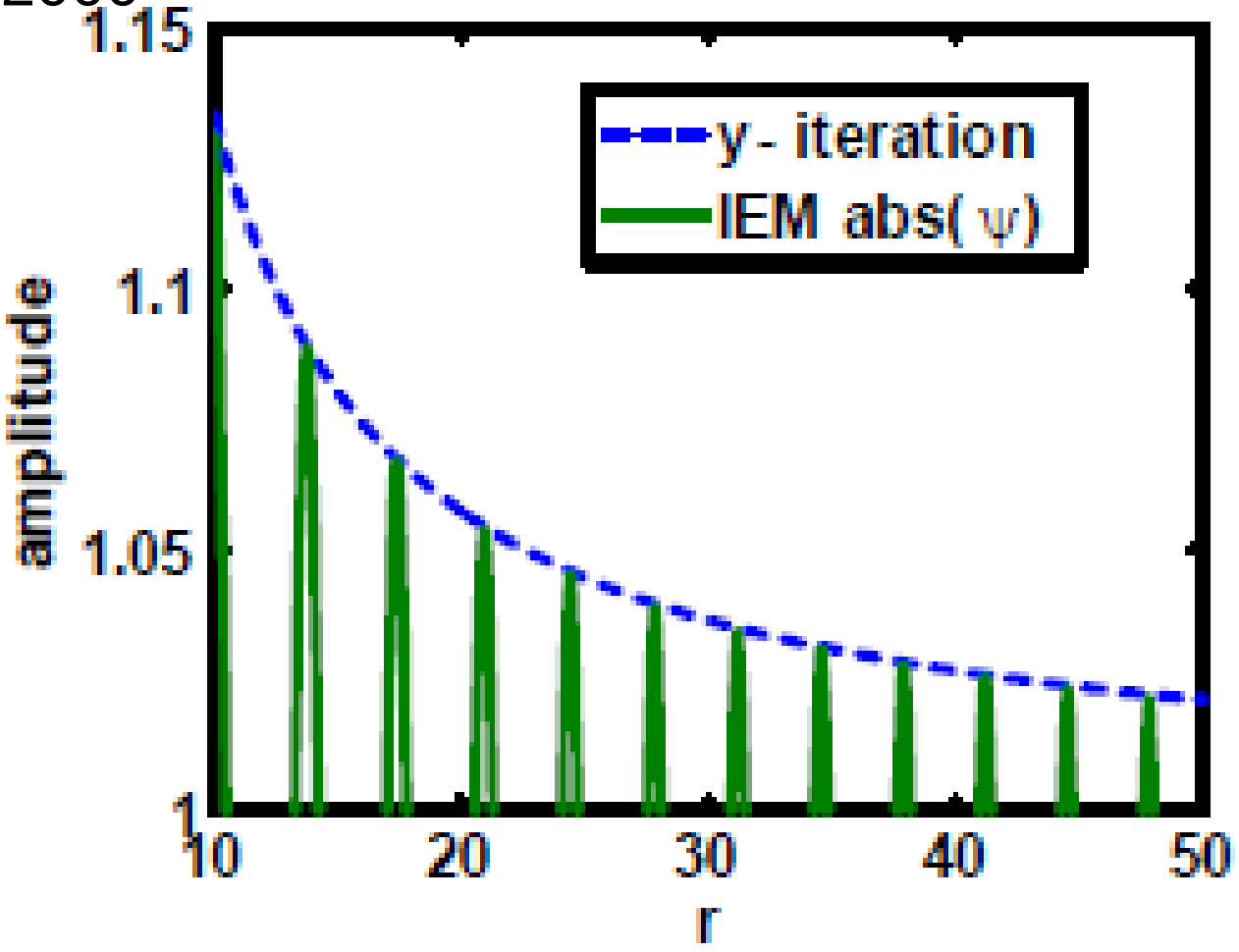
GR: Comp. Phys. Comm. **191** (2015) 33; **203** (2016) 138

$$y(x) = \sum_{n=0}^{N} a_n \, T_n(x)$$

$$N+1 \; Chebyshev Polynomials$$

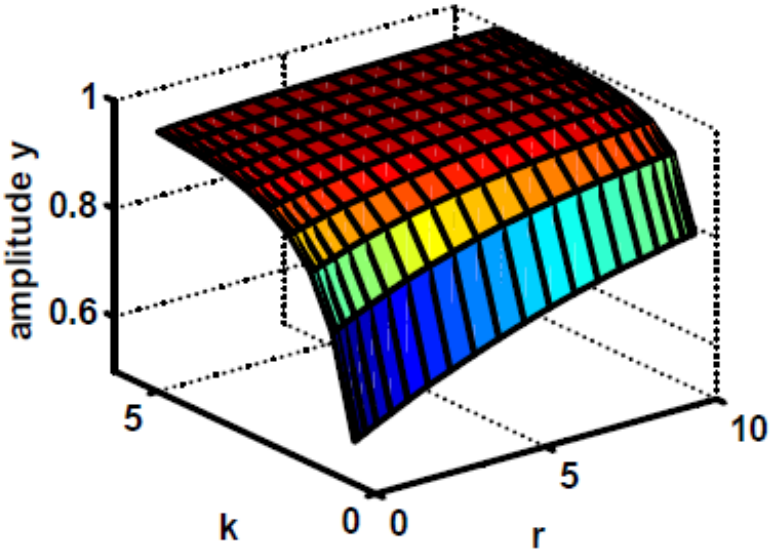
$$N+1 \; non-equidistant \;\; support \; points$$

Amplitude agrees with a S-IEM wave function for a **repulsive** rounded Coulomb Pot'l, eta = + 2, 10 <r <2000

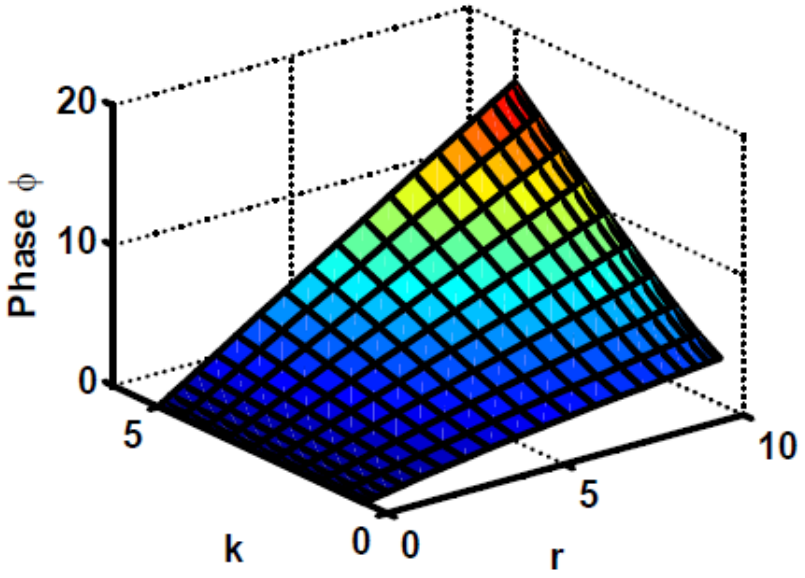


Atractive Coulomb Potential

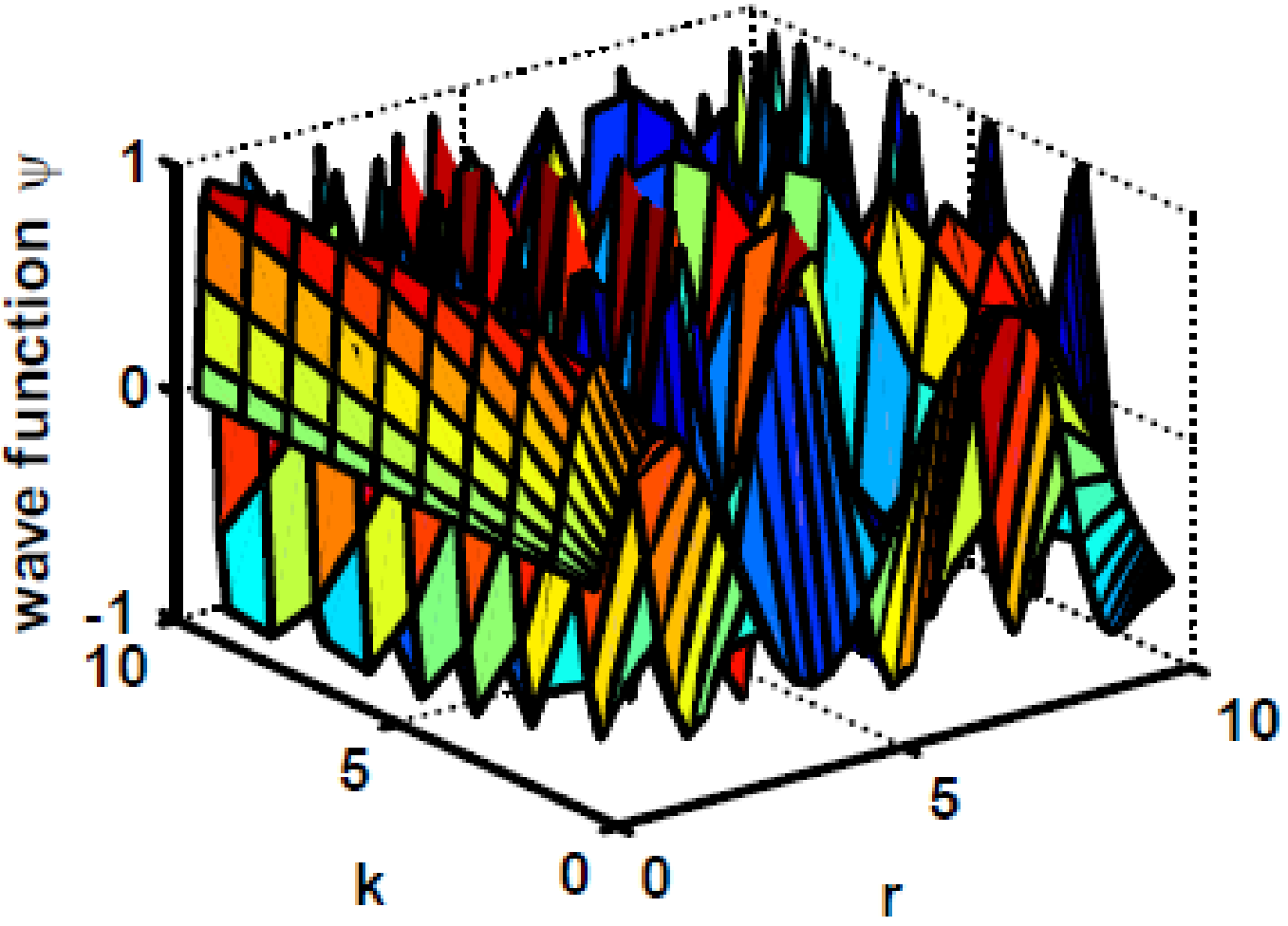
Amplitude y

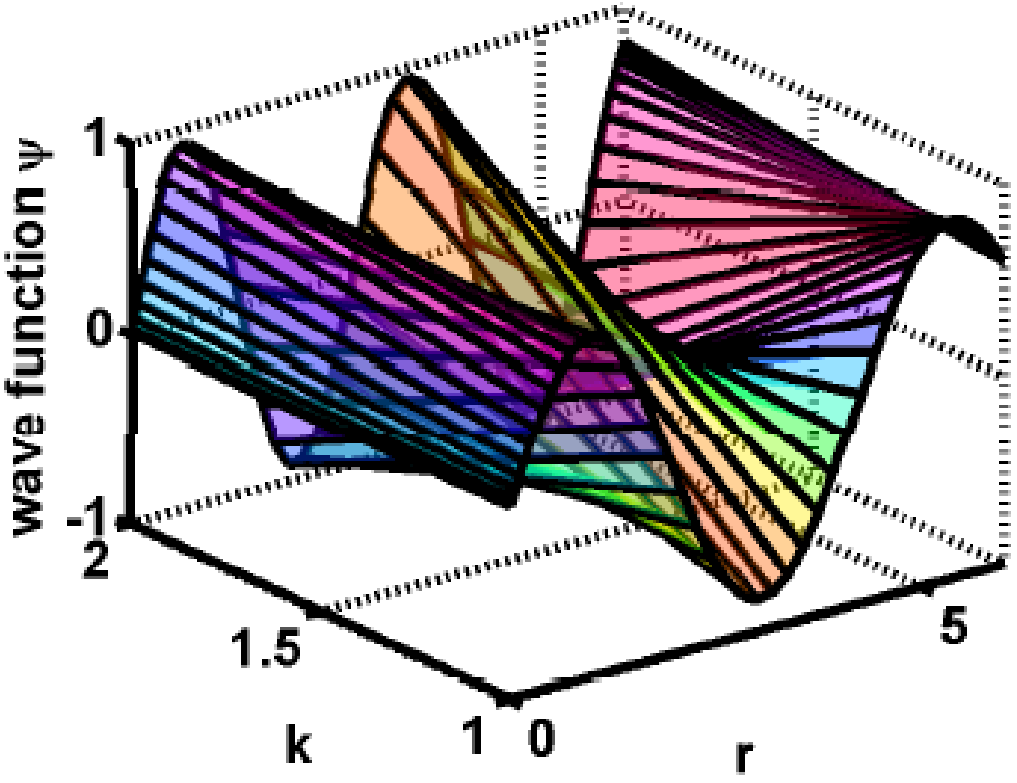


Phase



Wave function = y sin(phi)




wave function ψ
1
0
-1
2
1.5
k
1
0
r
5

Summary and conclusions

The spectral-Chebyshev integral eq. method in coord. space

a) only requires the value of the input potentials and Green's functions at the N+1 support points, and not integrals thereof.

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Summary and conclusions

The spectral-Chebyshev integral eq. method in coord. space

a) only requires the value of the input potentials and Green's functions at the N+1 support points, and not integrals thereof.

b) Does not require a matrix representation of the Kinetic Energy operator, since it uses analytical Green's fcts. (no pole singularities)

c) Converges rapidly to high accuracy, as N increases, and permits one to specify the expected accuracy ahead of time.

d) Spectral method explained in Am. J. Phys., 79 (2011) 417.

BOOK

: G.Rawitscher, V.Filho, T.Pexioto (2016).

A Practical Guide to Spectral Computational Methods, Springer, ISBN:978-3-319-42702-7.