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Numerical computation of scattering phase shifts for a screened Coulomb potential

J P Klozenberg

Mullard Research Laboratories, Redhill, Surrey RH1 5HA, UK

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Abstract. The theory of the phase equation for elastic scattering, with spherical symmetry, is applied to the problem of evaluating efficiently the scattering phase shifts in a partial-wave analysis. A fortran source version of the subroutine is available from the author.

1. Introduction

The problem of scattering of charged particles from a single fixed scattering centre is one which often arises in semiconductor physics. If it is assumed that the scattering is elastic then the force experienced by a particle due to the influence of the scattering centre may be represented by a potential $V(r)$. In the spherically symmetric case considered in this paper, V then depends only on the radial distance r in a system of spherical coordinates r, θ, ϕ with origin at the scattering centre.

The fortran program PHASE which has been written to solve this scattering problem requires the following potential function:

$$V(r) = \begin{cases} -V_1 \dfrac{\lambda}{r} e^{-r/\lambda} & r > \rho_0 \\ -V_0 & r < \rho_0. \end{cases} \tag{1}$$

The method of partial waves (Mott and Massey 1949) is used. This assumes that the wavefunction ψ_k has the expansion

$$\psi_k(r, \theta) = \sum_{l=0}^{\infty} a_l(k) \mathrm{P}_l(\cos\theta) \frac{u_{l,k}(r)}{r} \tag{2}$$

where P_l is the Legendre polynomial of order l and the radial wavefunction $u_{l,k}(r)$ satisfies the equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + k^2 - \frac{2\mu}{\hbar^2} V(r) \right) u_{l,k} = 0 \tag{3}$$

where $k^2 = 2\mu E/\hbar^2$. As $r \to \infty$ the solutions of equation (3) have the asymptotic form

$$u_{l,k} \sim \sin(kr - \tfrac{1}{2}\pi l + \delta_l) \tag{4}$$

where the phase shift δ_l is a function of k. Integration of the radial wave equation to a distance where the asymptotic form (4) is valid is time consuming (Blatt 1957). The

subroutine PHASE uses a different method (Kynch 1952) which is described in the following section. It gives a much faster computation than direct integration of the radial wave equation.

2. The phase equation

The solutions of the radial wave equation (3) when $V = 0$ are the Ricatti–Bessel functions (Abramowitz and Stegun 1965) $j_l(kr)$ and $n_l(kr)$.

We introduce two new functions S_l, a_l by writing

$$u_l = (j_l + S_l n_l) a_l \tag{5}$$

and impose the condition

$$j_l \frac{da_l}{dr} + n_l \frac{d}{dr}(S_l a_l) = 0. \tag{6}$$

This we are free to do because, given u_l and S_l (or a_l), then a_l (or S_l) is uniquely determined. Then

$$\frac{du_l}{dr} = \left(\frac{dj_l}{dr} + S_l \frac{dn_l}{dr}\right) a_l \tag{7}$$

(the suffix k on u_l has been dropped for convenience) and when substituted into (3) we get the phase equation:

$$\frac{dS_l}{dr} = -\frac{2\mu V}{\hbar^2 k}(j_l + S_l n_l)^2. \tag{8}$$

We have used the Wronskian relation

$$j_l \frac{dn_l}{dr} - n_l \frac{dj_l}{dr} = \frac{1}{k} \tag{9}$$

in deriving equation (8). Equation (8) is useful because we can establish the following asymptotic result:

$$\lim_{kr \to \infty} S_l(kr) = \tan \delta_l. \tag{10}$$

This may be deduced from the following equation:

$$\frac{da_l}{dr} + \frac{2\mu}{\hbar^2} u_l n_l V = 0 \tag{11}$$

and the resulting asymptotic relation

$$a_l(kr) \to \text{constant} \qquad \text{as } kr \to \infty \tag{12}$$

together with the asymptotic forms

$$\begin{aligned} j_l(kr) &\sim \sin(kr - \tfrac{1}{2}\pi l) \\ n_l(kr) &\sim \cos(kr - \tfrac{1}{2}\pi l). \end{aligned} \tag{13}$$

Comparison of equations (5) and (4) then leads to equation (10).

Naturally $\delta_l(kr)$ is called the phase function and equation (8) the phase equation. The method was first discussed in the literature by Morse and Allis (1933) for S-wave scattering. Provided the potential function falls off reasonably rapidly with distance equation (8) may be integrated much more quickly than the wave equation to the point where the limiting form (equation (10)) is obtained to within a prescribed accuracy.

3. Numerical integration of the phase equation

Summary

To simplify the mathematics a set of dimensionless variables is defined in § 3.1. Because the function evaluations can be expensive a predictor–corrector method was chosen for the numerical integration of the phase equation. The non-stiff part of Gear's program DIFSUB (Gear 1971) was used for this purpose.

In § 3.2 the problem of the phase function passing through singularities at odd multiples of $\frac{1}{2}\pi$ is discussed and the method of Calogero (1963) is described.

To evaluate Ricatti–Bessel functions j_l backward recursion is required if large l values are to be treated. For this purpose the Harwell subroutine FF05A (Hopgood 1971), with slight modification, has been incorporated into subroutine PHASE. It implements the algorithm of Corbató and Uretsky (1959) as well as generating the function n_l. For small values of the independent variable r the functions j_l and n_l can give rise to underflow and overflow respectively. Normalized functions $\hat{j}_l$ and $\hat{n}_l$ are defined to overcome this problem and the phase function correspondingly transformed. These topics are covered in § 3.3. To start the integration initial values of the function S_l are required. This part of the problem is treated briefly in § 3.4.

3.1. Dimensionless equations

A scaling length a is defined in terms of the shielded potential:

$$\frac{1}{a^2} = \frac{\mu V_1}{\hbar^2}. \tag{14}$$

Dimensionless variables, denoted by a bar are then

$$\begin{aligned} \bar{r} &= r/a \\ \bar{\lambda} &= \lambda/a \\ \bar{k} &= ka \\ \bar{E} &= 2E/V_1 \end{aligned} \tag{15}$$

so that $\bar{E} = \bar{k}^2$. The potential has the form

$$\bar{V}(\bar{r}) = \begin{cases} -2\dfrac{\bar{\lambda}}{\bar{r}} e^{-\bar{r}/\bar{\lambda}} & \bar{r} > \rho_0/a \\ -2\dfrac{V_0}{V_1} & \bar{r} < \rho_0/a. \end{cases} \tag{16}$$

For convenience the variable $t = \bar{k}\bar{r}$, ie $t = kr$ is used in the subroutine.

This gives the standard Ricatti–Bessel form for the wave equation when the potential vanishes. Equation (3) then becomes

$$\left(\frac{d^2}{dt^2}-\frac{l(l+1)}{t^2}+1-\frac{\overline{V}(t)}{k}\right)u_l = 0 \tag{17}$$

and equation (8) becomes

$$\frac{dS_l}{dt} = -\frac{\overline{V}(t)}{k}(j_l+S_l n_l)^2 \tag{18}$$

3.2. Singularities of the phase equation

If the phase function $\delta_l(t)$ is considered as the dependent variable then by substituting

$$S_l(t) = \tan(\delta_l(t))$$

in equation (18) we get

$$\frac{d\delta_l}{dt} = -\frac{\overline{V}(t)}{k}(j_l\cos\delta_l+n_l\sin\delta_l)^2\,. \tag{19}$$

For the potential given by (1) $\delta_l(t)$ is in fact an increasing function of t. For strong potentials it is therefore possible for δ_l to pass many times through odd integer multiples of $\frac{1}{2}\pi$. At such points $S_l \to \infty$ and numerical integration of equation (18) is not possible. Numerical tests show, however, that integration of equation (19), which has no such singularities, takes twice as long as for equation (18). This is because of the additional cost in function evaluations arising from the cos δ_l and sin δ_l terms. For greater efficiency the method of Calogero (1963) has been implemented in PHASE. Integration of equation (18) is interrupted when $|S_l| > 1$. A simple change of dependent variable is made

$$\tilde{S}_l = 1/S_l \tag{20}$$

and the transformed equation

$$\frac{d\tilde{S}_l}{dt} = -\frac{\overline{V}(t)}{k}(j_l\tilde{S}_l+n_l)^2 \tag{21}$$

is integrated from the change-over point. When a further stage is reached at which $|\tilde{S}_l| > 1$ the reverse technique is used.

3.3. Normalized functions

When $t \ll 1$ the value of n_l may be large enough to cause overflow for moderate l. In addition the phase equation has a singularity of order l at $t = 0$. To overcome these difficulties normalized Riccati–Bessel functions are computed when $t < 1$:

$$\begin{aligned}\hat{j}_l &= j_l/t^{l+1}\\ \hat{n}_l &= n_l t^l.\end{aligned} \tag{22}$$

Normalized dependent variables to replace S_l and $\tilde{S}_l$ are then introduced as follows:

$$\hat{S}_l = S_l/t^{2l+1}$$
$$\hat{\tilde{S}}_l = \tilde{S}_l t^{2l+1} \tag{23}$$

so that $\hat{\tilde{S}}_l = 1/\hat{S}_l$.

The phase equations are then respectively

$$\frac{d\hat{S}_l}{dt} = -\frac{2l+1}{t}\hat{S}_l - \frac{t\bar{V}}{k}(\hat{j}_l + \hat{S}_l\hat{n}_l)^2 \tag{24}$$

and

$$\frac{d\hat{\tilde{S}}}{dt} = \frac{2l+1}{t}\hat{\tilde{S}} + \frac{t\bar{V}}{k}(j_l\hat{\tilde{S}} + n_l)^2 . \tag{25}$$

The last two equations now have only first-order singularities at $t = 0$. The modification to the Harwell subroutine required to generate $\hat{j}_l, \hat{n}_l$ is easily implemented, especially when it is observed that $t < 1$ lies above the transition line for all l values. The phase equations (18), (21), (24) and (25) cover all the cases we shall need.

3.4. Initial values of S_l

The case $\rho_0 > 0$ is easy to deal with because the wave equation can be solved in terms of the regular Ricatti–Bessel function. When $\rho_0 = 0$ a power series solution is required.

3.5. Programming details

Integration of the phase equation is made in steps of $2\bar{\lambda}\bar{k}$ (in dimensioned quantities $2\lambda k$). After two steps have been computed the relative differences are tested for each l value and when these become smaller than the predetermined relative accuracy EPS the limiting values of δ_l ($l = 0$ to $L_{\max}$) are returned to the calling program. In practice EPS = 0·01 gives 0·01 relative accuracy in δ_l over the range of parameters tested, $0 < \lambda \lesssim 2$, $10^{-3} \leqslant \bar{E} \leqslant 10^3$ ($0 \leqslant l \leqslant 20$). If the starting point t is less than unity (this always occurs if $\rho_0 = 0$) then integration is halted within the subroutine at $t = 1$ and automatically restarted with the initial values computed at $t = 1$. This method is necessary because the phase equation has been transformed for $t < 1$ giving in effect a discontinuity at $t = 1$.

The subroutine has been written for values of $L_{\max} \leqslant 20$ but this restriction can easily be removed. If $\rho_0 > 0$ the user may replace the shielded potential $V_1 e^{-r/\lambda}\lambda/r$ by any other non-negative function of r/λ where λ is a positive parameter. Only one line of the program need be changed and this is clearly indicated in the source listing.

4. Results

To give some idea of the way in which the phase $\delta_l(t)$ depends on the dimensionless distance t we show the results in figure 1 of the step-by-step integration of the phase equation (18) with $l = 0$, 1 and 2 for $\bar{E} = 50$, $\bar{\lambda} = 1$, $\rho_0 = 0$. The steep gradients at small distances, and less importantly the oscillatory behaviour, means that the program spends most of its computing time reaching the point $t = 15$. The relatively larger distance

over which $\delta_l(t)$ for $l = 0, 1, 2$ tend to their constant values takes proportionately much less computing time, for in this region the function $\delta_l(t)$ is obviously uncomplicated enabling larger integration steps to be taken. In figure 2 the phase shift δ_l is shown as a function of energy for $l = 0, 1, 2$ for $\bar{\lambda} = 0{\cdot}5$, $\rho_0 = 0$.

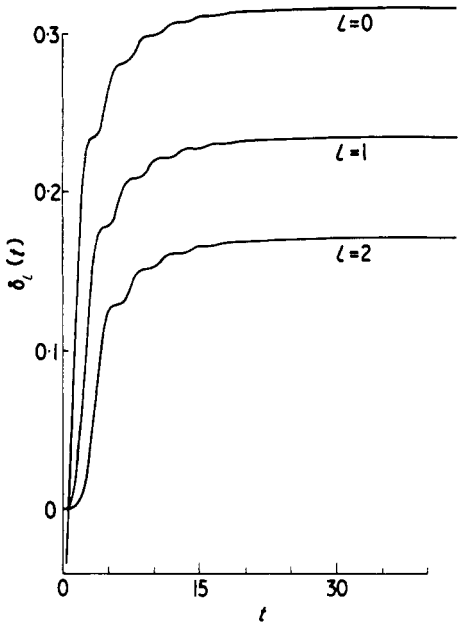

Figure 1. The phase function $\delta_l(t)$ for $l = 0$, 1 and 2 for $\bar{\lambda} = 1$, $\bar{E} = 50$.

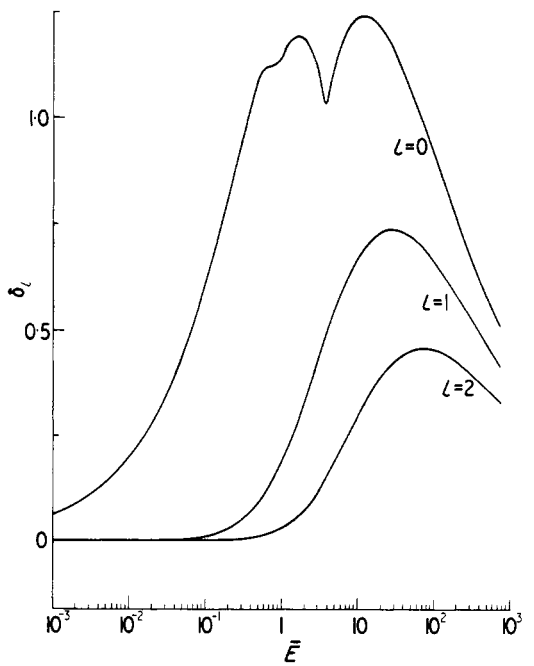

Figure 2. The phase shift δ_l as a function of energy for $l = 0$, 1 and 2; $\bar{\lambda} = 0{\cdot}5$.

In table 1 below we give the computer time taken, for 10 equally spaced energies in the range $0{\cdot}1 < \bar{E} < 1$ for the case $\bar{\lambda} = 1$ to evaluate $\delta_l(l = 0 \text{ to } L_{max})$.

Table 1.

L_{max}	Time (s)	Time per L value (s)
2	9	0·30
4	16	0·32
10	50	0·45
20	150	0·71

The timings are for the 1904A using a program compiled in an optimized mode (compiler XFEW MK 3B). (The user should note carefully the fact that on the above machine for our program optimized code runs at least twice as fast as non-optimized code.)

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