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Tunneling through a barrier with the phase–amplitude method

George Rawitscher

Physics Department, University of Connecticut, Storrs CT 06269, United States

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ABSTRACT

A previous study (Rawitscher, 2015) of the solution of Milne's non linear equation for the phase and amplitude of a one-dimensional wave function is extended to the case where the incident energy is less than the potential (Barrier region). The numerical method again consists in implementing a spectral expansion of the amplitude in terms of a number of Chebyshev polynomials. The method is applied to a Morse-type potential, for energies in a resonance region, and for one energy below the resonance region, and a strong repulsive Coulomb potential. The results are compared with highly accurate direct solutions of the Schrödinger equation, and were found to be accurate to 1:10^{-6}.

1. Introduction

The tunneling of a wave function through a potential barrier is a well known phenomenon in quantum mechanics. It has played an important role in the interpretation of various physical phenomena, such as the decay of a nucleus through α-particle emission, the fission [1] or fusion [2,3] of a heavy nucleus at energies below the Coulomb barrier, optical model scattering calculations [4–6], in the physics of ultra-low temperature atoms [7], and may have applications in other fields of physics [8] as well. Since the 1930s the Wentzel, Kramers, Brillouin (WKB) approximation provided a very useful tool in the calculation of barrier penetration probabilities. A good pedagogical description of the WKB approximation with several good references can be found in the book by Griffith [9]. Since the WKB expression contains factors $\exp(\pm\int^r \kappa(r')dr')$, where κ is the local wave number, which are exponentially sensitive to the errors of the WKB, it would be very helpful to find improvements to this approximation. Many such improvements have been obtained [10], and it is the purpose of the present note to present yet another improvement based on the phase–amplitude (Ph–A) description of the solution of a one-variable Schrödinger equation.

Milne's equations for the Ph–A description [11] have a non-linear term which presents difficulties for the numerical solution. Seaton and Peach [12] have presented an iterative solution that proved to be very accurate once a spectral expansion [13,14] for the calculation of the amplitude was introduced [15]. However the latter formulation was up to now applied only to attractive potentials, in the region where the local wave number is real, in contrast to a barrier region, where the local wave number is purely imaginary. It is the purpose of the present paper to remedy that lack, and show that the appropriate modification of the Ph–A method also works for the radial region that is forbidden classically. However, the restrictions for the validity of the WKB approximation are valid also for the method presented here, i.e., the method is accurate only in a region sufficiently far away from the turning points such that the variations of the potential in a distance of the local wave length are small compared to the potential itself [9].

In Section 2 the Ph–A formulas pertinent to the barrier region will be derived, in Section 3 the iterative solution method will be described, in Section 4 the connection formulas across the turning points will be presented, in Section 5 a numerical application to a Morse-type potential will be described for incident energies near and below the resonance region. Section 6 contains results for the long range Coulomb potential, Section 7 contains some numerical considerations, and Section 8 contains the summary and conclusions.

The resonance properties for the Morse potential case have been investigated previously [16], and a comparison of the accuracy of various computational methods that calculate the scattering phase shifts in the resonance region was presented in Ref. [17]. The accuracy analyses was possible, because the phase shifts are known analytically for the Morse potential case. The resonance region presents a challenging test of accuracy, because some of the wave functions do decrease with distance r in that region, while the errors of the computational method introduce *increasing* contributions in the barrier region. It was shown in

E-mail address: George.Rawitscher@uconn.edu.

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Fig. 2 of Ref. [17] that using a sixth order Numerov method for the solution of the Schrödinger equation the results were six orders of magnitude *less* accurate than that of a solution based on a spectral integral equation method denoted as S-IEM [18]. The latter method will also be used in the present investigation as a comparison benchmark result for the numerical examples.

2. The equations

The one-dimensional radial Schrödinger equation for a partial wave function ψ is written as

$$d^2\psi/dr^2 + k^2\psi = V\,\psi \tag{1}$$

where V is the spherically symmetric potential, that includes the angular momentum contribution $L(L+1)/r^2$, and k is the wave number. The corresponding energy of the incident particle is k^2, which is assumed to be positive. In the present notation the factor $2m/\hbar^2$ has already been multiplied into quantities given in energy units, such that the resulting values for V and E have units of inverse length squared, while k is given in units of inverse length, and r is given in units of length. The units will however not be indicated in the graphs below. In the barrier region, where $V > E$, the local wave number κ is given by

$$\kappa(r) = \sqrt{\tilde{w}(r)}, \tag{2}$$

where

$$\tilde{w}(r) = V(r) - k^2 > 0. \tag{3}$$

If one inserts into Eq. (1) the ansatz

$$\psi^{(-)}(r) = y^{(-)}(r)\exp(-\Phi^{(-)}(r)) \tag{4}$$

or

$$\psi^{(+)}(r) = y^{(+)}(r)\exp(\Phi^{(+)}(r)) \tag{5}$$

or

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

one finds that

$$y^{(+)} = y^{(-)} = y \tag{6}$$

and

$$\Phi^{(+)} = \Phi^{(-)} = \Phi(r) \tag{7}$$

where the common amplitude y obeys the equation

$$\frac{d^2}{dr^2}y - \tilde{w}\,y = -\frac{k^2}{y^3} \tag{8}$$

and the common phase Φ is given by the simple quadrature

$$\Phi(r) = \int_a^r \frac{k}{y^2(r')}dr'. \tag{9}$$

The two turning points at the extremities of the barrier region are T_1 and T_2, and the region suitable for the Ph–A method is located in $[a, b]$, which is contained between T_1 and T_2. (Hence $T_1 < a \le r \le b < T_2$.) The complete Ph–A wave function in $[a, b]$ is given by

$$\psi(r) = y(r)\left[A\,e^{-\Phi(r)} + B\,e^{+\Phi(r)}\right]; \quad a \le r \le b, \tag{10}$$

where the coefficients A and B are determined by the connection formulas across the turning points. The validity of Eqs. (6)–(10) can be verified by inserting Eq. (10) into Eq. (1), and setting to zero each of the terms multiplied respectively the factors A or B.

Once the phase is defined according to Eq. (9), then the relationship between phase Φ and amplitude y is determined uniquely, but other relationships are also possible [19], as is the case for the Calogero's Ph–A formalism, described in Appendix A of Ref. [15]. The region of validity of the WKB approximation requires that the local wave length $\lambda(r) = 2\pi k/[E - V(r)]$ changes little in the distance of the local wave length, i. e., that

$$\frac{\Delta\lambda}{\lambda} = \frac{2\pi k}{(V-E)^2}\frac{dV}{dr} \ll 1. \tag{11}$$

However the conditions of applicability of the Ph–A method are more stringent, because the convergence of the iterations depends on the smallness of the quantity $(d^2y/d^2r)/y$ compared to the potential V.

3. Iterative solution

In this section the iterative method of Seaton and Peach [12] is extended to the barrier region, where $\tilde{w} = V - k^2 > 0$. By re-writing Eq. (8) and taking square roots, one obtains

$$\frac{k}{y_{n+1}^2} = (\tilde{D}_n + \tilde{w})^{1/2}, \quad n = 0, 1, 2.. \tag{12}$$

where $\tilde{w}$ is defined in Eq. (3), where

$$\tilde{D}_n = -\frac{d^2y_n/dr^2}{y_n} \tag{13}$$

and where $D_0 = 0$. The resulting value of y_1 is identical to the WKB approximation

$$y_1 = y_{\rm WKB} = (V/k^2 - 1)^{-1/4}, \quad a \le r \le b \tag{14}$$

and hence the phase and the wave function (10) becomes identical to their WKB values. Since there would be a numerical loss of accuracy when calculating the second order derivative of y, it is preferable to obtain $\tilde{D}_n$ by a recursion relation which in the present case takes the form

$$\tilde{D}_{n+1} = -\frac{5}{16}\frac{(\tilde{D}_n' + \tilde{w}')^2}{(\tilde{D}_n + \tilde{w})^2} + \frac{1}{4}\frac{(\tilde{D}_n'' + \tilde{w}'')}{(\tilde{D}_n + \tilde{w})}, \quad n = 0, 1, 2, \ldots, \tag{15}$$

where "primes" denote derivatives with respect to r. For $n = 0$, one has $\tilde{D}_0 = 0$, and hence all its derivatives are zero. The derivatives of $\tilde{w}$ are equal to the derivatives of V, which can be calculated analytically if the analytic expression for V is known, as is the case in the numerical example below. The advantage of obtaining $\tilde{D}_{n+1}$ by means of Eq. (15) instead of by calculating the second derivative of y_{n+1} directly is that the quantity $\tilde{D}_{n+1}$ and its derivatives are small compared to $\tilde{w}$ and its derivatives, and hence the effect of the errors of the Chebyshev expansion of $\tilde{D}_{n+1}$ and its derivatives becomes reduced. A numerical comparison of the potential V and the quantity D is presented in connection with an application of the Ph–A method to a Coulomb potential.

There are two methods for obtaining $\tilde{D}$. One consists by inserting the values of $\tilde{D}_{n-1}$ and its derivatives into Eq. (15) in order to obtain $\tilde{D}_n$. Next, the derivatives of $\tilde{D}_n$, calculated numerically, are inserted into the right hand side of Eq. (15) and the iteration for $\tilde{D}_n$ continues until the iteration converges for $n_{\max}$. By inserting the result into Eq. (12) one obtains the values of $y_{n_{\max}}$ for all support points, hence the phase for all support points can be obtained from the quadrature indicated in Eq. (9) from which the functions $\psi^{(\pm)}$ can be obtained. This procedure is especially economical if a spectral expansion of all the functions in terms of Chebyshev polynomials is implemented, as described below. The coefficients A and B required for the full wave function in Eq. (10) are obtained by a connection formula across the left turning point, as described below.

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