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# A spectral Phase–Amplitude method for propagating a wave function to large distances

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ABSTRACT

The phase and amplitude (Ph–A) of a wave function vary slowly with distance, in contrast to the wave function that can be highly oscillatory. Hence the Ph–A representation of a wave function requires far fewer computational mesh points than the wave function itself. In 1930 Milne presented an equation for the phase and the amplitude functions (which is different from the one developed by Calogero), and in 1962 Seaton and Peach solved these equations iteratively. The objective of the present study is to implement Seaton and Peach's iteration procedure with a spectral Chebyshev expansion method, and at the same time present a non-iterative analytic solution to an approximate version of the iterative equations. The iterations converge rapidly for the case of attractive potentials. Two numerical examples are given: (1) for a potential that decreases with distance as $1/r^3$, and (2) a Coulomb potential $\propto 1/r$. In both cases the whole radial range of [0–2000] requires only between 25 and 100 mesh points and the corresponding accuracy is between $10^{-3}$ and $10^{-6}$. The 0th iteration (which is the WKB approximation) gives an accuracy of $10^{-2}$. This spectral method permits one to calculate a wave function out to large distances reliably and economically.



## 1. Introduction

When the Phase–Amplitude (Ph–A) method was first introduced by Milne in 1930 [1], and then taken up by many authors, see Ref. [2], the main motivation was the paucity of numerical mesh points required, compared to the calculation of the wave function itself. This is because both phase and amplitude functions are slowly varying, as opposed to the wave function that can be highly oscillatory. This point was verified by many authors, in particular by Calogero and Ravenhall [3] who state that the solution for the phase is more stable than the solution of the wave function. An additional argument in favor of the Ph–A representation is that it lends itself to analytic expressions to address particular problems. For example, the Ph–A representation facilitates the incorporation of the effect of long range potentials [4,5] or the calculation of resonances [2]. It is also helpful in the quantum defect calculation of atomic wave functions [6], the calculation of Gaunt Factors [7], as well as the description of an electron with an ion embedded in a plasma [8], among others. The emission of an electron from an atom, either by incident photons, or by other processes such as beta decay of the nucleus also makes extensive use of Calogero's Ph–A description [9]. However that method studied by Calogero [10] is different from the one described here, as is further discussed in Appendix A. The Ph–A description of a carrier wave in radio or television also plays a significant rôle in the compactification of the signal transmission in the field of Information Technology [11]. An additional advantage of the present Ph–A representation is that it provides a method to improve the Wentzel, Kramers Brillouin (WKB) [12,13] approximation of a wave function, an important point since the WKB approximation has led, over the years, to a much improved understanding of the solution of the Schrödinger equation. A further advantage for the case of long range potentials is that Milne's Ph–A method lends itself to provide the normalization of a conventionally obtained wave functions calculated only out to short distances, such that the amplitude of that wave function would asymptotically approach unity, if carried out to large distances. This normalization method does not require a Wronskian-type matching procedure to two analytically known basis functions.

The Ph–A representation consists in writing a wave function $\psi(r)$ in the form

$$\psi(r) = y(r)\sin[\phi(r)], \tag{1}$$

where $y$ is the amplitude and $\phi$ is the phase, and $r$ the distance from the origin. Here $\psi$ is a partial wave function that depends only on

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the single variable $r$. If an overlap matrix element

$$M = \int_0^\infty \psi_1(r) U(r) \psi_2(r) dr \tag{2}$$

between two wave functions is required, then in the finite difference method of obtaining integrals, both $\psi_1$ and $\psi_2$ have to be calculated on a sufficiently fine mesh, which can be time consuming and prone to errors. However, the Ph–A representation can provide an estimate of $M$ by decomposing the integrand of the overlap matrix element into a slowly oscillating ($S$) and a fast oscillating ($F$) part

$$M = M^{(S)} - M^{(F)}. \tag{3}$$

The decomposition makes use of a trigonometric identity for the product of two sine functions with the result

$$M^{(F)} = \frac{1}{2} \int_0^\infty y_1(r) U(r) y_2(r) [\cos(\phi_1 + \phi_2)] dr. \tag{4}$$

$$M^{(S)} = \frac{1}{2} \int_0^\infty y_1(r) U(r) y_2(r) [\cos(\phi_1 - \phi_2)] dr. \tag{5}$$

The matrix element $M^{(S)}$ ($S$ stands for slow variation, $F$ for fast variation of the integrand) can be calculated on a small set of radial mesh points since the integrand oscillates slowly. Further, since $|M^{(F)}| < |M^{(F)}|$, a rough estimate for $M$ is provided by $M^{(S)}$ alone. Here $U(r)$ is an overlap function that depends on the physics application envisaged.

In 1962 Seaton and Peach [14] presented an iterative scheme to solve Milne's non-linear differential equation [1] for the amplitude and phase. It is the purpose of the present work to implement this iterative method by means of a spectral [15,16] expansion of the amplitude in terms of Chebyshev polynomials. A further purpose is to examine the accuracy of the resulting Ph–A wave function by comparison with the direct solution of the Schrödinger equation for the wave function, the latter is also obtained by an accurate spectral integral equation method [17,18], denoted as IEM in what follows. The combination of both objectives has not been presented previously. The great advantage of a spectral expansion is that the calculations utilize all the support points located in a given partition simultaneously, with the result that the errors are shared uniformly across the partition in the case of Chebyshev expansions [19,20]. For the present numerical examples the calculation is done in one great radial partition, extending from $r = 0$ to $r = 2000$, containing between 25 and 201 Chebyshev support points, depending on the accuracy required. By contrast, other algorithms (such as finite elements, finite differences, or the IEM method described below) divide such a large radial interval into a number of partitions, with the result that the accumulated error from all previous partitions is propagated into the next one, the last partition having the largest error [21]. An analysis of the accumulation of the Finite Element errors is presented in Appendix B. In addition, for calculations that require the storage of many wave functions with high precision [22–25] the use of the Ph–A representation can be very advantageous because the amount of storage required can be substantially smaller than what is needed for other algorithms.

In Section 2 the iterative method is explained, Section 3 contains details of the computational spectral method, Section 4 describes a non-iterative analytic solution to an approximate set of iterative equations, Section 5 establishes a connection between a wave function and the corresponding values of the phase and amplitude, Section 6 contains numerical results, the calculation of overlap integrals is described in Section 7, the Summary and Conclusions are given in Section 8. In Appendix A it is shown that the Ph–A combination defined by Calogero is not the same as the one defined by Milne, even though both methods lead to the same wave function $\psi$, and in Appendix B it is argued that a Gauss–Lobatto finite element method cannot reach large distances with the same accuracy as the Ph–A method.

## 2. Iterative solution of Milne's phase–amplitude equation

The Schrödinger equation to be solved for a partial wave function $\psi$ is

$$d^2\psi/dr^2 + k^2\psi = V_T\ \psi. \tag{6}$$

The total potential $V_T$ is

$$V_T(r) = L(L+1)/r^2 + V(r), \tag{7}$$

where $V(r)$ is the atomic or nuclear potential (including the Coulomb potential) in units of inverse length squared, and $L$ is the orbital angular momentum quantum number. Milne's non-linear equation for the amplitude $y(r)$ is given by [1]

$$d^2y/dr^2 + k^2 y = V_T\ y + k^2/y^3, \tag{8}$$

where the nonlinearity is given by the last term in Eq. (8). In Eqs. (6) to (8) the factor $\hbar^2/2m$ has already been divided into the potential and into the energy, so that both are given in units of inverse length squared, and the wave number $k$ is given in units of inverse length. The unit of length can be either fm for nuclear physics applications, or the Bohr radius $a_0$ for atomic physics applications, but will not be explicitly indicated. The phase $\phi(r)$ is obtained from the amplitude $y$ by [1]

$$\phi(r) = \phi(r_0) + k \int_{r_0}^{r} [y(r')]^{-2}\, dr', \tag{9}$$

but it can also be obtained without the knowledge of $y$ [7]. Eqs. (8) and (9) can be obtained by inserting Eq. (1) into Eq. (6), noting that the terms involving the phase $\phi(r)$ can be separated from the terms involving the amplitude $y(r)$, and each collection of terms can be set to zero independently. An overall normalization is still arbitrary, but it can be fixed by demanding close agreement with the WKB approximation [12,13]. Eqs. (8) and (9) lead to a phase–amplitude representation of the wave function that is different from the one described by Calogero [10], in that Eqs. (8) and (9) do not require the definition of auxiliary basis functions, as is the case for the Calogero method, and the phase is obtained from the amplitude, while the reverse is the case for the Calogero method. Details are given in Appendix A.

Eq. (8) has been solved non-iteratively in the past by using some form of a finite difference computational method, such as one of Milne's predictor–corrector methods [26], or [8] by a Bulirsch–Stoer limit method [27], none of which will be used in the present study.

The iterative method of Seaton and Peach [14] consists in rewriting Eq. (8) in the form

$$\frac{k^2}{y^4} = w + \frac{1}{y}\frac{d^2y}{dr^2} \tag{10}$$

where

$$w(r) = k^2 - V_T, \tag{11}$$

and calculating the solution of Eq. (10) by means of the iteration [14]

$$\frac{k}{y_{n+1}^2} = \left[ w + \frac{1}{y_n}\frac{d^2y_n}{dr^2} \right]^{1/2}, \quad n = 0, 1, 2, \ldots. \tag{12}$$

Here $n$ denotes the order of the iteration, and the initial value of $y$ is given by the WKB approximation [12,13]

$$\frac{k}{y_0^2} = w^{1/2}. \tag{13}$$

The advantage of formulating the iteration according to Eq. (12) is that $y$ varies slowly with $r$, automatically approaching unity at