Phase-Amplitude Representation of a wave function, revisited

G. Rawitscher

University of Connecticut

EFB-23, Aug . 8, 2016

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

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

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

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

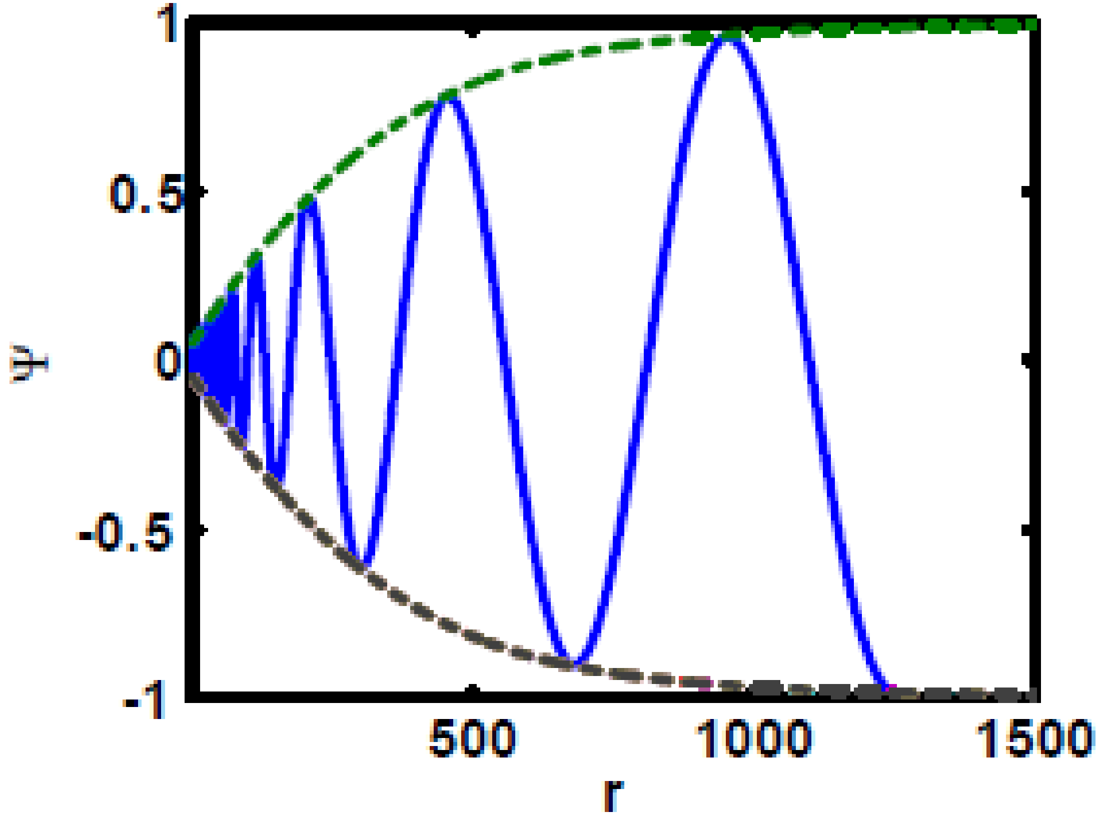
Spectral expansion

$$y(x) = \sum_{n=1}^{N+1} a_n \, T_{n-1}(x) \qquad -1 \leq x \leq 1$$

$N+1$ Chebyshev Polynomials

$N+1$ non-equidistant support points

Oscillatory case, E > V



Phase for a Coulomb potential

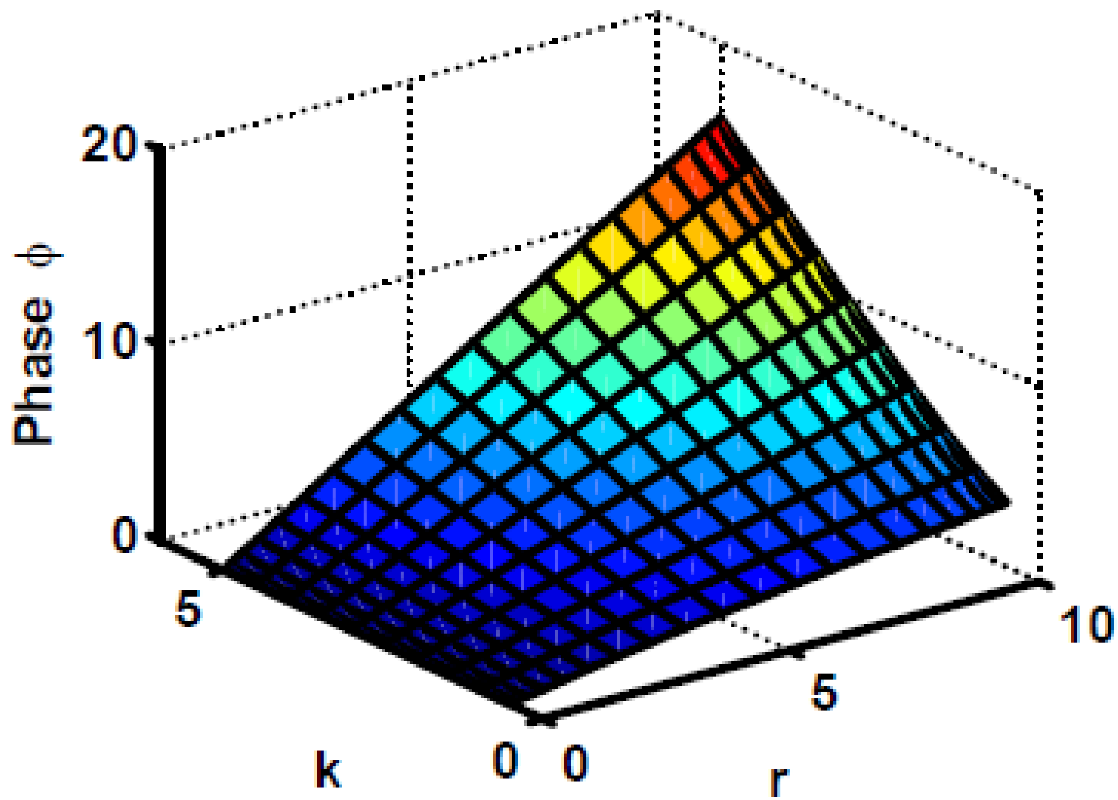
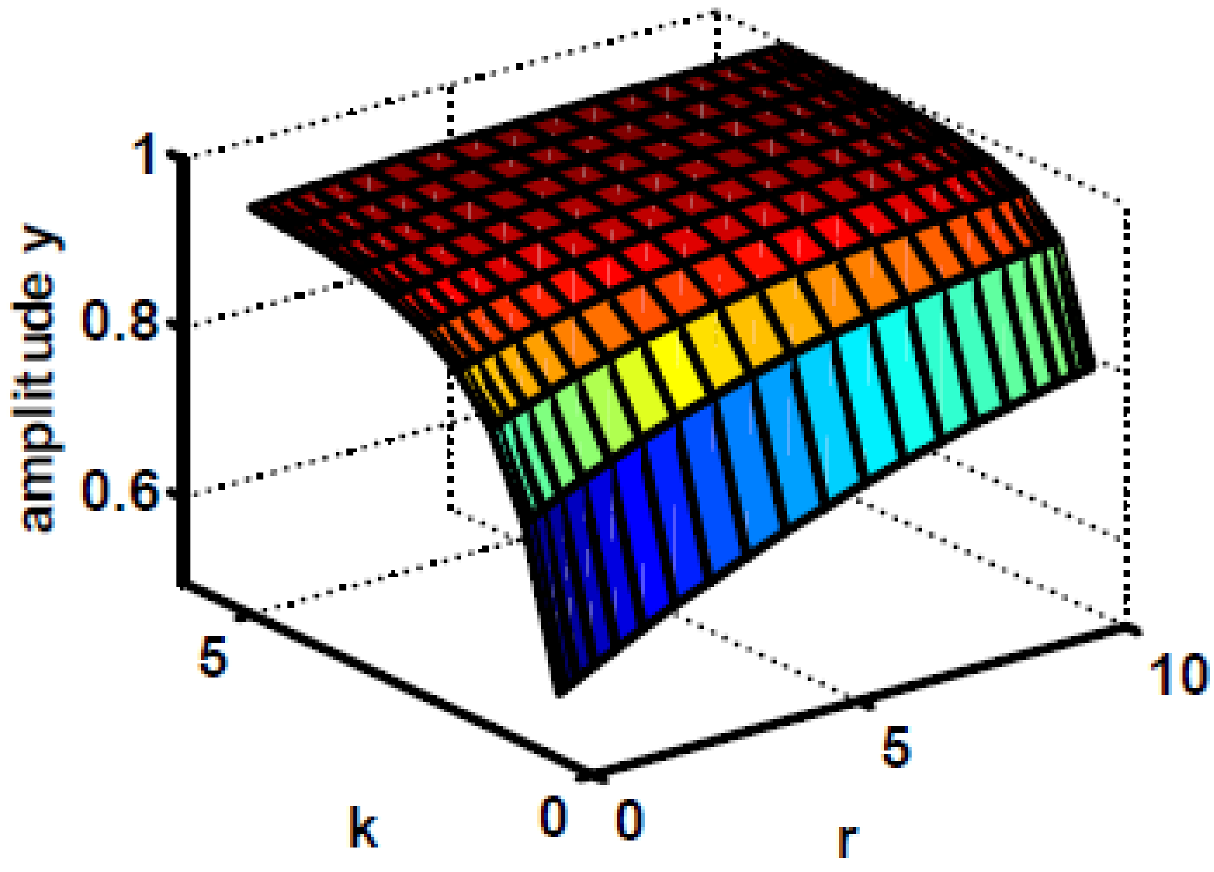
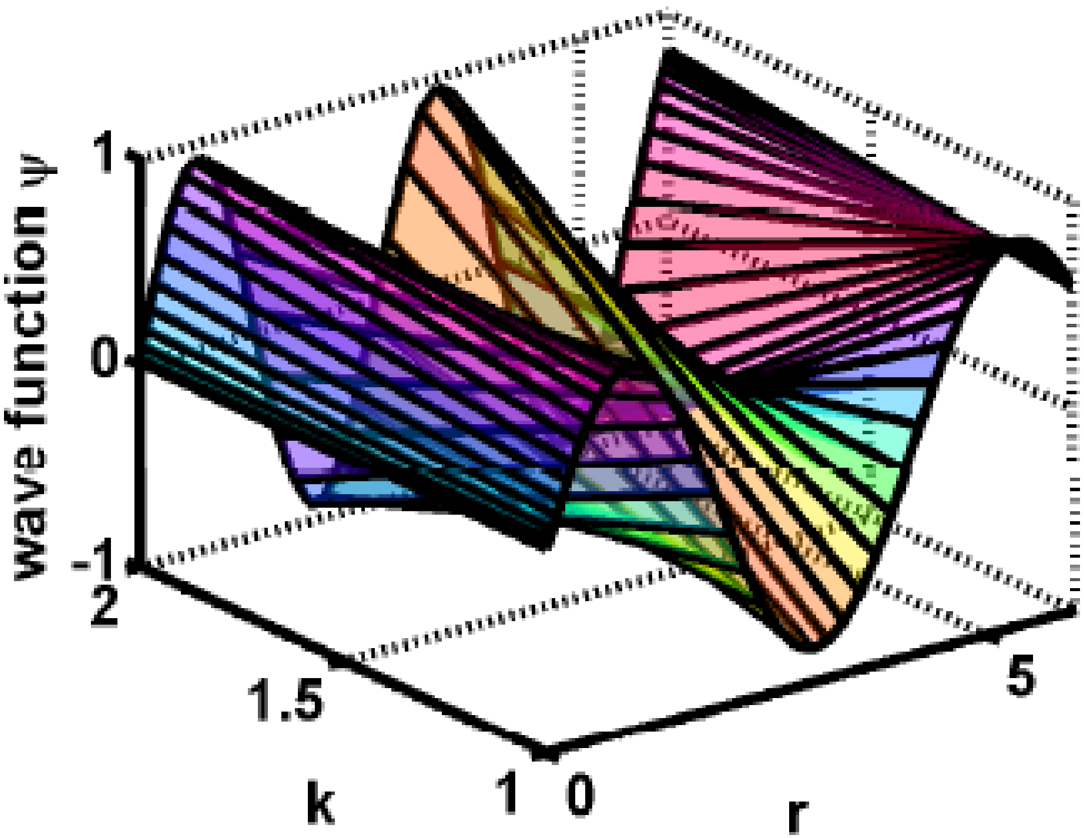


Figure 2: Fig

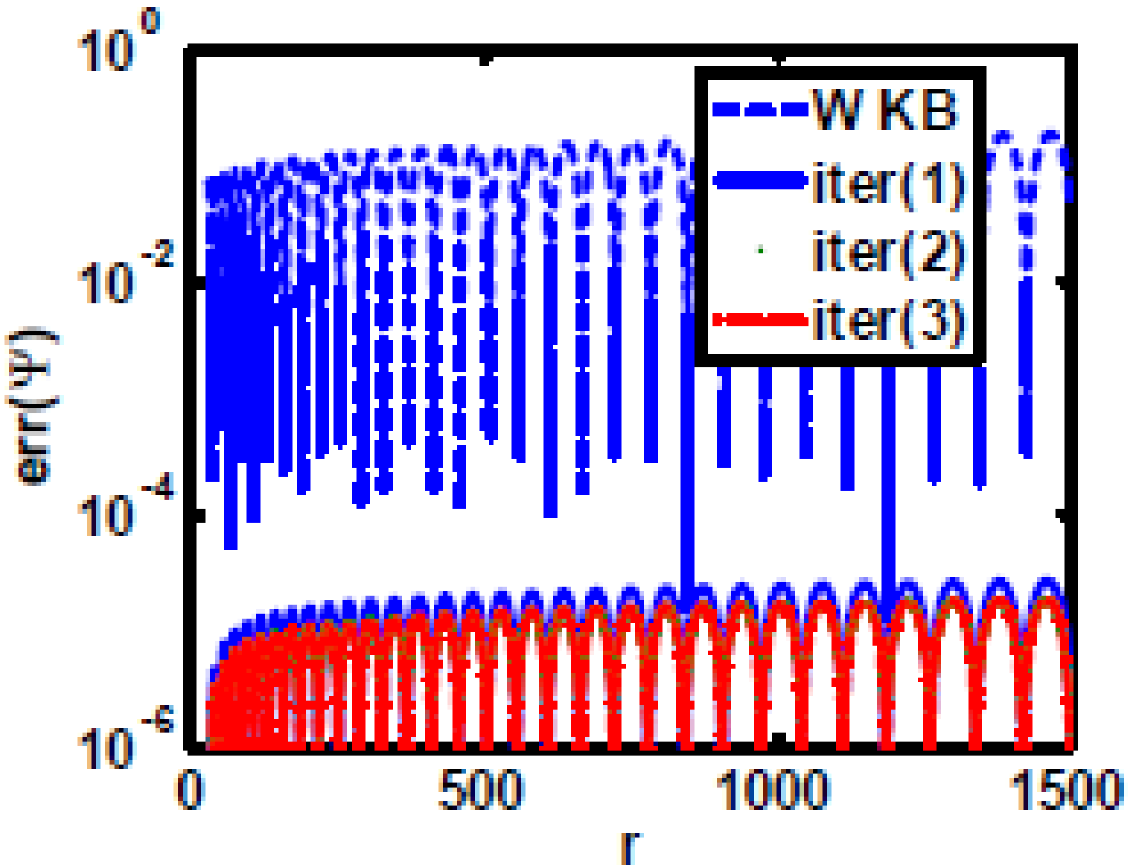
Amplitude for a Coulomb Potential



The wave function

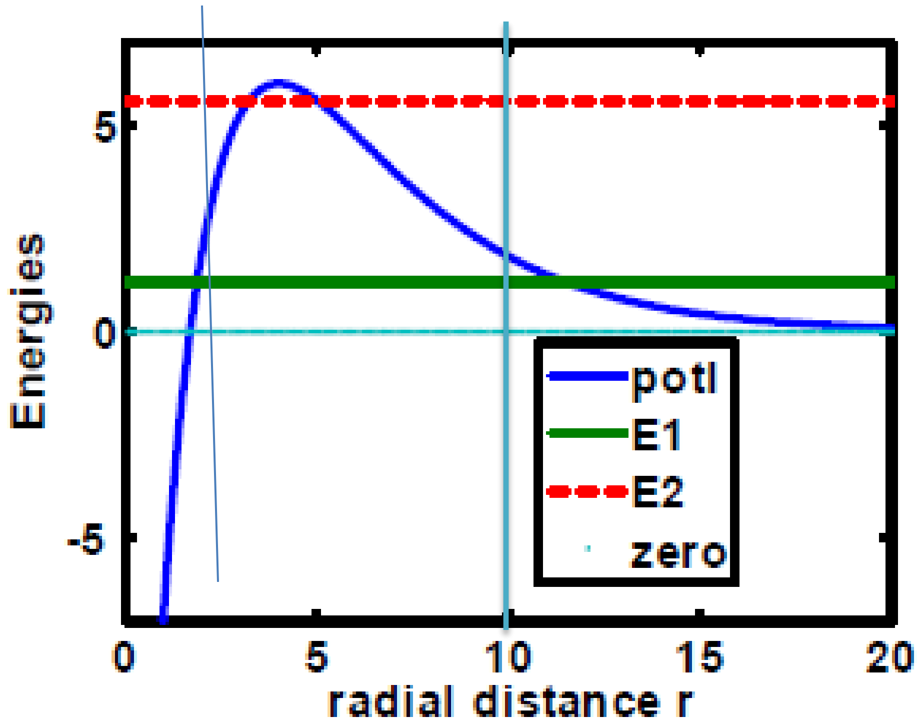


Accuracy for an **attractive** rounded Coulomb pot'l, eta = -1, N = 51, 30 < r < 1500



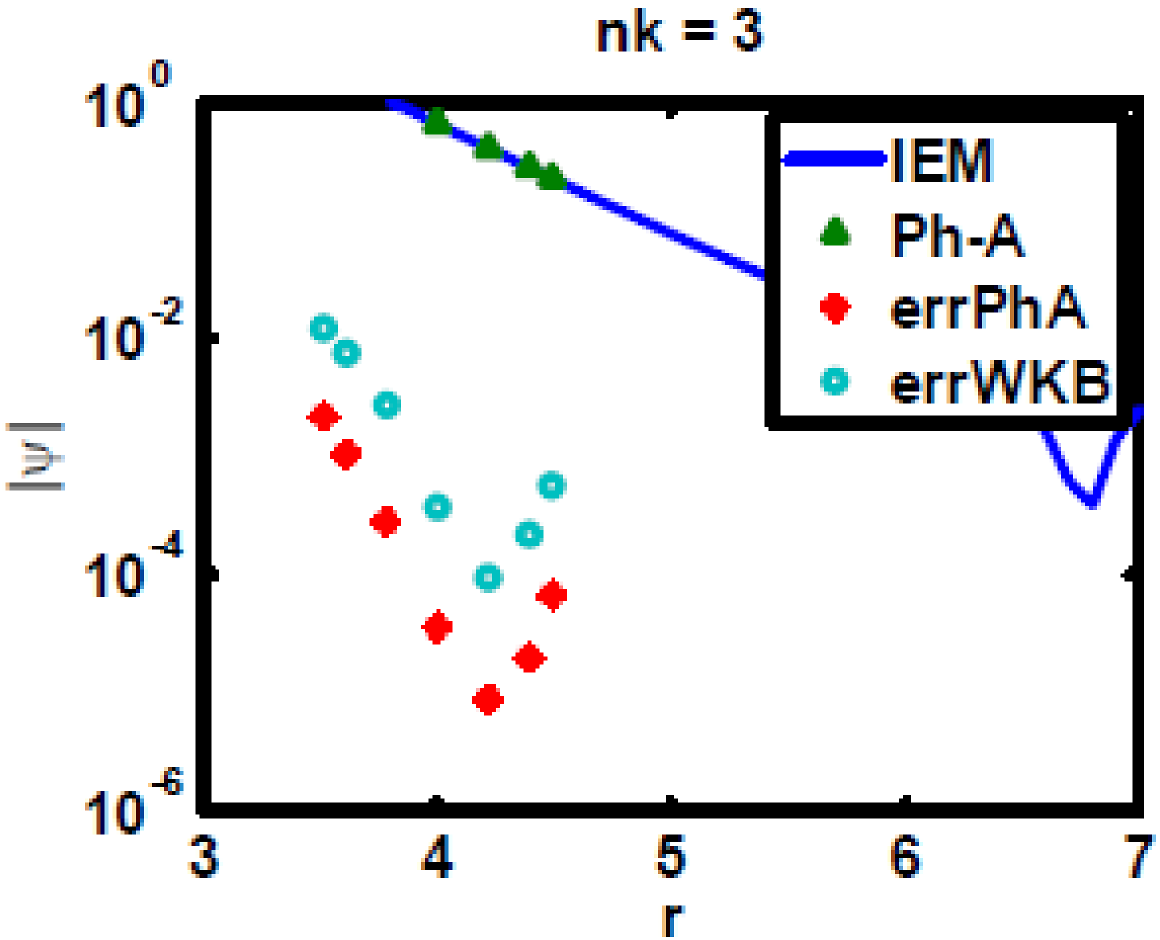
E < V ; Barrier Region

$$\psi^{(\pm)}(r) = \tilde{y}(r)\exp(\ \pm\ \Phi(r))$$



Resonance #1, k = 1.0853

Error of the Ph-A wave function



Ph-A linear Equation.

Ph-A linear Eq.

$$u(r) = y^2(r)$$ Define u

$$u''' + 4(k^2 - V)u' - 2V'u = 0.$$

$$v(r) = u' = du/dr$$ Define v

$$d^2v/dr^2 + 4(k^2 - V)v = 2(dV/dr)\left(\int_0^r v(r')dr'\right)$$

Second order linear Eq.

$$d^2v/dr^2 + 4(k^2 - V)v = 2(dV/dr)\left(\int_0^r v(r')dr'\right)$$

k^2 = energy
V = scattering potential
v = function to be solved
y^2 = square of amplitude = integral of v

Solve by expanding into Laguerre polynomials

The basis functions in terms of Laguerre polynomials

$$\Lambda_n(r) = \sqrt{\kappa}e^{-(\kappa r/2)}\ L_n(\kappa r),\ \ n = 1, 2, \ldots,\ \ 0 \leq r \leq \infty$$

They are orthogonal

$$\int_0^\infty \Lambda_n(r)\Lambda_m(r) = \int_0^\infty e^{-x}L(x)L(x)dx = \delta_{n,m}$$

Plot of some basis Functions

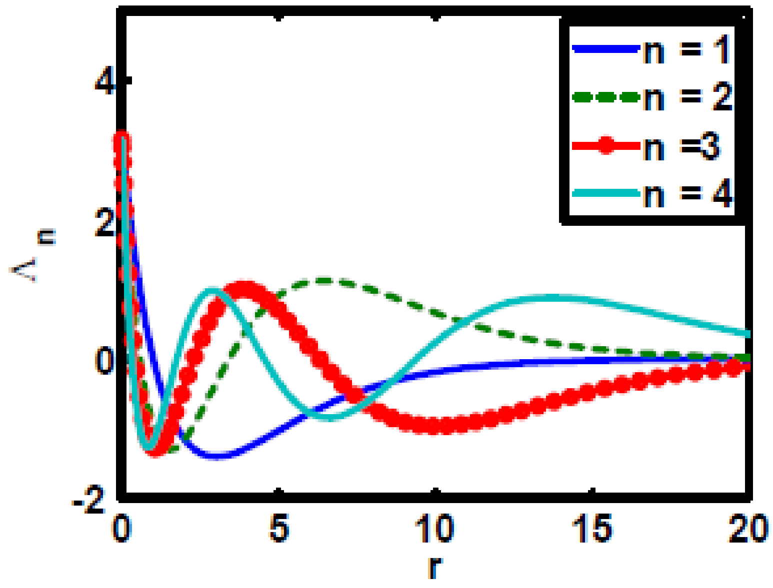


FIG. 1. The basis functions Λ_n , $n = 1, 2, 3, 4$, as defined by Eq. (7), with $\kappa = 10$.

Galerkin method

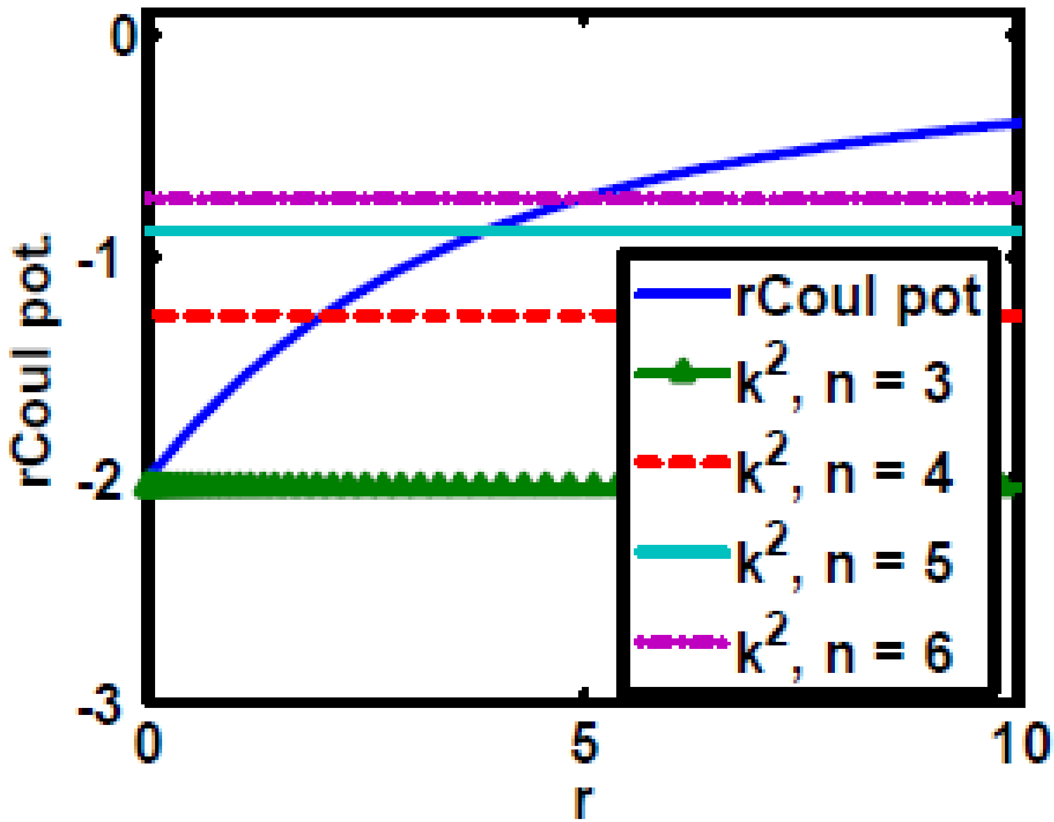
$$\mathcal{O} = d^2/dr^2 - 4V - 2(dV/dr)\left(\int_0^r dr'\right)$$ Operator

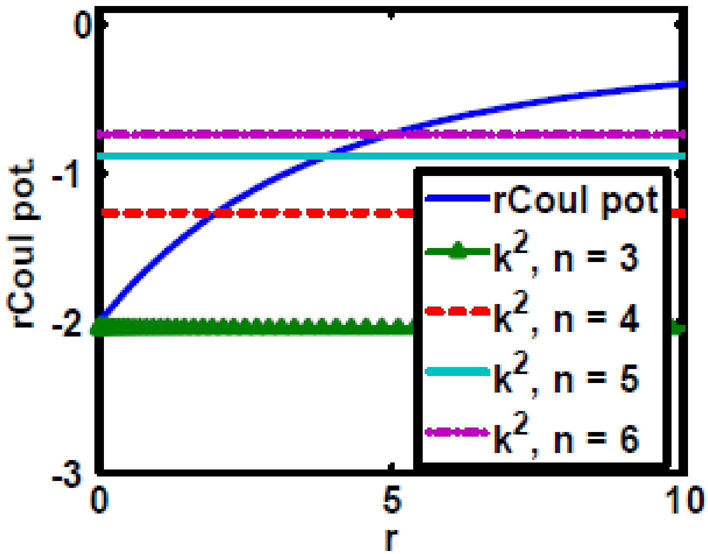
$$\sum_{n'=0}^{\Lambda_N} c_{n'}\langle \Lambda_n \mathcal{O} \Lambda_{n'} \rangle = -4k^2 \left(\sum_{n'=0}^{\Lambda_N} c_{n'} \langle \Lambda_n \Lambda_{n'} \rangle\right.$$

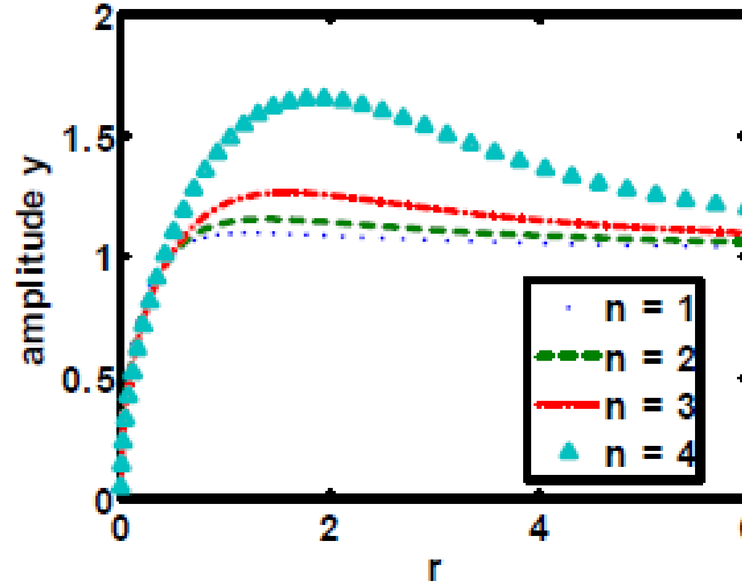
Matrix eigenvalue equation

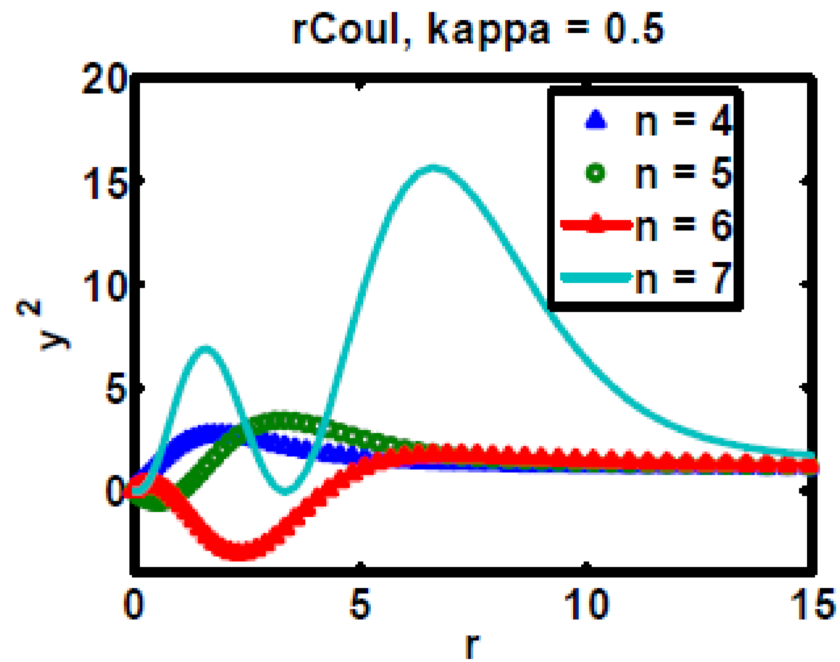
Result for a “rounded” Coulomb potential

n	k^2
1	-4.505
2	-3.030
3	-2.034
4	-1.262
5	-0.8842
6	-0.7393
7	-0.4456




rCoul pot
k^2, n = 3
k^2, n = 4
k^2, n = 5
k^2, n = 6
rCoul pot
r
0
-1
-2
-3
0
5
10


amplitude y
r
n = 1
n = 2
n = 3
n = 4
0
0.5
1
1.5
2
0
2
4
6


rCoul, kappa = 0.5
y^2
r
n = 4
n = 5
n = 6
n = 7
0
5
10
15
20
0
5
10
15

Some of the y^2 functions become negative as shown for the case $n=6$.
This because a turning point is included but a physical interpretation of the meaning of $y(r)$ is still a work in progress

Summary and Conclusion

1. The iterative method of Seaton and Peach for solving Milne's phase amplitude non linear equation converges very well, and has been overlooked in the recent literature.

2. The novelty here is to use a spectral Chebyshev expansion method for calculation of the iterations, rather than using the usual finite difference methods for solving the non-linear y equation

3. For the case $E > V$ get good accurate results 1:10 ^ -6
   For the case $E < V$ the iterations do **NOT** converge near turning pts..

4. A better linear method is under exploration

BOOK : G.Rawitscher, V.Filho, T.Pexioto (2016).
A Practical Guide to Spectral Computational Methods, Springer, ISBN:978-3-319-42702-7.