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A polynomial approximation for the scattering wavefunction of an arbitrary spherically symmetric potential*

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A new variational approach is proposed to calculate scattering phase shifts. In this approach, the variational parameter is contained not explicitly in the trial function but in the boundary conditions that the scattering wavefunction should satisfy. It was found that a high accuracy could be reached. Furthermore, the scattering wavefunction appears as a polynomial of finite orders in the interior region. This expression is convenient for applications.

Keywords: scattering phase shift, variational approach
PACC: 0365, 0380, 0260

1. Introduction

It is not difficult to calculate the phase shifts of scattering wavefunctions for arbitrary potentials; it can be done, for example, by solving the difference equations numerically. However, in various existing numerical methods, the wavefunctions are mostly given in the form of numbers, which is inconvenient if the wavefunction is to be utilized in further theoretical treatment. As a remedy, an alternative approach is suggested for calculating the scattering wavefunctions for arbitrary potentials with spherical symmetries. In this approach, the scattering wavefunction in the inner region is expressed as a polynomial of finite ranks. This expression is found to be very accurate.

2. Theoretical approach

Letting the potential contain a short-range interaction $U(r)$ plus a long-range Coulomb repulsion, we define a sufficiently long-range b such that $U(r)$ can be considered to be zero for $r \geq b$. We denote the scattering wavefunction as $f(r)$, and we study its behaviour in the region $r \leq b$. In the outer region, the scattering wavefunction is simply composed of regular and irregular Coulomb functions and can therefore be obtained by a continuous extension from the inner to the outer regions.

In general, a scattering state may not be represented by a polynomial of finite ranks. However, if we are concerned only the region $r \leq b$, it can be approximately expressed in this form with a very high accuracy, as shown below.

When the units are properly chosen, the scattering wavefunction satisfies the Schrödinger equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{l(l+1)}{r^2} - \frac{\beta}{r} - U(r)\right] f(r) = 0, \quad (1)$$

where l is the partial wave, k^2 is twice the energy and β (a positive value) is associated with the strength of the Coulomb repulsion.

For $r \geq b$, it is well known that[1]

$$\begin{aligned} f(r) =& f_{\mathrm{out}}(r) \\ =& A(r)\cos[\theta(r)+\delta] + B(r)\sin[\theta(r)+\delta]. \end{aligned} \quad (2)$$

Here

$$\theta(r) = kr - \eta\ln(2kr) - \frac{l\pi}{2}, \quad (3)$$

$$\eta = \frac{\beta}{2k}, \quad (4)$$

$$A(r) = \frac{l(l+1)+\eta^2}{2kr} + \frac{3\eta[l(l+1)+\eta^2] + \eta[l(l+1)-2+\eta^2]}{8k^2r^2} + \cdots, \quad (5)$$

$$B(r) = 1 + \frac{\eta}{2kr} + \frac{3\eta^2 - [l(l+1)+\eta^2][l(l+1)-2+\eta^2]}{8k^2r^2} + \cdots \quad (6)$$

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and

$$\delta = \delta_{\rm C} + \delta_U, \tag{7}$$

where

$$\delta_{\rm C} = \arg[\Gamma(l+1+{\rm i}\eta)] \tag{8}$$

is the Coulomb phase shift and δ_U is an additional phase shift arising from the short-range potential. More detailed expressions for $A(r)$ and $B(r)$ can be found in Ref.[1] and are accurately calculated.[2]

Our aim is to determine δ. For this purpose, we let the interior wavefunction be expanded as

$$f(r) = f_{\rm in}(r) = r^l \sum_m C_m r^m, \tag{9}$$

where the index m ranges from 1 to N (an integer to control the accuracy). This expansion is valid only in the region $r \le b$. Inserting Eq.(9) into Eq.(1), we have

$$\sum_m \left[(m+l)(m+l-1)r^{m+l-2} + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{\beta}{r} - U(r)\right) r^{m+l}\right] C_m = 0. \tag{10}$$

We define a set of $N-2$ distances r_n uniformly distributed in the region $(0, b)$ as

$$r_n = \frac{n}{N-2} b, \tag{11}$$

where n is an integer ranging from 1 to $N-2$. Putting r at r_n, we obtain from Eq.(10) a set of $N-2$ equations

$$\sum_m \left[(m+l)(m+l-1)r_n^{m+l-2} + \left(k^2 - \frac{l(l+1)}{r_n^2} - \frac{\beta}{r_n} - U(r_n)\right) r_n^{m+l}\right] C_m = 0. \tag{12}$$

The unknown δ is considered as a variational parameter and is assigned a series of suggested values. For each given δ, we can obtain two additional equations from the continuity at the border b, namely

$$b^l \sum_m C_m b^m = A(b)\cos[\theta(b)+\delta] + B(b)\sin[\theta(b)+\delta] \tag{13}$$

and

$$b^{l-1} \sum_m (m+l) C_m b^m = \left[A'(b) + \left(k - \frac{\eta}{b}\right) B(b)\right] \cos[\theta(b)+\delta] + \left[B'(b) - \left(k - \frac{\eta}{b}\right) A(b)\right] \sin[\theta(b)+\delta]. \tag{14}$$

A' and B' are the derivatives of $A(r)$ and $B(r)$ with respect to r and can be calculated accurately. In total, we have N equations that are sufficient to determine the set of coefficients C_m. Having solved these equations, we insert the resultant C_m into Eq.(9). Then, we obtain the function $f_{\rm in}(r, \delta)$ in the inner region. $f_{\rm in}$ so given depends evidently on δ and satisfies the Schrödinger equation only at the $N-2$ points but not in the entire region. Therefore, it is generally not a solution. When it is inserted into Eq.(1), we have

$$\left[\frac{{\rm d}^2}{{\rm d}r^2} + k^2 - \frac{l(l+1)}{r^2} - \frac{\beta}{r} - U(r)\right] f_{\rm in}(r, \delta) = g(r, \delta), \tag{15}$$

where the function $g(r, \delta)$ deviates from zero in general, but contains nodes at r_n. For $g(r, \delta)$, we define an error function

$$\epsilon(\delta) = \int_0^b {\rm d}r |g(r, \delta)|. \tag{16}$$

Evidently, if $\epsilon(\delta) \to 0$, $f_{\rm in}(r, \delta)$ would tend to the exact solution.

It turns out that, for various types of potential, $\epsilon(\delta)$ is highly sensitive to δ. We see that, if δ goes through a certain optimal value $\delta_{\rm min}$, $\epsilon(\delta)$ undergoes a dramatic fall to a minimum at $\delta_{\rm min}$. This is an interesting discovery about the property of the error function. The magnitude of $\epsilon(\delta_{\rm min})$ depends on N. As expected, the larger N is, the smaller $\epsilon(\delta_{\rm min})$. Using these features, it is necessary just to choose a sufficiently large N and then calculate ϵ as a function of δ. From the drastic fall of ϵ , $\delta_{\rm min}$ can be identified and $f_{\rm in}(r, \delta_{\rm min})$ can be obtained. The smaller $\epsilon(\delta_{\rm min})$ is, the more accurate $f_{\rm in}$ and $\delta_{\rm min}$.

3. Concrete results and comparison

In order to see how well this procedure works, we study the first case with a pure repulsive Coulomb potential (i.e. $U(r) = 0$). In this case, we can compare the numerical results with the exact value $\delta_{\rm C}$ (refer to Eq.(8)). We let $k = 1, l = 2$ and $\beta = 2$. When b=10 and N=15 and 13 are respectively adopted, $\epsilon(\delta)$ is plotted in Fig.1 as a function of δ. The lower curve with $N = 15$ has a sharp minimum at $\delta_{\rm min}$ which is extremely close to the exact value $\delta_{\rm C}$=0.947406. Thus, in our approach, an N=15 polynomial is sufficient to give a highly accurate phase shift. Associated with this phase shift, $\epsilon(\delta_{\rm min})$ is extremely small

($< 10^{-6}$). This implies that the corresponding polynomial $f_{\rm in}(r, \delta_{\rm min})$ is extremely close to the exact wavefunction in the inner region. It is noted that the scales in Fig.1 are extremely small, thus $\epsilon(\delta)$ is highly sensitive to δ and therefore our approach is highly efficient. Incidentally, the accuracy of this approach depends seriously on the accuracy of $A(b)$ and $B(b)$ (refer to Eqs.(5) and (6)). In our examples, these values are given with eight significant figures.

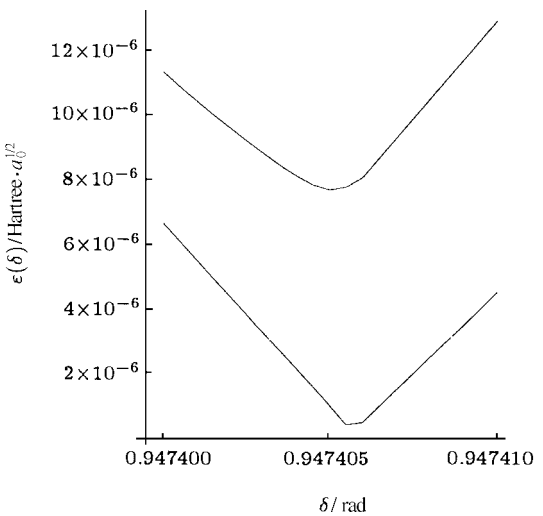


Fig.1. $\epsilon(\delta)$ as a function of δ in the case of pure Coulomb scattering for N=15 (lower curve) and N=13 (upper curve). Here, 1 Hartree=27.21eV, and a_0 is the Bohr radius.

Now, we observe the second case in which, in addition to the repulsive Coulomb potential, an attractive short-range potential

$$U(r) = -U_0 \mathrm{e}^{-r^2} \tag{17}$$

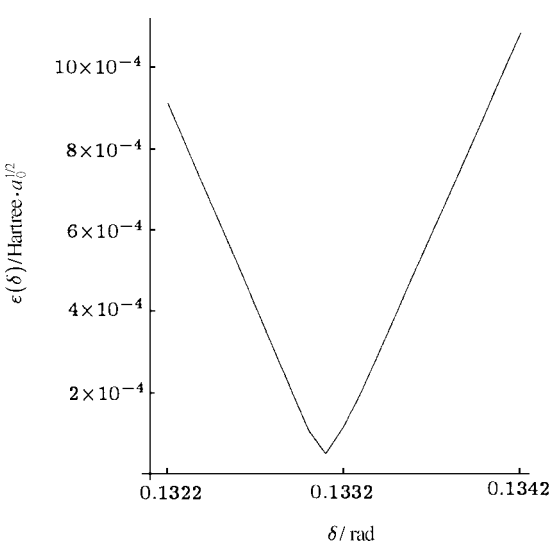


Fig.2. $\epsilon(\delta)$ as a function of δ in the case of a Coulomb repulsive potential together with a short-range attractive potential for $N = 23$.

is incorporated. We let $k = 1$, $l = 0$, $\beta = 4$ and $U_0 = 4$. When $b = 5$ and N=23, $\epsilon(\delta)$ is plotted in Fig.2 as a function of δ. In this case the behaviour of the wavefunction is more complicated due to the interference of the repulsive and attractive potentials. Accordingly, a larger N is needed and the accuracy is lower than the previous case but is still satisfactory, i.e. there are is still a large decrease of $\epsilon(\delta)$ and a very small $\epsilon(\delta_{\rm min})$. Thus, our approach remains effective and accurate.

When U_0 varies, the resulting δ (i.e. $\delta_{\rm min}$) is given in Fig.3 as a function of U_0, where the increase of U_0 causes a nonlinear increase of δ , following an approximate relation of the type $\delta_{\rm min} = {U_0}^{1.456}$.

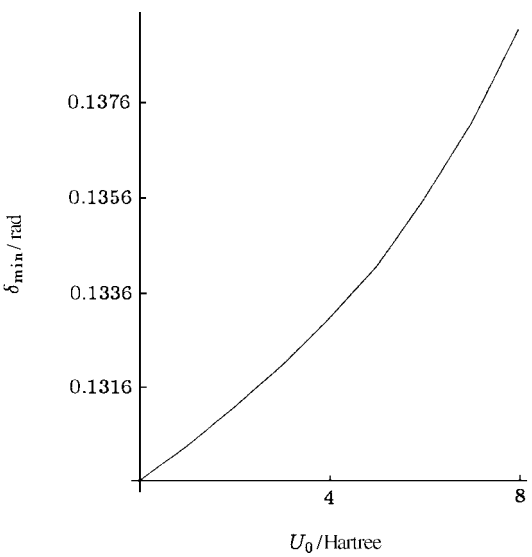


Fig.3. $\delta_{\rm min}$ as a function of U_0 for $N = 23$.

When the Coulomb potential does not exist, the above regular and irregular Coulomb functions should be changed to the Bessel functions of the first and second kinds. Accordingly, Eqs.(3), (5) and (6) should be changed to

$$\theta(r) = kr - \frac{l\pi}{2}, \tag{18}$$

$$A(r) = \sum_m \frac{(-1)^m (l+2m+1)!}{(2m+1)!(l-2m-1)!} \frac{1}{(2kr)^{2m+1}} \tag{19}$$

and

$$B(r) = \sum_m \frac{(-1)^m (l+2m)!}{(2m)!(l-2m)!} \frac{1}{(2kr)^{2m}}. \tag{20}$$

Here the summations over m are from zero to $\left[\frac{l-1}{2}\right]$ in Eq.(19) and to $\left[\frac{l}{2}\right]$ in Eq.(20), respectively.[3]

To summarize, a new approach is proposed to calculate the scattering phase shifts. It uses a new type of variational technique with three features:

(i) In the usual variational approaches, specific trial functions are defined in the whole region and the variational parameters are contained in these. However, in the present approach, the trial function is defined only in a limited region and the variational parameter is not evidently contained in it, but in the boundary conditions that the wavefunction has to satisfy.

(ii) In contrast to the usual approaches in which some selected observable(s) are optimized (for instance, the expectation value of a Hamiltonian is minimized in the bound-state problems),[4,5] in the present approach, the error function $\epsilon(\delta)$ is minimized.

(iii) The calculated results emerging from the usual variational procedures might not be very sensitive to the variational parameters; in the present approach, however, it is highly sensitive. The V-type curves, as shown in Figs.1 and 2, are generally not seen in other variational methods. It is the high sensitivity that leads to the high accuracy.

4. Conclusions

It has been pointed out that the phase shift can be calculated by other methods. Mostly, it is calculated by solving the difference equation using the Runge–Kutta method (or similar methods).[6] Nonetheless, the present approach has two advantages:

(i) The accuracy in solving a difference equation cannot be improved step-by-step by increasing the grids because, in doing so, errors would be accumulated. In contrast, using the present method, once $A(b)$ and $B(b)$ have been calculated accurately enough (which is relatively easy), the accuracy can be improved step-by-step by increasing N, as shown in Fig.1, until a satisfactory result is obtained.

(ii) Another remarkable advantage is that the wavefunction has a polynomial expression in the present approach. As mentioned above, this would facilitate further applications of the wavefunction.

It is noted that the $N-2$ points r_n are chosen to be uniformly distributed. This choice is simple. In fact, if the potential is more complicated, it is suggested that more points be chosen in the region where $U(r)$ rapidly varies. Furthermore, if a larger value of N has been adopted (e.g. $N > 25$), it is recommended to use the quadruple precision rather than the double precision in numerical calculations.

This approach may be generalized to solve bound-state problems, which will be discussed elsewhere.

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