Phase-Amplitude Representation of a wave function, revisited

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The Schroedinger partial wave equation

\[ \frac{d^2 \psi}{dr^2} + k^2 \psi = V_T \psi \]

\[ V_T(r) = \frac{L(L + 1)}{r^2} + V(r) \]
Milne's eqs. (1930)

For the amplitude and phase, $E > V$

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

$$\frac{d^2 y}{dr^2} + k^2 y = V_T y + \frac{k^2}{y^3}$$

$$\phi(r) = \phi(r_0) + k \int_{r_0}^{r} [y(r')]^{-2} dr'$$
Solution of the amplitude Eq. Spectral expansion

\[ y(x) = \sum_{n=0}^{N} a_n T_n(x) \]

\begin{align*}
N + 1 \text{ Chebyshev Polynomials} \\
N + 1 \text{ non-equidistant support points}
\end{align*}
\[ \frac{k}{y_{n+1}^2} = \left[ w + \frac{1}{y_n} \frac{d^2 y_n}{dr^2} \right]^{1/2}, \quad n = 0, 1, 2, \ldots \]

\[ w(r) = k^2 - V(r), \]

\[ \frac{k}{y_0^2} = w^{1/2^{\text{WKB}}} \]
Oscillatory case, $E > V$
Amplitude for a Coulomb Potential
Phase for a Coulomb potential
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, \( \eta = -2, k = 1; \bar{z} = -4 \): 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 approx 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.

Amplitude agrees with a S-IEM wave function for a repulsive rounded Coulomb Potential, \( \eta = +2 \), \( 10 < r < 2000 \)
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

\[ E < V \]

\[ \psi(r) = A\psi^{(+)} + B\psi^{(-)}(r) \]

\[ \psi^{(\pm)}(r) = \tilde{\gamma}(r)\exp(\pm\Phi(r)) \]
Iterations, \( V > E \)

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

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

\[
\tilde{D}_n = -\frac{d^2\tilde{y}_n/dr^2}{\tilde{y}_n}
\]

\[
D_0 = 0
\]

\[
\Phi(r) = \int_a^r \frac{k}{\tilde{y}^2(r')} dr'
\]
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 $k = 1.08526787 + (n - 1) \times 10^{-8}$, with $n = 1, \ldots 4$. 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

\[ k(n) = 1.50713 + (n-1) \times 0.5 \times 10^{-5}, \quad V_0=4; r_e=4; \alpha=0.3. \]
How narrow is a resonance?

\[ \text{Eta} = 40 \]
Ph-A linear Eq.

\[ u(r) = y^2(r) \]

Define \( u \)

\[ u'''' + 4(k^2 - V)u' - 2V'u = 0. \]

Define \( v \)

\[ v(r) = u' = \frac{du}{dr} \]

\[ d^2v/dr^2 + 4(k^2 - V)v = 2\left(\frac{dV}{dr}\right)\left(\int_0^r v(r')dr'\right) \]
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