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A note on calculation of the potential from scattering phase shifts

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Abstract. An improvement is suggested for calculating the potential from scattering phase shifts using the general equations of inverse scattering theory. It is shown that all the necessary coefficients which eventually determine the potential can in principle be obtained from a lesser number of significant phase shifts. The resulting improvement in practical calculation is shown by examples.

1. Introduction

Newton (1962) first developed a theory for determining the potential from a knowledge of phase shifts at a given energy. Since then, this inverse scattering problem at fixed energy has been studied extensively (Newton 1966, Chadan and Sabatier 1977). Sabatier and Quyen Van Phu (1971) gave a numerical method for the calculation of the potential. Quite a number of numerical tests have also been performed. Sabatier's procedure was improved upon by Coudray (1977) and was applied to the case of complex optical potentials as well. Munchow and Scheid (1980) have recently suggested a modified form of the Newton–Sabatier method. This has the advantage that the information given by the phases is fully and optimally used to reproduce the potential. Usually the number of coefficients b_l which go to determine this potential is the same as the number of partial waves included in the initial data. In this report we show how to calculate all the coefficients, b_l, from the smaller number of known significant phase shifts. By including more coefficients a better approximation to the original potential can be obtained. The deduction of relevant equations for the higher coefficients is straightforward and no further assumptions appear to be necessary. However, in practice, the largest number of coefficients that can be reliably calculated numerically depends on the capacity of the computer to invert the required matrices.

2. Conventional method

In a rationalised form the radial Schrödinger equation can be expressed as

$$D(\rho)\phi_l(\rho) = l(l+1)\phi_l(\rho) \tag{1}$$

where

$$D(\rho) = \rho^2[\mathrm{d}^2/\mathrm{d}\rho^2 + 1 - U(\rho)], \qquad \phi_l(\rho) = rR_l(r),$$
$$\rho = (2\mu E/\hbar^2)^{1/2} r = kr, \qquad U(\rho) = V(r)/E.$$

Let $\phi_l^{(0)}(\rho)$ be the wavefunction when the potential is zero. The Schrödinger equation

$$\rho^2[d^2/d\rho^2+1]\phi_l^{(0)}(\rho)=l(l+1)\phi_l^{(0)}(\rho) \tag{2}$$

has the regular solutions

$$\phi_l^{(0)}(\rho)=F_l(\rho)=\rho j_l(\rho). \tag{3}$$

In the presence of the unknown potential U, the large distance behaviour of (1) determines the phase shifts. Let R be the range of this potential and k the centre of mass momentum, so that $\rho_0=kR$ is the effective distance over which the potential has appreciable effect. For distances $\rho \gg \rho_0$ the wavefunction is

$$\phi_l(\rho)=A_lT_l(\rho)=A_l[\cos\delta_lF_l(\rho)+\sin\delta_lG_l(\rho)]. \tag{4}$$

$F_l(\rho)$ and $G_l(\rho)$ are the regular and irregular solutions of (2). The coefficients A_l are the unknown quantites to be determined.

For solving inverse scattering problems Newton (1962) has defined a kernel

$$K(\rho,\rho')=\sum_{l=0}^{\infty}C_l\phi_l(\rho)\phi_l^{(0)}(\rho') \tag{5}$$

which turns out to be the solution of the Gel'fand–Levitan linear integral equation

$$K(\rho,\rho')=g(\rho,\rho')-\int_0^{\rho}d\rho''\,\rho''^{-2}K(\rho,\rho'')g(\rho'',\rho') \tag{6}$$

where

$$g(\rho,\rho')=\sum_{l=0}^{\infty}C_l\phi_l^{(0)}(\rho)\phi_l^{(0)}(\rho'). \tag{7}$$

This integral equation is uniquely satisfied by defining the potential as

$$U(\rho)=-(2/\rho)(d/d\rho)(\rho^{-1}K(\rho,\rho)). \tag{8}$$

The Schrödinger wavefunctions then satisfy the integral equation

$$\phi_l(\rho)=\phi_l^{(0)}(\rho)-\int_0^{\rho}d\rho'\,\rho'^{-2}K(\rho,\rho')\phi_l^{(0)}(\rho'). \tag{9}$$

Substituting (5) in the above equation we get a coupled system of equations, namely

$$\phi_l(\rho)=\phi_l^{(0)}(\rho)-\sum_{l'=0}^{\infty}C_lL_{ll'}(\rho)\phi_{l'}(\rho) \tag{10}$$

where the matrix $L_{ll'}$ is

$$L_{ll'}(\rho)=\int_0^{\rho}\phi_l^{(0)}(\rho')\phi_{l'}^{(0)}(\rho')\frac{d\rho'}{\rho'^2}.$$

Equivalently (10) can be written as

$$\sum_{l=0}^{\infty}[\delta_{ll'}T_{l'}(\rho)A_{l'}+L_{ll'}(\rho)T_{l'}(\rho)b_{l'}]=\rho j_l(\rho) \tag{11}$$

where we have abbreviated $b_l=C_lA_l$. Knowing the coefficients from equations (11), the kernel $K(\rho,\rho)$ and the potential are obtained from (5) and (8) respectively.

In potential problems the number of significant phase shifts is roughly $L \simeq kR$. Normally the phase shifts become negligibly small at a partial wave somewhat higher than L. In earlier work, Munchow and Scheid (1980) limited the l' summation in (11) to L. But several values of ρ were used, which actually overdetermines the solutions. The solutions are then optimised by a standard procedure (Pipes and Harvill 1970). The resulting M becomes a matrix of dimensionality $2(L+1)$ columns and $N(L+1)$ rows. The coefficients $(\{A_l \ldots\}, \{b_l \ldots\})$ are determined from the relation

$$X = (\{A_l \ldots\}, \{b_l \ldots\}) = (M^+ M)^{-1} M^+ F,$$

where M^+ is the Hermitian adjoint matrix of M and F is a vector with $N(L+1)$ components where N is the number of ρ's and L is the number of partial waves.

However, the total number of coefficients C_l is only L. As a result the series for $K(\rho, \rho)$ of (5) is truncated at this point. Unfortunately the coefficients C_{L+1}, $C_{L+2} \ldots$ are not small, even for a case where the reference potential is zero. This has been demonstrated by Sabatier (1966). As the higher coefficients are not zero, truncation of the series for $K(\rho, \rho)$ will not lead to a correct U. In § 3 we suggest how we can find the C_l's larger than $l > L$. The total number of coefficients will increase the number of terms in the series and the potential is more likely to reproduce the actual one and the correction ΔU to U will be considerably reduced.

3. Determination of higher coefficients

In this section we demonstrate how the higher A_l's and b_l's can also be calculated from the lower coefficients using the general theory. For simplicity let us write down (11) only for two radial distances ρ_1 and ρ_2. Then one can eliminate A_l from the two equations and get the simpler form

$$\sum_{l'=0}^{\infty} M_{ll'}(\rho_1, \rho_2) b_{l'} = \chi_l(\rho_1, \rho_2) \tag{12}$$

where

$$M_{ll'}(\rho_1, \rho_2) = T_l(\rho_2) L_{ll'}(\rho_1) T_{l'}(\rho_1) - T_l(\rho_1) L_{ll'}(\rho_2) T_{l'}(\rho_2)$$

and

$$\chi_l(\rho_1, \rho_2) = F_l(\rho_1) T_l(\rho_2) - F_l(\rho_2) T_l(\rho_1).$$

For

$$l \leqslant L,$$

$$\sum_{l'=0}^{L} M_{ll'} b_{l'} + \sum_{K=L+1}^{\infty} M_{lk} b_k = \chi_l \tag{13}$$

and by construction for $l > L$,

$$\sum_{l'=0}^{L} M_{kl'} b_{l'} + \sum_{k'=L+1}^{\infty} M_{kk'} b_{k'} = 0. \tag{14}$$

The important observation we make is that from (14) the coefficients for $l > L$, b_k can be obtained in terms of the coefficients for $l \leqslant L$, from

$$b_k = -\sum_{k'} \sum_{l'} (M^{-1})_{kk'} M_{k'l'} b_{l'}. \tag{15}$$

Then from (13) with the help of (14) we easily have

$$b_l = \sum_{l'} (H^{-1})_{ll'} \chi_{l'} \tag{16}$$

where

$$H_{ll'} = M_{ll'} - \sum_{k} \sum_{k'} M_{lk} (M^{-1})_{kk'} M_{k'l'}. \tag{17}$$

In (15)–(17), $(M^{-1})_{kk'}$ stands for the (k, k') element of the inverse of the matrix M, only in the subspace generated by the indices k and k', which are greater than L, but not that of the inverse of the whole matrix M of dimensionality $(L_{\max}+1)$. The coefficients from known phase shifts b_l, $l \leq L$ are calculated from (16) by inverting the matrix of dimensionality $(L+1)\times(L+1)$. The higher coefficients $b_k, k > L$ are then computed from (15) in terms of lower coefficients b_l by inversion of a matrix of dimensionality $(L_{\max}-L)\times(L_{\max}-L)$.

The upper limit L of the general method can thus be effectively pushed to larger values of L till $L_{\max}$, depending on the limitation of the computer. The equation for $\phi_l(\rho)$ takes the form

$$\phi_l(\rho) = \sum_{l'=0}^{L} [(1+LC)^{-1}]_{ll'} \left[\phi_{l'}^{(0)}(\rho) - \sum_{l''=L+1}^{L_{\max}} \rho L_{l'l''}(\rho) C_{l''} A_{l''} j_{l''}(\rho) \right] \qquad \text{for } 0 \leq l \leq L$$

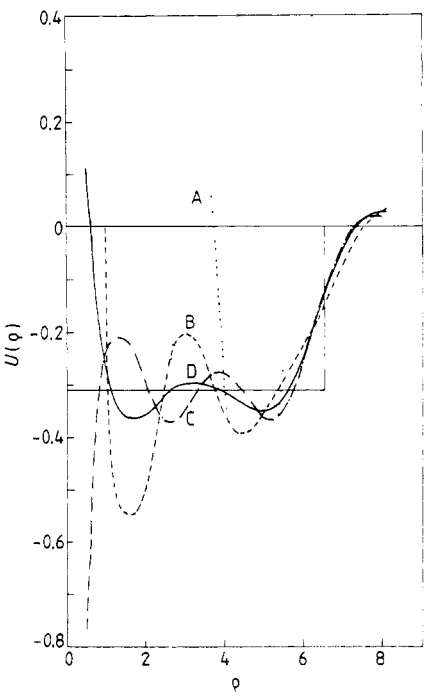

Figure 1. Calculation of potential with differing number of coefficients b_l; curves A, B, C, D represent the potential obtained by including 10, 14, 15, 16 coefficients respectively, at laboratory energy 55 MeV. $\rho_0 = 6.54$; $U_0 = -0.31$.

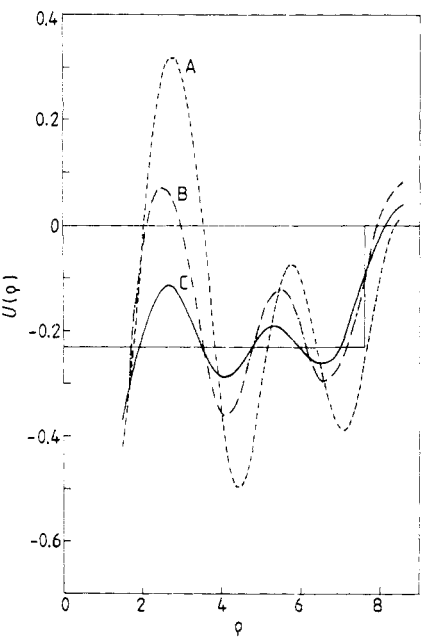

Figure 2. Calculation of potential with differing number of coefficients b_l; curves A, B, C represent the potential obtained by including 10, 14, 15 coefficients respectively at laboratory energy 75 MeV. The original square well potential is shown in the figures. $\rho_0 = 7.59$; $U = -0.2336$.

and for $l > L$

$$\phi_l(\rho) = A_l \rho j_l(\rho). \tag{18}$$

Knowing all the wavefunctions ϕ_l, the unknown potential is then calculated from (5) and (8).

4. Examples

To illustrate the improvement we choose a square well potential of depth -14 MeV with a range of five fermi, at laboratory energies 55 MeV and 75 MeV. In both cases the number of significant phase shifts is around ten.

From figures 1 and 2 it is easily seen that the reproduced potentials oscillate violently and are quite away from the expected square well. As soon as we include more than ten coefficients the oscillations stabilise around the square well. The numbers of additional coefficients are only four, five and six (due to the limitation of our existing computer IBM 1130). Significant improvement can easily be noticed. Thus we are convinced that such additional coefficients are needed for the determination of a more accurate potential without much addition of computer time.

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