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Variable Phase Method for the Calculation of the Scattering Phase Shift: The Bound-State Region*

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Variable phase methods for the calculation of the scattering phase shift in non-relativistic, quantum mechanical potential scattering are investigated with emphasis on their use for negative energies (bound-state region) and general (not necessarily integral) angular momenta. Of the various phase methods known to be valid for positive energies (scatering region), some remain valid and some become invalid for negative energies. One of the phase methods demonstrated to be valid for both positive and negative energies is fast for numerical computation of the scattering phase shift and so is useful for phenomenological investigations.

I. INTRODUCTION

The variable phase method for the calculation of the scattering phase shift in non-relativistic, quantum mechanical scattering theory is approximately 50 years old, but, as emphasized by Calogero in this monograph on the technique [1], it is a method still not widely used and appreciated. The variable phase method, or as we shall sometimes call it, the phase-function method, has the advantages: (1) it is simple mathematically, (2) it is interpretable in direct physical terms, and (3) it is a powerful method for the numerical calculation of the scattering phase shift. These points are examined in Calogero's book and references therein, especially for positive energies (the scattering region) and physical, integer values of the angular momentum. In the present note we investigate phase-function techniques for the calculation of the scattering phase shift for negative energies (the bound-state region) and all, not

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necessarily integer, angular momenta. In particular, there are three phase-function methods which have been studied and applied in the positive energy region, but which have not been carefully investigated and applied in the negative energy region. We examine the applicability and physical interpretation of these three methods in the bound-state region. Our result (for negative energies) is that the first of these methods (usually the slowest for numerical computation) remains valid, the second breaks down entirely, while the third method (the fastest for numerical computation) requires reanalysis and reinterpretation before it can be used.

A fast and accurate method for the calculation of the scattering phase shift for both negative and positive energies is useful because of the trend in physics to treat the bound-state and scattering regions as parts of one, unified physical situation. As is well known, knowledge of the phase shift in the scattering region yields directly the scattering cross section, and other valuable information such as, e.g., the locations and widths of all the resonance states of the system. Perhaps not quite so well known, however, is the usefulness of the phase shift in the bound-state region [1, 2]. For positive energies the phase shift is defined as the shift in the argument of the asymptotic wave function due to the presence of the scattering potential; this interpretation remains valid for negative energies except that the phase shift is now complex instead of real, and now the asymptotic wave function contains two pieces, one growing exponentially with the radial distance and one shrinking exponentially with the radial distance, instead of one sinusoidally oscillating piece. The physical bound states are those states which have energies such that the growing exponential is absent in the asymptotic wave function so that the wave function is normalizable; these special energies are the energy eigenvalues of the quantum system. Since the phase shift is complex for negative energies, it can determine the relative amounts of the growing and shrinking exponentials in the asymptotic wave function. The physical bound-state condition, i.e., absence of the growing exponential, is achieved at those energies where the imaginary part of the scattering phase shift tends to minus infinity [1, 2]. Thus, knowledge of the phase shift for negative energies yields immediately the system energy eigenvalues by simply noting those energies where the imaginary part of the phase shift goes to minus infinity; this procedure can be carried out graphically or on a computer.

II. Phase Function Formalism

We summarize in this section the basic formulae of the phase-function method that we will use for the calculation of the scattering phase shift [1].

Starting from the radial Schrödinger equation (prime means differentiation with respect to r),

$$u_l''(r) + \left[k^2 - \frac{l(l+1)}{r^2} - V(r) \right] u_l(r) = 0, \tag{1}$$

and the requirement that

$$\lim_{r\to 0} r^2 V(r) = 0, \tag{2}$$

it follows that the boundary condition $u_l(0) = 0$ is enough to specify the wave function $u_l(r)$ up to a multiplicative constant. The scattering phase shift δ_l can then be defined using the asymptotic behavior of $u_l(r)$:

$$u_l(r) \xrightarrow[r\to\infty]{} \text{const} \cdot \sin(kr - \tfrac{1}{2}l\pi + \delta_l). \tag{3}$$

The phase-function method is based on the amplitude function $\alpha_l(r)$ and the phase function $\delta_l(r)$ which are defined in terms of the wave function and its first derivative by

$$u_l(r) = \alpha_l(r)[\cos\delta_l(r)\hat{f}_l(kr) - \sin\delta_l(r)\,\hat{n}_l(kr)], \tag{4}$$

$$u_l'(r) = k\alpha_l(r)[\cos\delta_l(r)\hat{f}_l'(kr) - \sin\delta_l(r)\,\hat{n}_l'(kr)], \tag{5}$$

where $\hat{f}_l$, $\hat{n}_l$ are the Ricatti–Bessel functions [1, 3]. Note in particular that (5) does not follow from (4), so that (4) and (5) are independent expressions which unambiguously determine $\alpha_l(r)$ and $\delta_l(r)$. Considerations based on Eqs. (1), (3)–(5) then give the phase shift δ_l in terms of the asymptotic limit of the phase function $\delta_l(r)$:

$$\delta_l = \lim_{r\to\infty} \delta_l(r). \tag{6}$$

The amplitude and phase functions, $\alpha_l(r)$ and $\delta_l(r)$, are not the only such functions that can be defined. Two other sets, which are useful conceptually and computationally and which we use below, are defined by

$$u_l(r) = \alpha_l^{\gamma}(r)\sin[kr + \gamma_l(r)], \tag{7}$$

$$u_l'(r) = k\alpha_l^{\gamma}(r)\cos[kr + \gamma_l(r)], \tag{8}$$

and

$$\bar{u}_l(r) = \alpha_l^{\beta}(r)\sin[kr + \beta_l(r)], \tag{9}$$

$$\bar{u}_l'(r) = k\alpha_l^{\beta}(r)\cos[kr + \beta_l(r)], \tag{10}$$

where $\bar{u}_l(r)$ satisfies the radial Schrödinger equation (1) with $V(r) = 0$ and the usual boundary condition $\bar{u}_l(0) = 0$.

From the above equations, one obtains the corresponding first order, non-linear differential equations

$$\delta_l'(r) = -k^{-1}V(r)[\cos\delta_l(r)\hat{f}_l(kr) - \sin\delta_l(r)\,\hat{n}_l(kr)]^2, \tag{11}$$

$$\gamma_l'(r) = -k^{-1}\left[\frac{l(l+1)}{r^2} + V(r)\right]\sin^2[kr + \gamma_l(r)], \tag{12}$$

$$\beta_l'(r) = -k^{-1}\frac{l(l+1)}{r^2}\sin^2[kr + \beta_l(r)], \tag{13}$$

with accompanying boundary conditions $\delta_l(0) = \gamma_l(0) = \beta_l(0) = 0$ and $\gamma_l'(0) = \beta_l'(0) = -kl/(l+1)$. Since $\delta_l(r)$ is the phase function associated with the potential $V(r)$ and leads asymptotically to the phase shift δ_l, inspection of Eqs. (11)–(13) suggests that $\gamma_l(r)$ is the phase function of the full effective potential $V(r) + l(l+1)/r^2$, and that $\beta_l(r)$ is the phase function of the angular momentum barrier $l(l+1)/r^2$. Thus, further, one might expect $\gamma_l(r)$ and $\beta_l(r)$ to lead asymptotically to a "total" phase shift γ_l and an "angular-momentum-barrier" phase shift β_l. This is, in fact, the case in the scattering region ($E > 0$), but such an interpretation is unclear in the bound-state region ($E < 0$), as is discussed in detail in Sections IV and V.

Finally, the following expressions for the phase functions in terms of the wave functions are useful in later discussion:

$$\delta_l(r) = \tan^{-1}\left\{\frac{\hat{j}_l(kr)\,u_l'(r) - k\hat{j}_l'(kr)\,u_l(r)}{\hat{n}_l(kr)\,u_l'(r) - k\hat{n}_l'(kr)\,u_l(r)}\right\}, \tag{14}$$

$$\gamma_l(r) = \tan^{-1}\left\{\frac{ku_l(r)\cos kr - u_l'(r)\sin kr}{ku_l(r)\sin kr + u_l'(r)\cos kr}\right\}, \tag{15}$$

$$\beta_l(r) = \tan^{-1}\left\{\frac{\hat{j}_l(kr)\cos kr - \hat{j}_l'(kr)\sin kr}{\hat{j}_l(kr)\sin kr + \hat{j}_l'(kr)\cos kr}\right\}. \tag{16}$$

Note that $\hat{j}_l(kr)$ in (16) is just the $\bar{u}_l(r)$ of (9), (10), since $j_l(kr)$ is the solution of the radial Schrödinger equation with $V(r) = 0$ and $\bar{u}_l(0) = 0$.

III. Phase Shifts in the Scattering Region ($E > 0$)

In this section we give the three main phase-function calculational techniques for obtaining the phase shift δ_l in the positive energy, scattering region [1].

For $E > 0$ (and $l > 0$), Calogoro shows that the amplitude and phase functions all have well-defined limits as $r \to \infty$. Using the differential equations (11)–(13) together with their respective boundary conditions, one finds that δ_l is a real constant (the value of which depends, of course, upon $V(r)$), and that

$$\beta_l \equiv \lim_{r\to\infty} \beta_l(r) = -\tfrac{1}{2}l\pi, \tag{17}$$

$$\gamma_l \equiv \lim_{r\to\infty} \gamma_l(r) = -\tfrac{1}{2}l\pi + \delta_l. \tag{18}$$

Results (17), (18) may also be obtained by using the asymptotic forms of $u_l(r)$ and $j_l(kr)$ and their derivatives in expressions (15) and (16). The fact that $\beta_l = -\frac{1}{2}l\pi$ and $\gamma_l = -\frac{1}{2}l\pi + \delta_l$ lends credence to the interpretation of β_l and γ_l as the angular-momentum barrier and total phase shifts, respectively, given in Section II; see also Eq. (3).

Thus, immediately, one has two techniques for calculating δ_l: (i) integrate (11) from $r = 0$ to $r = \bar{r}$ such that $V(r) \simeq 0$ for $r > \bar{r}$. Then from (11) it is clear that $\delta_l(r)$

does not change appreciably beyond $\bar{r}$ and one can use (6) to get δ_l: $\delta_l \simeq \delta_l(\bar{r})$ to a high order of accuracy; (ii) integrate (12) from $r=0$ to $r=\bar{\bar{r}}$ such that $V(r)+l(l+1)/r^2 \simeq 0$ for $r > \bar{\bar{r}}$. Then (12) shows that $\gamma_l(r)$ does not change appreciably beyond r and one can use (18) to get δ_l: $\gamma_l = -\frac{1}{2}l\pi + \delta_l \simeq \gamma_l(\bar{\bar{r}})$, again to a high order of accuracy. Methods (i) and (ii) both work for phase shift computations; however, method (i) requires the evaluation of the Ricatti–Bessel functions at each step of the integration, which is very costly especially in the cases of non-integral and complex l, and method (ii) requires integration out to very large $\bar{\bar{r}}$ because $l(l+1)/r^2$ falls off so slowly; this also is impractical in many cases.

There is a combined method (which we call method (iii)) which contains the computational virtues of methods (i) and (ii), but not their weakness: (iii) integrate (12) from $r=0$ to $r=\bar{r}$ such that $V(r) \simeq 0$ for $r > \bar{r}$. To a high order of accuracy the phase shift is then given by $\delta_l \simeq \delta_l(\bar{r})$, where

$$\delta_l(\bar{r}) = \tan^{-1}\left\{ \frac{\cos[k\bar{r}+\gamma_l(\bar{r})]\,\hat{j}_l(k\bar{r}) - \sin[k\bar{r}+\gamma_l(\bar{r})]\,j_l'(k\bar{r})}{\cos[k\bar{r}+\gamma_l(\bar{r})]\,\hat{n}_l(k\bar{r}) - \sin[k\bar{r}+\gamma_l(\bar{r})]\,\hat{n}_l'(k\bar{r})} \right\}. \tag{19}$$

(Equation (19), which is exact for all $\bar{r}$, follows from (7), (8), and (14).) Thus, in method (iii) one does not integrate a long way and one evaluates the Ricatti–Bessel functions only once; this method is a fast and accurate method for the numerical computation of γ_l in the scattering region ($E > 0$).

IV. The Bound-State Region ($E < 0$): $\beta_l(r)$

The formalism and computational procedures summarized in the previous two sections require reexamination when applied in the bound-state, negative energy region. As an illustration of the "problem" that occurs, we consider in this section the angular-momentum phase function $\beta_l(r)$ for $E < 0$.

In Section III, we noted for $E > 0$ that $\beta_l \equiv \lim_{r\to\infty} \beta_l(r) = -\frac{1}{2}l\pi$. For $E < 0$ however, $k = i\kappa$ (κ real, >0 and $E = k^2 = -\kappa^2$), and inspection of (13) shows that $\beta_l(r)$ tends to $-i\infty$ as $r \to \infty$; i.e., $\beta_l(r)$ is unbounded because $l(l+1)/r^2$ does not decrease fast enough to subdue the exponential increase of $\sin^2[i\kappa r + \gamma_l(r)]$. Thus, the result $\beta_l = -\frac{1}{2}l\pi$ obtained and easily interpreted for $E > 0$ does not appear to hold for $E < 0$, at least according to (13). On the other hand, use of the asymptotic approximation [1, 3]

$$\hat{j}_l(kr) \xrightarrow[|kr|\to\infty]{} \sin(kr - \tfrac{1}{2}l\pi), \qquad |kr| \gg l \tag{20}$$

(which is good for complex kr) in (16) yields $\beta_l = \lim_{r\to\infty} \beta_l(r) = -\frac{1}{2}l\pi$. To summarize, for $E < 0$, (13) yields $\beta_l = -i\infty$, while (16) apparently yields $\beta_l = -\frac{1}{2}l\pi$. Thus, two questions are raised: first, since (13) and (16) are equivalent, why do they appear to yield different results for β_l for $E < 0$?, and second, if (13) is correct and $\beta_l(r)$ really does tend to $-i\infty$ for $E < 0$, what is the meaning of $\beta_l(r)$ for negative energies?

To begin, the contradiction between (13) and (16) on the value of β_l is only apparent; both expressions actually agree and give $\beta_l = -i\infty$ for $E < 0$. This can be seen by noting that, while (20) is indeed correct, Eq. (16) is a particularly delicate combination of solutions, and more terms are required in the asymptotic approximation for $\hat{f}_l(kr)$. With additional terms included, (20) becomes [1, 3]

$$\hat{f}_l(kr) = \sin(kr - \tfrac{1}{2}l\pi) + \frac{A_1}{kr}\cos(kr - \tfrac{1}{2}l\pi) + \frac{A_2}{(kr)^2}\sin(kr - \tfrac{1}{2}l\pi) + \cdots, \tag{21}$$

valid for $|kr| \to \infty$ ($A_1 = \frac{1}{8}(4(l+\frac{1}{2})^2 - 1)$, $A_2 = \frac{1}{16} \cdot A_1 \cdot (4(l+\frac{1}{2})^2 - 9)$). We now use (21) in (16), which yields the asymptotic expression for $\beta_l(r)$ (valid for $|kr| \to \infty$):

$$\beta_l(r) = \tan^{-1}\left\{\frac{\sin(-\frac{1}{2}l\pi) + [A_1/(kr)^2]\cos(kr - \frac{1}{2}l\pi)\sin kr + \cdots}{\cos(-\frac{1}{2}l\pi) - [A_1/(kr)^2]\cos(kr - \frac{1}{2}l\pi)\cos kr + \cdots}\right\}. \tag{22}$$

This expression is valid for both our cases, and yields immediately

$$\begin{aligned} \beta_l &= -\tfrac{1}{2}l\pi \qquad \text{for } E > 0, \quad k = k, \\ \beta_l &= -i\infty \qquad \text{for } E < 0, \quad k = i\kappa. \end{aligned} \tag{23}$$

Thus, (13) and (16) agree on β_l for $E < 0$.

Before turning to the question of the physical meaning of β_l and $\beta_l(r)$ for $E < 0$, we discuss why β_l is infinite for negative energies. If we consider, e.g., motion under a simple Yukawa potential of the form $V(r) = -ge^{-\mu r}/r$, then, as is well known [2], the phase shift δ_l is meromorphic in a strip of the k plane given by $|\operatorname{Im} k| < \mu/2$. This can be seen, e.g., in Eq. (11), where the right-hand side contains terms of the form $e^{-\mu r} \cdot e^{2|\operatorname{Im} k|r}$ which are non-vanishing for large r unless $|\operatorname{Im} k| < \mu/2$. The same phenomenon is at work in the $\beta_l(r)$ equation (13) except that in (13), $l(l+1)/r^2$ vanishes so slowly that it can never subdue $e^{2|\operatorname{Im} k|r}$ unless $\operatorname{Im} k = 0$. Thus, in the case of the angular-momentum phase function $\beta_l(r)$ considered here, the strip in which β_l is finite and equal to $-\frac{1}{2}l\pi$ has zero width, i.e., consists only of the real-k axis. This explains result (23).

What is the physical meaning of the angular-momentum phase function $\beta_l(r)$ and phase shift β_l in view of the above discussion, especially Eq. (23)? First, if β_l is interpreted as the "angular-momentum-barrier phase shift," it is clear that the angular-momentum barrier causes the usual phase shift $-\frac{1}{2}l\pi$ for real k and an infinite phase shift for k complex. On the other hand, if the phase shift due to the angular-momentum barrier is defined from the argument of the wave function for large r as in (20), then this phase shift is $-\frac{1}{2}l\pi$ for all values of k. Thus, one may conclude that the interpretation of $\beta_l = \lim_{r\to\infty}\beta_l(r)$ as the "angular-momentum-barrier phase shift" is unclear, at least for negative energies.

In spite of the ambiguities in the meaning of β_l for $E < 0$, the phase function $\beta_l(r)$ remains a well-defined object. Expressions (9), (10), (13), and (16) are all valid for complex k, and may, in certain circumstances, be useful. This is shown in the next section for $\gamma_l(r)$, which is closely related to $\beta_l(r)$ and has many of the same characteristics.

V. The Bound-State Region: Calculation of the Phase Shift δ_l from $\gamma_l(r)$

Which of the three phase-function methods given in Section III for $E > 0$ are available for the calculation of the phase shift δ_l in the bound-state, negative energy region? First, method (i), based on the phase-function differential equation for $\delta_l(r)$, remains valid for $E < 0$. As discussed and used by Calogero, method (i) is a powerful tool for theoretical analyses of the character of the phase shift. However, for the numerical calculation of δ_l method (i) is exceedingly slow, especially for non-integral values of l where the computation of $\hat{j}_l(kr)$ and $\hat{n}_l(kr)$ is more difficult. Second, what is the validity of method (ii) in the $E < 0$ region? Method (ii) is based on the use of $\gamma_l = -\frac{1}{2}l\pi + \delta_l \simeq \gamma_l(\bar{r})$, where $\gamma_l(\bar{r})$ is found by integrating the $\gamma_l(r)$ differential equation (12). But now it is clear from (12) that (exactly as in the $\beta_l(r)$ case for $E < 0$ and for the same reasons) $\gamma_l \equiv \lim_{r\to\infty} \gamma_l(r) = -i\infty$ and so for $E < 0$, $\gamma_l \neq -\frac{1}{2}l\pi + \delta_l$ and cannot be used. Thus, method (ii) is not valid in the negative energy region. Finally, what about method (iii) for $E > 0$; does it remain useful? Since method (iii) is also based on the "total" phase function $\gamma_l(r)$ one might expect it to fail for $E > 0$ just as did method (ii); interestingly enough, however, it does not fail as we now show.

As discussed in Sections II and III, method (iii) is based on expressions (7), (8), (12), (15), and (19). All of these equations remain valid for $E < 0$, and so method (iii) remains a correct procedure for calculating the phase shift δ_l in the bound-state region. This statement is true despite the fact that $\gamma_l(r) \to_{r\to\infty} -i\infty$ when k has a non-zero imaginary part as it does for $E < 0$. As for the $E > 0$ case, one uses $\delta_l \simeq \delta_l(\bar{r})$, where $\delta_l(\bar{r})$ is given by (19), and $\gamma_l(\bar{r})$ follows from integrating (12). This calculation gives δ_l to a high order of accuracy provided, of course, that $\bar{r}$ is chosen such that $V(r) \simeq 0$ for $r > \bar{r}$ as before. In addition, as discussed in Section IV, for complex k one must keep $|\mathrm{Im}\, k| < \mu/2$ (where μ is the potential range parameter as, e.g., in $V(r) = -ge^{-\mu r}/r$) in order that δ_l remain defined by method (iii) [2].

The expressions for $\gamma_l \equiv \lim_{r\to\infty} \gamma_l(r)$ analogous to (23) for β_l are

$$\begin{aligned} \gamma_l &= -\tfrac{1}{2}l\pi + \delta_l \qquad \text{for } E > 0, \quad k = k, \\ \gamma_l &= -i\infty \qquad\qquad \text{for } E < 0, \quad k = i\kappa. \end{aligned} \tag{24}$$

Thus, like β_l, γ_l has a finite value only on the real-k axis, and this is true for the same reason as that in the β_l case, namely, that the $l(l+1)/r^2$ term cannot subdue the $e^{2|\mathrm{Im}k|r}$ terms in (12).

From the discussion in Sections II and III it appeared that a reasonable interpretation of $\gamma_l(r)$ and γ_l is a "total" phase function and "total" phase shift, respectively. Now, however, as in the case of β_l for $E < 0$, Eq. (24) casts doubt on the aptness of the name "total phase shift" for γ_l, at least for negative energies.

Apart from the general interest of having a second method for the calculation of δ_l, the main justification for presenting method (iii) for use in the bound-state region is that, when used on a computer, method (iii) is between one and two orders of magnitude faster than method (i); this statement is true for both $E < 0$ and $E > 0$, and is especially true for non-integral l. This means that in practical calculations a given problem may be soluble using method (iii) and insoluble using method (i). Numerical examples of complex angular-momentum trajectories derived from phase shifts calculated using method (iii) are shown in Ref. [4]; selected phase shifts are shown also in this reference. Extensive numerical illustrations of scattering phase shifts for various potentials are shown in Ref. [5]; these phase shifts are calculated using method (iii) for both positive and negative energies.

In conclusion, methods (i), (ii), and (iii) of Section III can be used to calculate the scattering phase shift δ_l in the scattering region $E > 0$, while only methods (i) and (iii) can be used in the bound-state region $E < 0$. Method (i) is conceptually cleaner than method (iii), while method (iii) is as much as several orders of magnitude faster than method (i) when both are used on a computer.

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