Phase-Amplitude Representation of a wave function, revisited

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Phys. 2016 Conference, New Orleans

June 27-29, 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

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

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

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

Solution of the amplitude Eq. **Spectral expansion**

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

$$N+1 \; Chebyshev Polynomials$$

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

Iterations Seaton & Peach, 1962

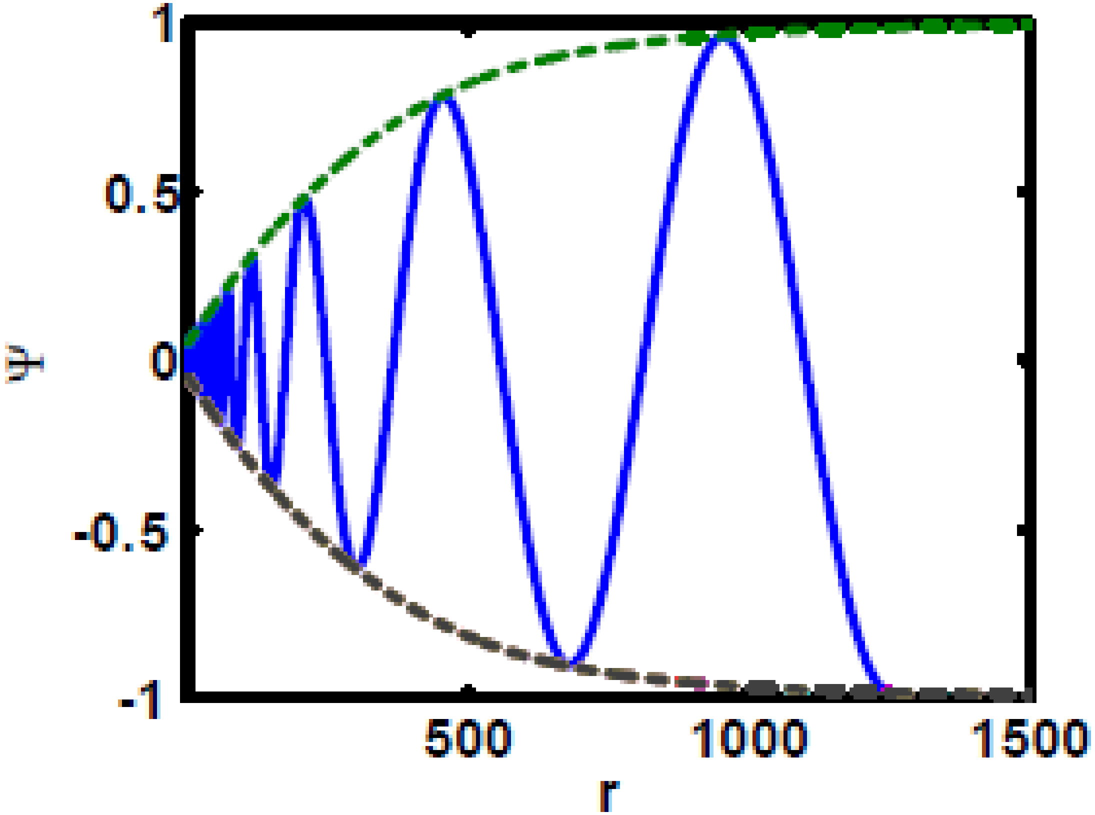
$$\frac{k}{y_{n+1}^2} = [w + \frac{1}{y_n}\frac{d^2 y_n}{dr^2}]^{1/2}, \quad n = 0, 1, 2,$$

$$w(r) = k^2 - V(r),$$

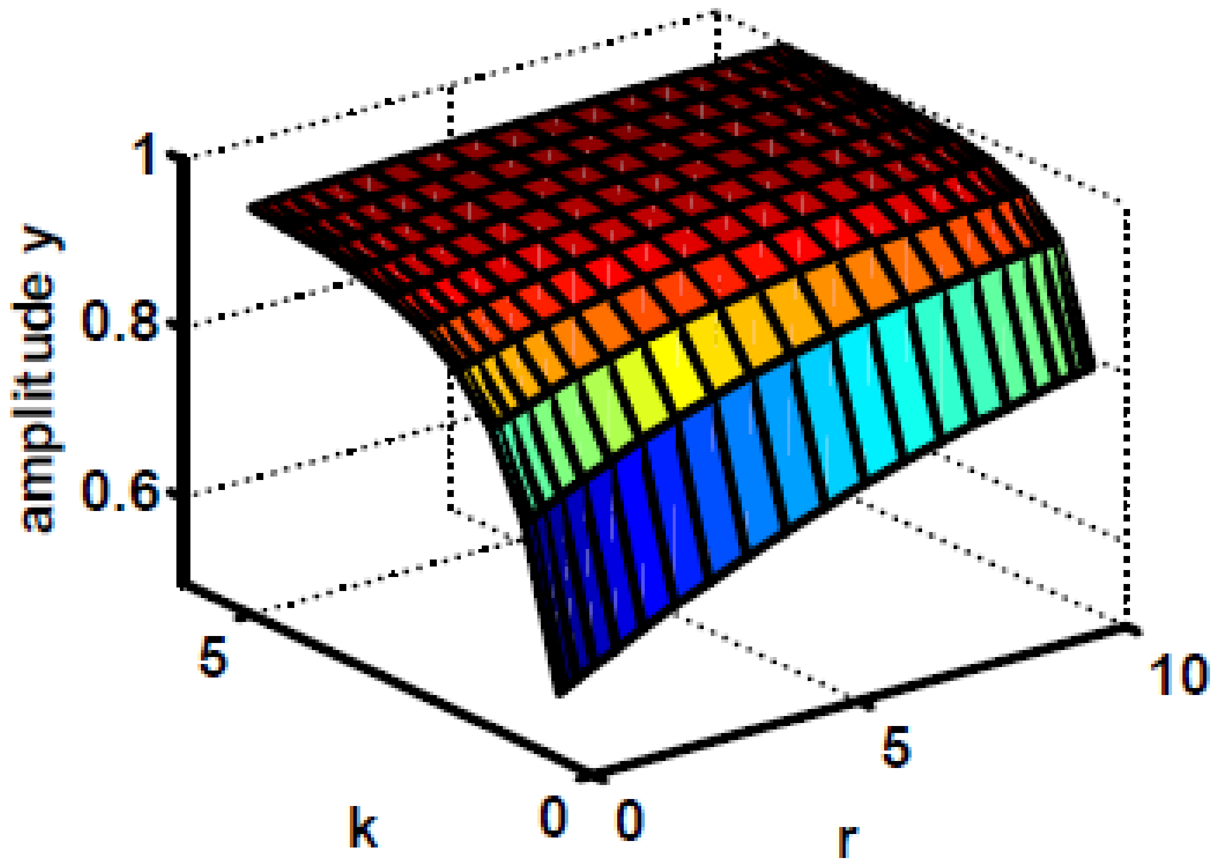
$$\frac{k}{y_0^2} = w^{1/2}$$

WKB

Oscillatory case, E > V



Amplitude for a Coulomb Potential



Phase for a Coulomb potential

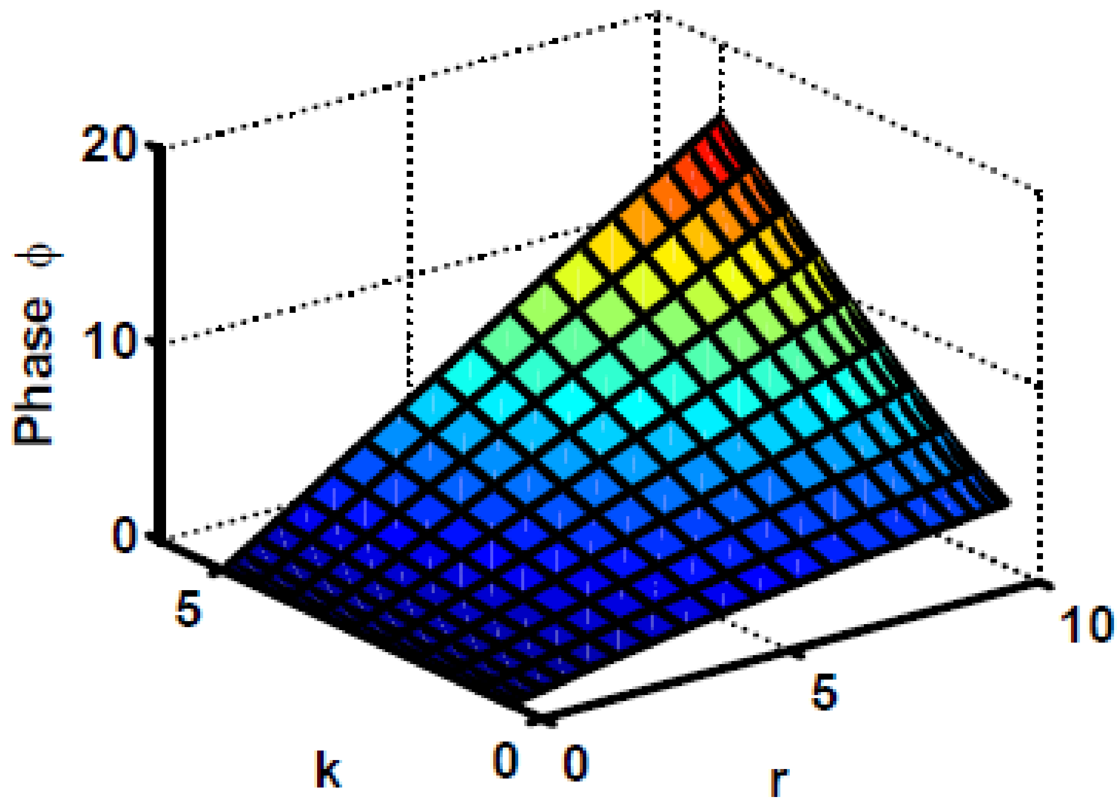
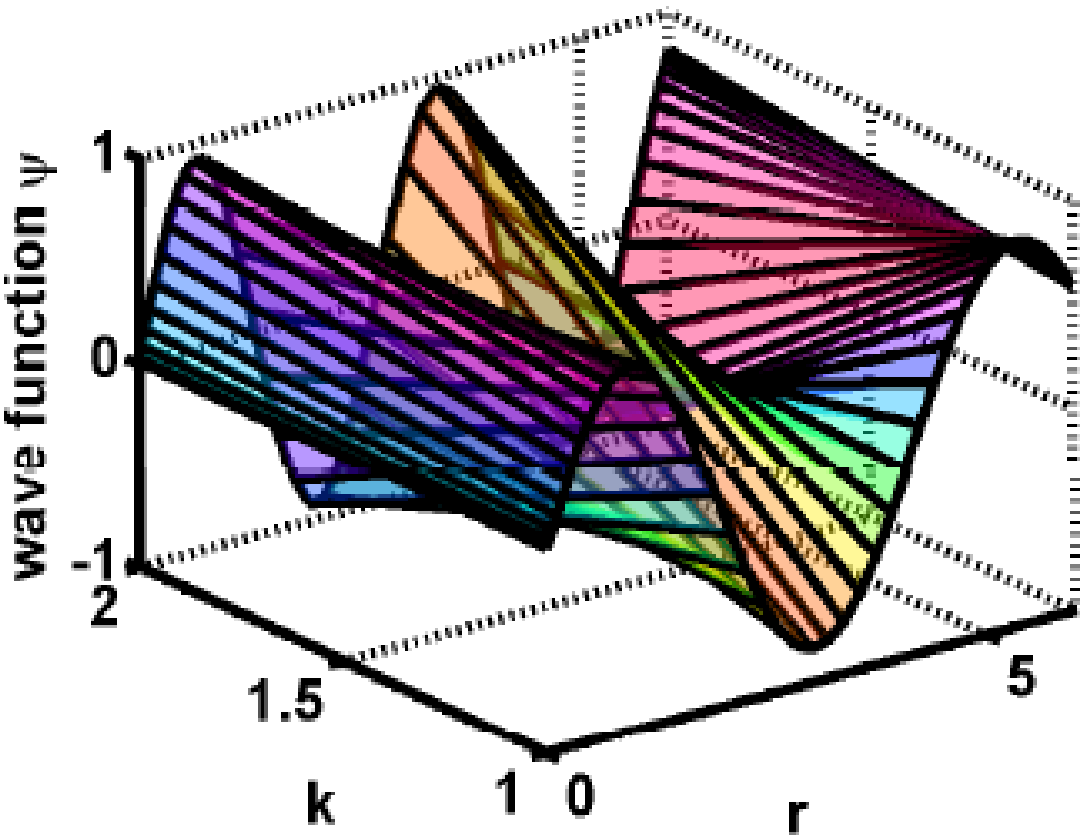


Figure 3: Fig

The wave function



The amplitude agrees well with a S-IEM wave –function calculation

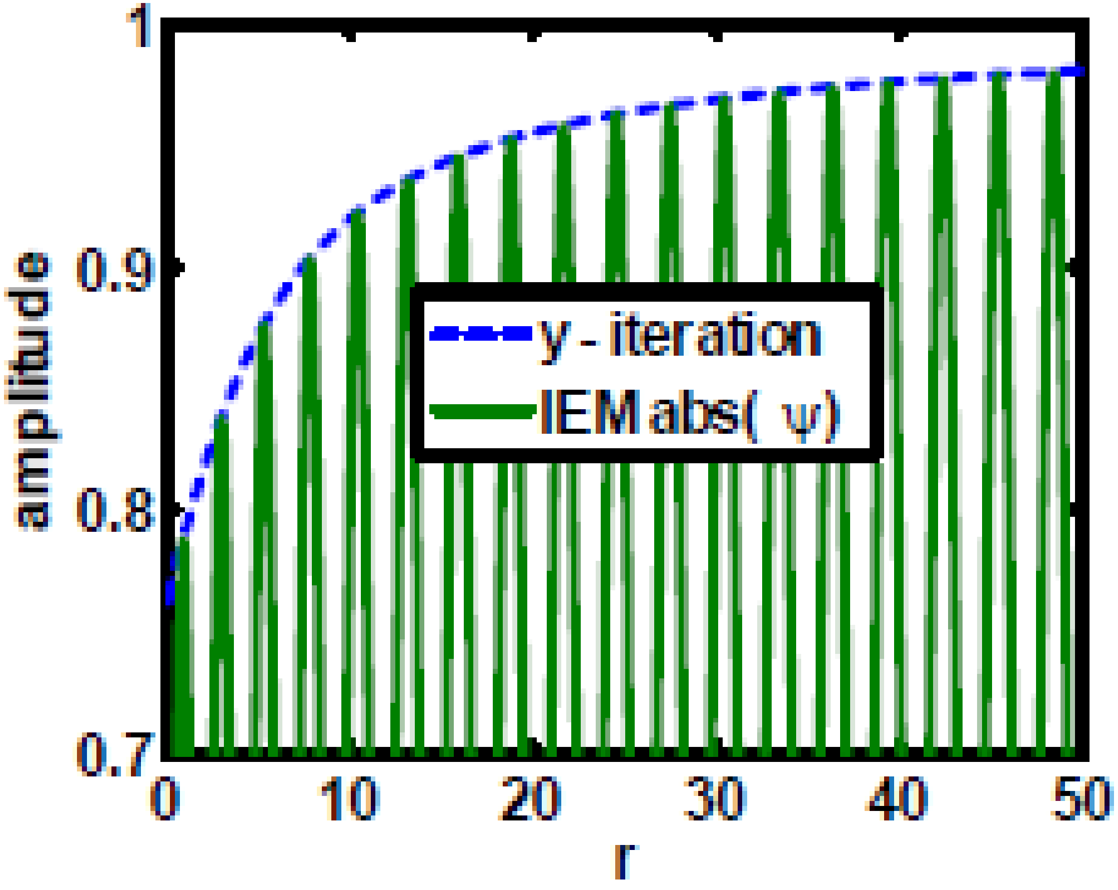


Figure 6: Wave function and amplitude for an **attractive** rounded Coulomb potential, eta = - 2, k = 1; zbar = - 4: The result labeled "y-iteration" is obtained with the MATLAB code "anal_norm.yiter_time.m", located in the Phase-A matlab directory. The calculation is started at r=0, and goes out to r = 2000. It has **101 Chebyshev support points**, and takes aprox 1 sec, not including the interpolation to a uniform mesh. The IEM calc is done with IEM_k_exp, started at r= 0, going through the barrier region, ending up at **r = 2000.**The amplitude y is calculated either from the iterative method described in Ref 1, and agrees with the iterative solution of a new linear equation, described below. The iteration is started with the WKB approximation.

[1] : G. Rawitscher, Comp. Phys. Commun 191 (2015) 33

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

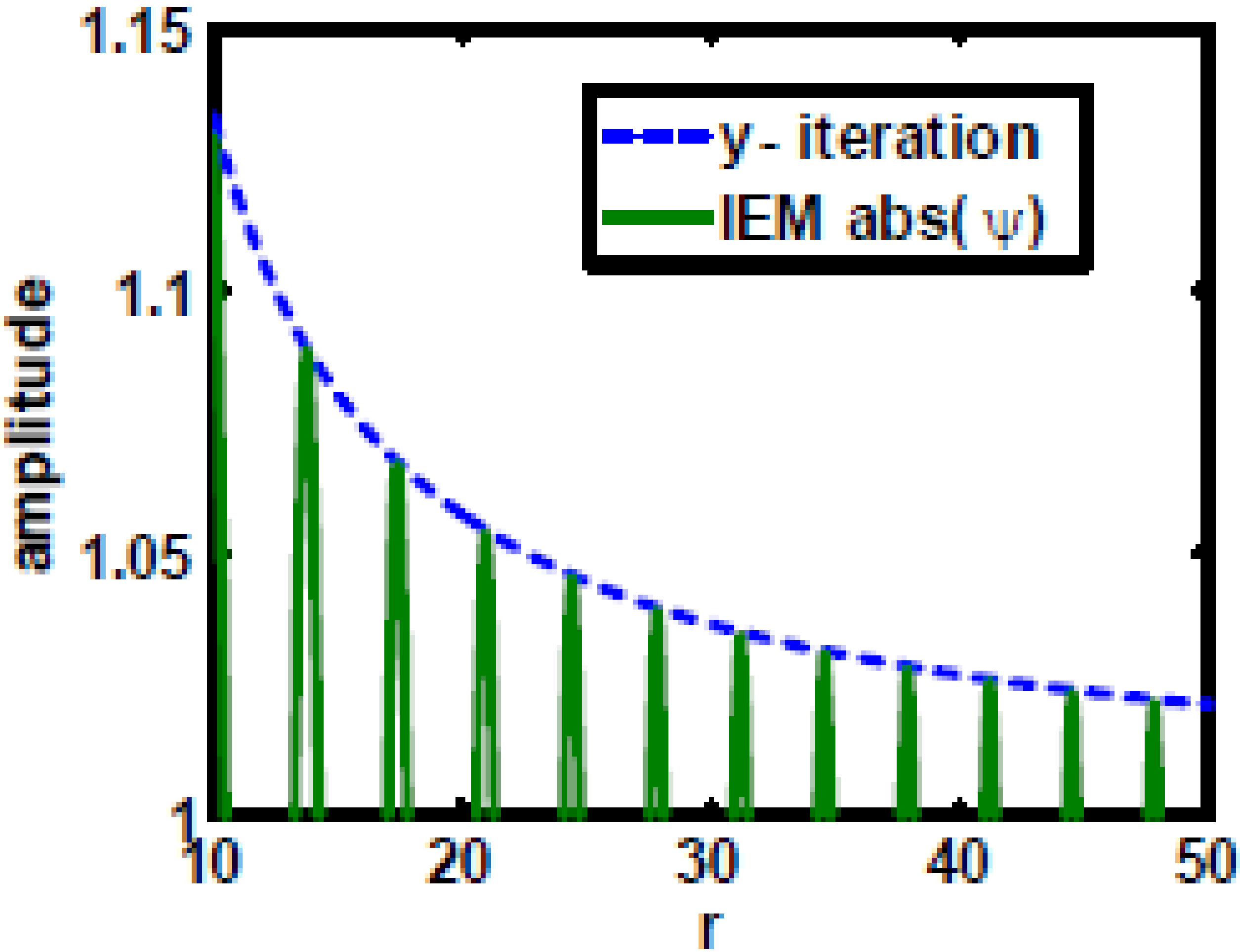
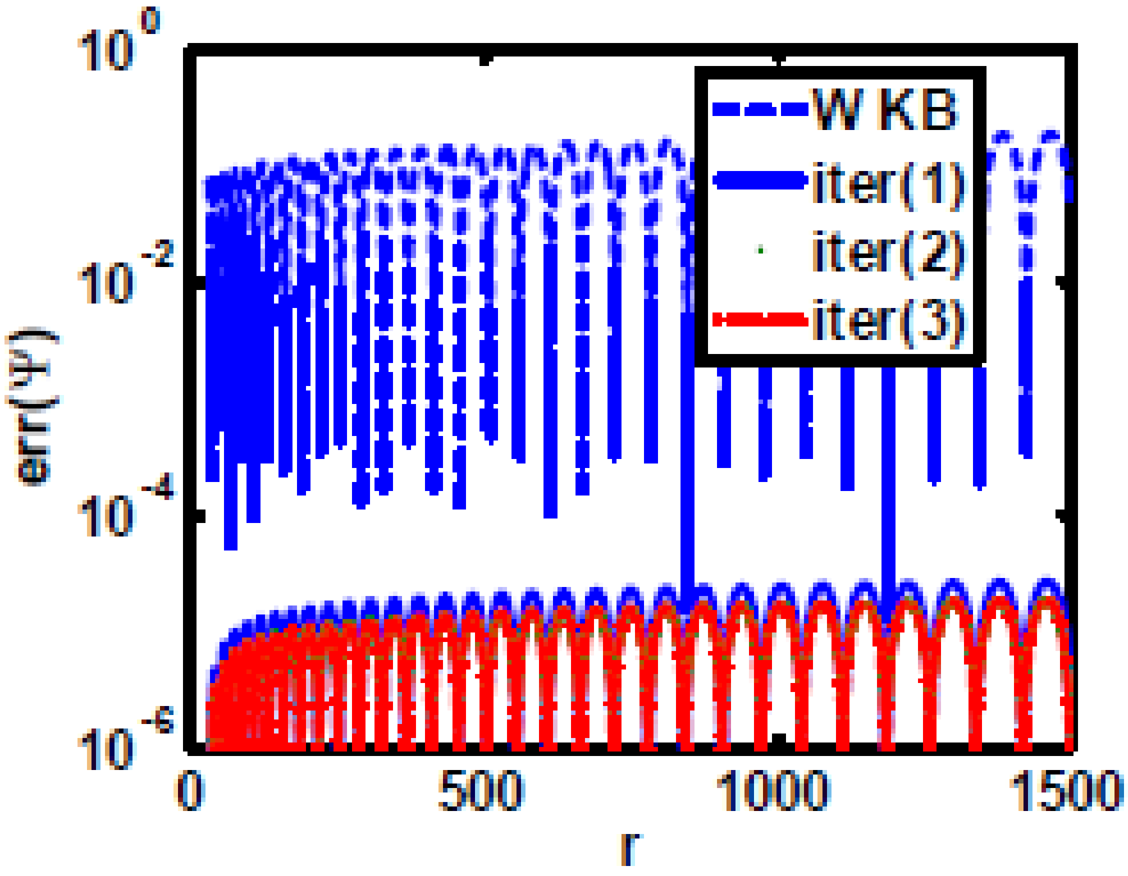


Figure 8: The accuracy of the Ph-A wave function for the rounded Coulomb potential, with rounding parameter $t = 2$ and for $\eta = -1$. The radial interval is $[30, 1500]$, the number of Chebyshev polynomials used in this interval is 51.

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



Forbidden Classical Region

E < V

$$\psi(r) = A\psi^{(+)} + B\,\psi^{(-)}(r)$$

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

Iterations, V > E

G.R., Comp. Phys. Comm **203** (2016) 138

Seaton & Peach iterations

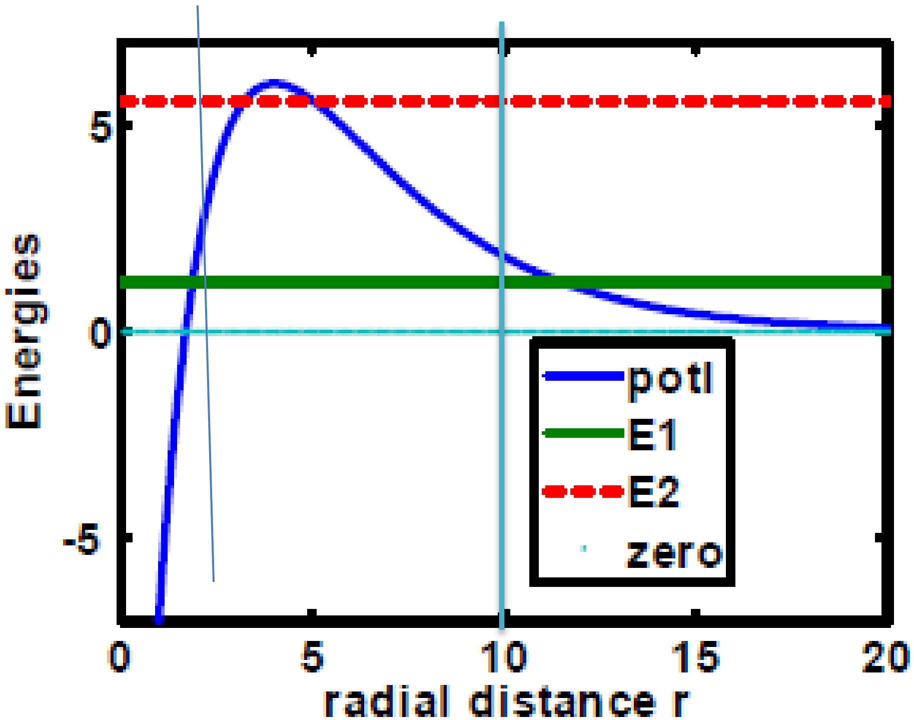
$$\tilde{w} = V - k^2 > 0$$

$$\frac{k}{\tilde{y}^2_{n+1}} = (\tilde{D}_n + \tilde{w})^{1/2}, \quad n = 0, 1, 2, \ldots$$

$$\tilde{D}_n = -\frac{d^2\tilde{y}_n/dr^2}{\tilde{y}_n} \qquad D_0 = 0$$

$$\Phi(r) = \int_a^r \frac{k}{\tilde{y}^2(r')} dr'$$

E < V ; Barrier Region



Resonance #1
Wave functions in the Barrier Region

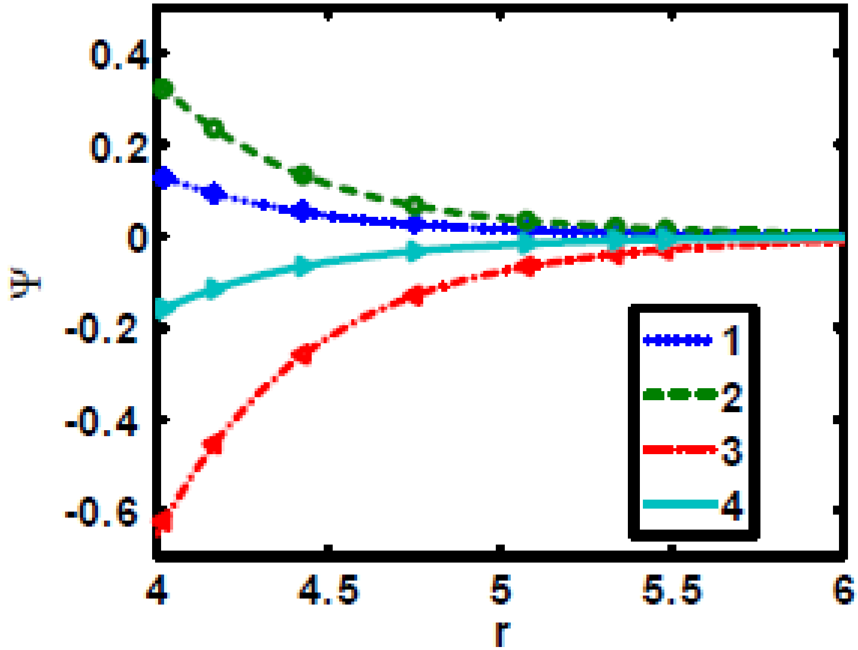
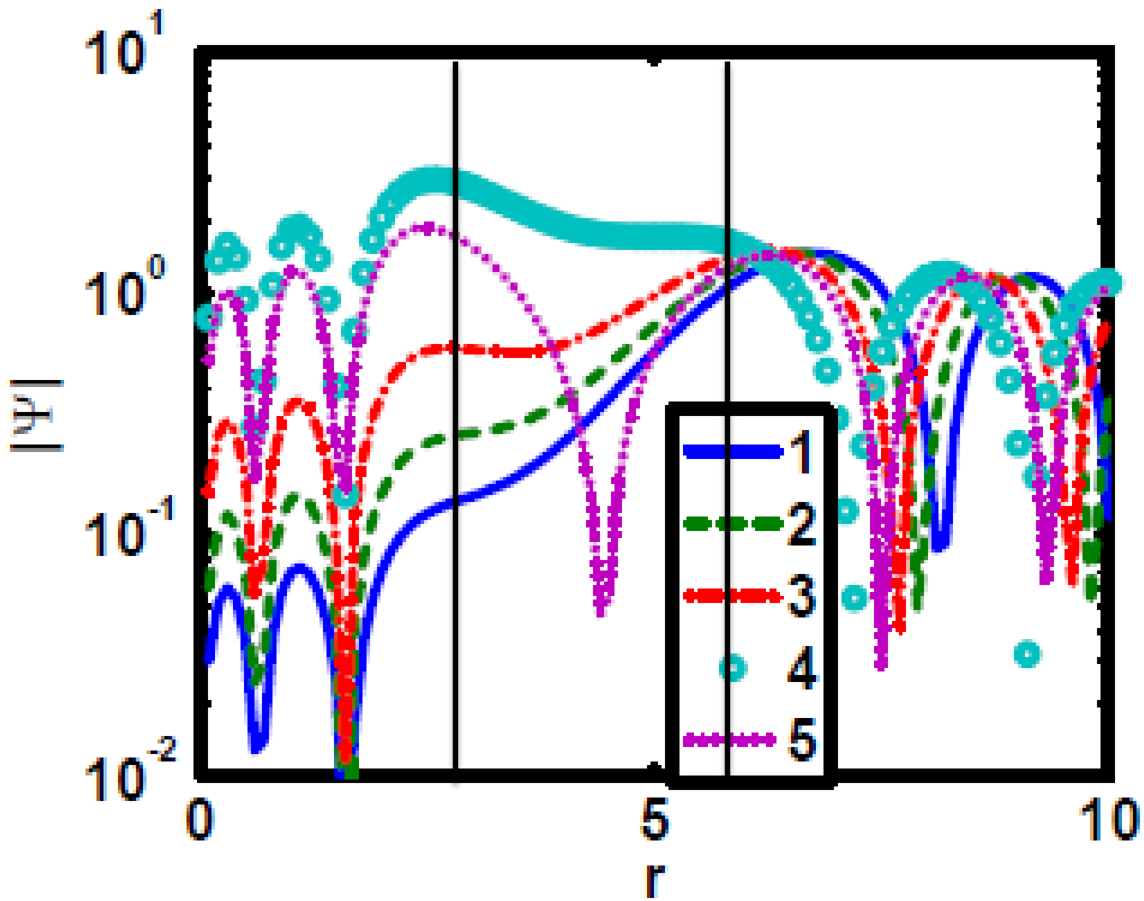


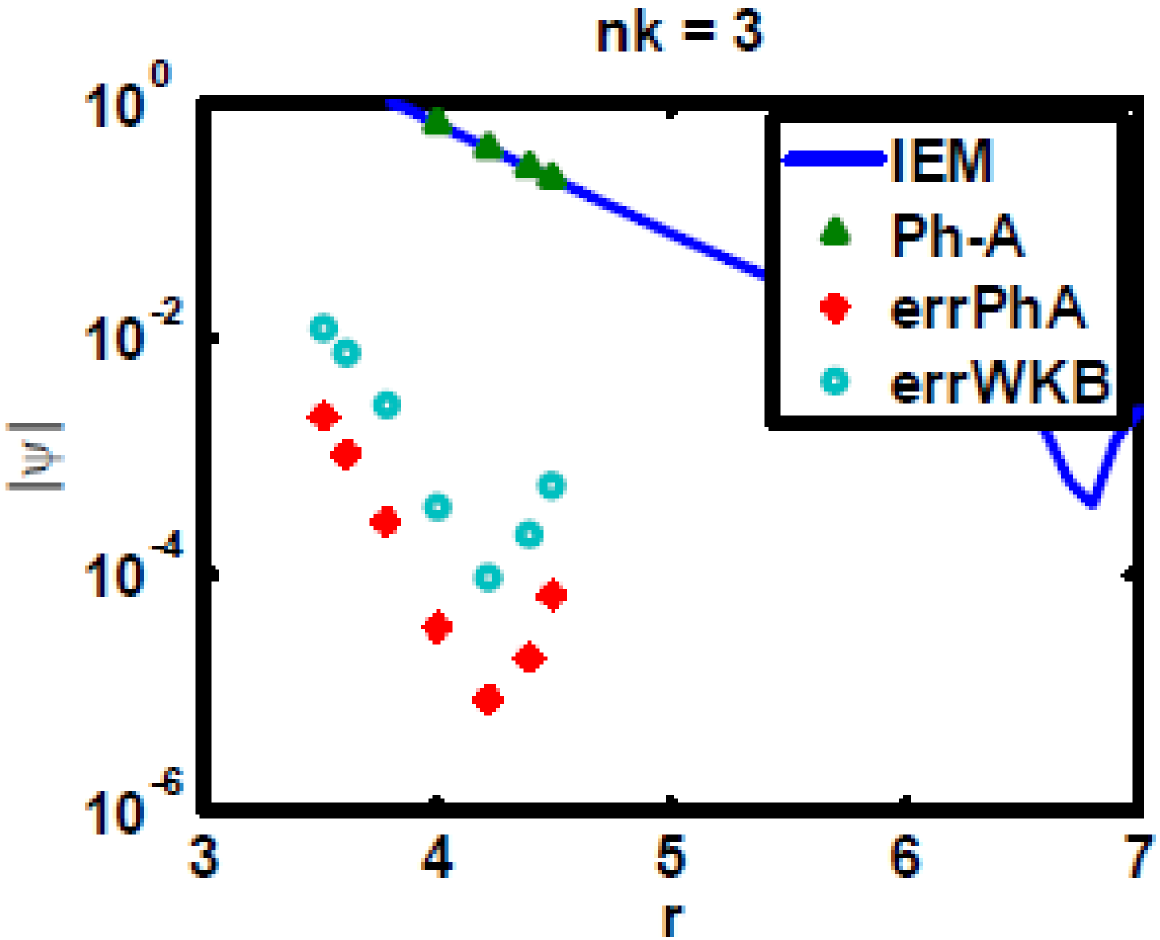
Figure 11: The continuous lines illustrate the wave function results in the barrier region obtained by solving the Schrödinger Eq. for the Morse potential (23) using the S-IEM method for $0 \leq r \leq 100$, for the various energies given by k^2. Here the wave numbers k spanning the resonance region are given by $k = 1.08526787 + (n-1) * 10^{-8}$, with $n = 1, ..4$. The barrier region extends from $r = 2$ to $r = 12$. The discrete symbols represent the results of an independent Phase-Amplitude calculation described in the text.

Reson. # 2, Near top of Barrier



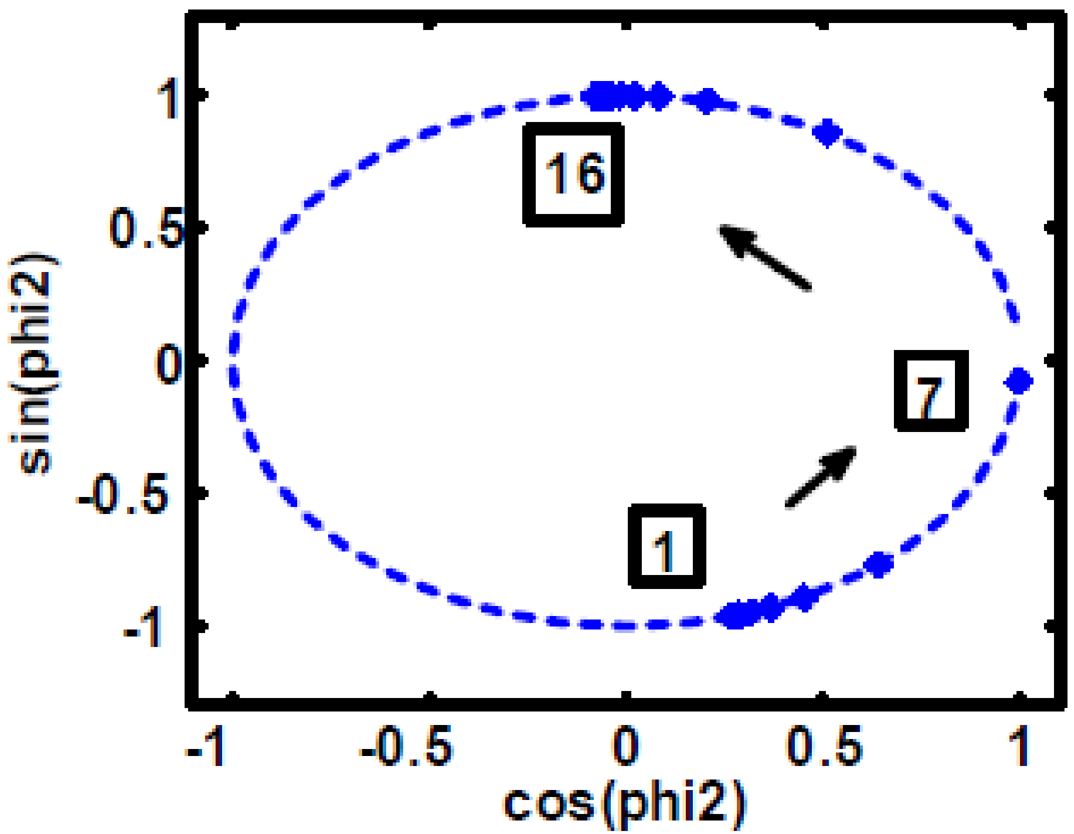
Resonance #1, k = 1.0853

Error of the Ph-A wave function



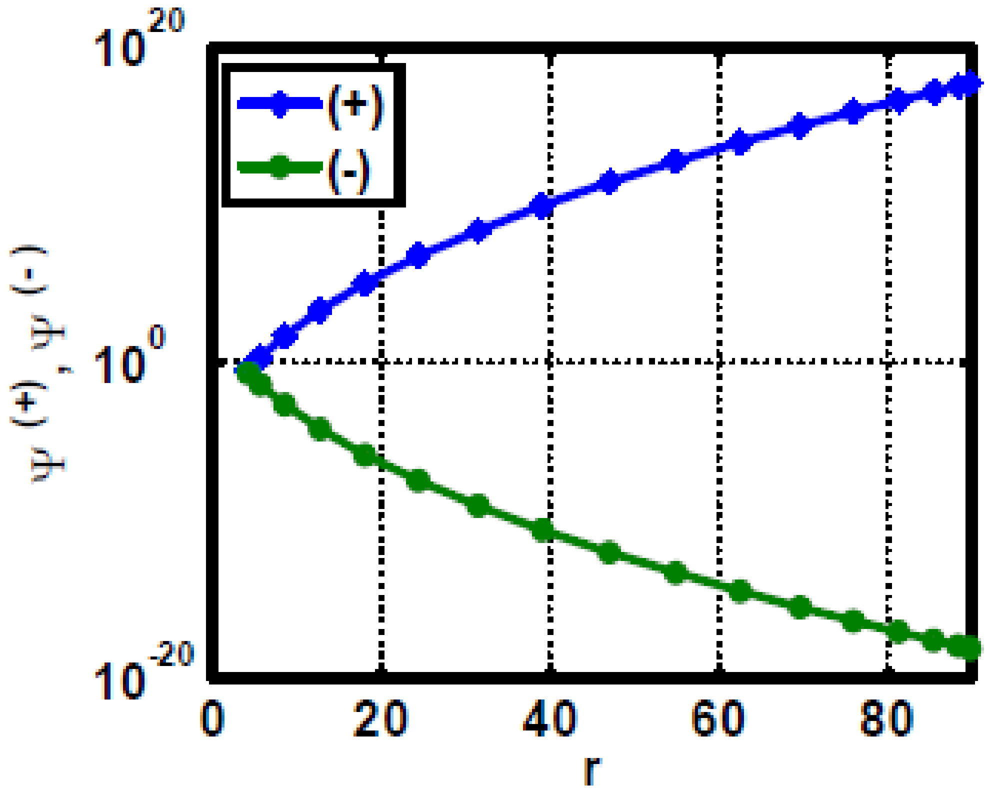
Phase-Shift

k(n) = 1.50713+(n-1)∗0.5×10^{-5}, V_o=4;r_{e}=4;α=0.3.



How narrow is a resonance?

Eta = 40



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

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

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..
   Better **linear** method under exploration

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