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Generating phase-equivalent potentials

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Abstract. A perturbation-iteration scheme is employed to generate central potentials in an effort to reproduce the elastic scattering phase shifts for a few standard central potential models such as the square well, the perturbed Gaussian and the Woods-Saxon. A comparison is made with earlier work in which the Newton-Sabatier method was used.

1. Introduction

Recently a number of proposals have come forward aimed at providing straightforward, practical procedures for the solution of the fixed-energy quantum-mechanical inverse scattering problem. It has been demonstrated that, if the interaction potential falls off faster than $r^{-3/2}$ for increasing r, then a knowledge of all the phase shifts at a particular energy is sufficient to construct a unique scattering potential. Unfortunately in practice, one has only a limited knowledge of these phase shifts, and hence there are insufficient data to generate a unique potential. One is also plagued by the difficulty of numerically implementing the inversion procedure, such as that of Newton and Sabatier, with sufficient accuracy to obtain a unique potential.

In particular, three approaches have recently been applied to generate either real or optical model local potentials starting from a limited knowledge of the scattering phase shifts at fixed energy. Deo *et al* (1984) have improved on the now familiar Newton-Sabatier method by determining the necessary coefficients using a smaller number of phase shifts than in the original procedure. Kermode *et al* (1986) utilise a polynomial representation for the wavefunction in each partial wave, together with a variational approach, to generate the potentials. Finally, Ioannides and MacKintosh (1985) have carried out calculations using a perturbative iterative technique, as proposed by MacKintosh and Kobos (1979), to generate optical model potentials using phase shifts computed from known potentials. They have found that the procedure works very well at high energies with light projectiles.

Our objective in this brief study is to conduct a second test of the applicability of the iterative scheme proposed by Ioannides and MacKintosh (1985) to invert a limited set of phase shift data. We have assumed a local central field potential, describing the scattering of a neutron off an alpha particle at various energies. The iterative method is considerably simpler in implementation than the use of Fredholm determinants to solve the equations which arise in the Newton-Sabatier approach. The latter scheme was the focus of a study by Coudray (1977) to determine the ability of that approach to reproduce local potentials from which the input phase shifts were computed. Coudray observed that the inversion calculation worked well at high energies, but produced oscillating potentials at low energies.

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In implementing the iterative approach we have modified the procedure slightly by choosing different basis functions for the expansion, and by utilising a procedure which rapidly computes very accurate wavefunctions and phase shifts. This, we believe, leads to more reliable results.

2. Background

The perturbative iterative scheme is based on the evaluation of the difference between the phase shifts computed from two slightly different potentials. For example, from the work of Sugar and Blankenbecler (1964), if w and $\bar{w}$ are the radial wavefunctions associated with potentials v and $\bar{v}$ respectively, then the phase shifts δ_l and $\bar{\delta}_l$ are related through

$$\sin(\delta_l - \bar{\delta}_l) = -\left(\frac{\pi}{2k}\right) \int_0^\infty \bar{w}(v - \bar{v}) w \, \mathrm{d}r. \tag{1}$$

If the potentials v and $\bar{v}$ depend on parameters λ and $\bar{\lambda}$ with $|\bar{\lambda} - \lambda|$ very small, i.e.

$$v = v(\lambda, r) \qquad \bar{v} = v(\bar{\lambda}, r) \tag{2}$$

then

$$\frac{\mathrm{d}\delta_l}{\mathrm{d}\lambda} = -\left(\frac{\pi}{2k}\right) \int_0^\infty [w(\lambda)]^2 \frac{\partial v}{\partial \lambda} \, \mathrm{d}r. \tag{3}$$

Alternatively, by choosing two potentials v_0 and v_1 which are very close to each other, and by defining

$$v(\lambda) = v_0 + \lambda(v_1 - v_0) \tag{4}$$

with $v_1 \geqslant v_0$, the phase shifts for v_0 and v_1 are related through

$$\delta_l(\lambda = 1) - \delta_l(\lambda = 0) = -\left(\frac{\pi}{2k}\right) \int_0^\infty \mathrm{d}r \, w^2(v_1 - v_0). \tag{5}$$

The difference between the solutions w and $\bar{w}$ may be neglected in the integral. The effective result of this is that the partial-wave phase shift is linearly dependent on small corrections to the interaction potential. The iteration procedure is initiated by choosing a reference potential $V_0(r)$ and computing the associated phase shifts δ_l^0. A set of basis functions $v_i(r)$ are then chosen, and for each modified potential $V_0(r) + v_i(r)$, the corresponding set of phase shifts δ_l^i are also computed. A best set of inversion amplitudes λ_i are then obtained by inverting the linear set of equations

$$\delta_l = \delta_l^0 + \sum \lambda_i (\delta_l^i - \delta_l^0). \tag{6}$$

The number of active partial waves, N_l, is chosen to be larger than the number of basis functions, N_b, so that the least-squares inversion procedure of Dalquist and Bjorck (1974) can be utilised.

Once a set of λ_i have been generated a new reference potential is computed:

$$V(r) = V_0(r) + \sum_{i=1}^{N_b} \lambda_i v_i(r). \tag{7}$$

The process is then repeated until there is convergence, such that the generated phase shifts match the input set as closely as possible. As a measure of the fit we have chosen to compute

$$\sigma = \left(\sum_{l=0}^{N_l} |\delta_l - \delta_l^0|^2 \right)^{1/2}. \tag{8}$$

This iterative process requires accurate calculations of the phase shifts at each stage. In order to be able to provide this accuracy, we have chosen to employ the method of analytic continuation as introduced recently by Holubec and Stauffer (1985). In this approach the radial scattering equation is written

$$z^2 u'' + Q(z)u = 0 \tag{9}$$

where

$$Q(z) = -l(l+1) + k^2 z^2 - z^2 V(z). \tag{10}$$

The method is based on expanding $Q(z)$ in a Taylor series:

$$Q(z) = \sum Q_i z^i = \sum \tilde{Q}_i (z - z_0)^i. \tag{11}$$

The coefficients Q_i and $\tilde{Q}_i$ are determined explicitly for each potential $V(z)$, and the wavefunction u is obtained by analytically continuing a Frobenius series. The expansion about the origin (for the regular solution) is given by

$$u_l(z) = \sum a_i z^{i+r} \qquad \text{with } r = l+1 \tag{12}$$

whereas the expansion about z_0 is given by

$$u_l(z) = \sum c_i (z - z_0)^i. \tag{13}$$

The coefficients a_i and c_i are expressed in terms of the Q_i and $\tilde{Q}_i$, so that no numerical integration procedures are employed. The wavefunction is generated by starting at the origin and then stepping out to larger r values, changing the value of z_0 as one progresses. This procedure is able to generate very accurate wavefunctions and hence accurate phase shifts.

In view of this choice of procedure to compute the phase shifts, we have chosen to use modified Laguerre polynomials $\phi_n(z)$ as our basis functions instead of the spline functions employed by Ioannides and MacKintosh:

$$\phi_n(z) = e^{-z/2} L_n(z) \tag{14}$$

where the Laguerre polynomials $L_n(z)$ are polynomials of order n. Thus we can readily obtain the coefficients for a power series expansion of $\phi_n(z)$ and hence use these in our computation of the phase shifts for the sum of the reference potential plus basis functions.

3. Results

We have applied the foregoing inversion process to some of the same potentials and scattering energies considered by Coudray (1977). These include the square well, the Gaussian, a perturbed Gaussian and the Woods-Saxon potentials. The problem treated

is that of a neutron scattering off an alpha particle. The procedure is initiated in each case by computing the phase shifts for the potential model chosen. These are referred to as the goal phase shifts δ_l^G, associated with the goal potential. A reference potential, V_0, is then chosen with parameters such that it produces phase shifts which are similar to those of the goal potential. In all the cases studied here, we have selected a Gaussian as the reference potential. The iteration process is then carried out, with the value of σ computed at the end of each stage. We found that the process converged very quickly, with only two or three iterations necessary before σ stabilised.

The results for the square well potential at a laboratory energy of 50 MeV are shown in figure 1, where the comparison is made with results obtained using the Newton-Sabatier approach. The well has a depth of 14 MeV and a radius of 5.0 fm. The oscillations found in our case are much deeper than those found by Coudray (1977). The phase shifts for this potential form, however, are still in very good agreement with the square well phase shifts, such that they are not distinguishable on a graph. Instead we have plotted the difference between the goal phase shifts (δ_l^G) and the computed phase shifts (δ_l) in figure 2.

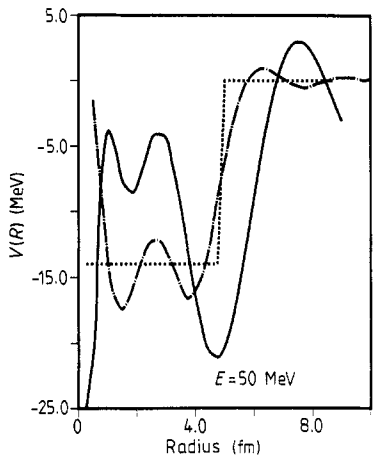

Figure 1. Generated potentials for the square well at 50 MeV. Our results (full curve) and those of Coudray (chain curve).

Increasing the energy to 400 MeV with the same square well as the goal potential, we find that the generated potential is quite different from that at 50 MeV. The small oscillations about the goal potential are not obtained in our case. Instead, a largely fluctuating, relatively smooth form is found. These results are shown in figure 3. The agreement of the phase shifts here is not as good as it is at 50 MeV, but it nevertheless is satisfactory.

The perturbed Gaussian potential

$$V(r) = -V_0 \exp[-(r/\mu)^2] - V_1 \exp\{-[(r-r_0)/\nu]^2\} \tag{15}$$

with $V_0 = 14$ MeV, $V_1 = 2$ MeV, $\mu = 3.5$ fm, $\nu = 0.4$ fm and $r_0 = 5$ fm was run at 30 MeV and 400 MeV. An extremely good match to the phase shifts was obtained at 30 MeV. As can be seen from figure 4, the generated potential does not reproduce the dip found in the goal potential, and also has large deviations in the region less than 3 fm. The

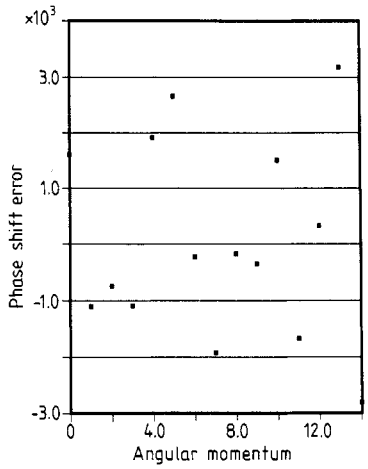

Figure 2. Difference between the goal and computed phase shifts for the square well potential at $E = 50$ MeV.

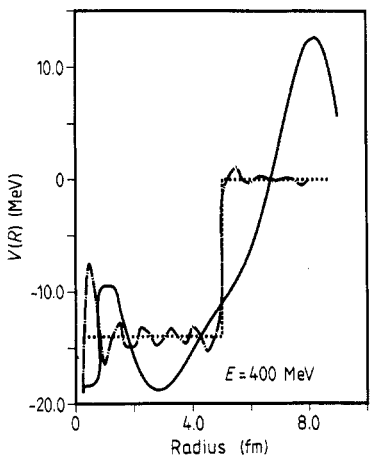

Figure 3. Same as for figure 1, at $E = 400$ MeV.

potential obtained at 400 MeV is similar, but deviates more in the rising part of the potential curve. In both cases V is relatively smooth.

The final case examined in this study was the Woods-Saxon potential at 150 MeV. The generated potential and the phase shift errors are shown in figure 5 and figure 6 respectively. The fit to the goal phase shift is quite good, and the potential deviates only slightly from the goal potential.

The procedure for the inversion is quite simple and the process converges quickly. Naturally, in this type of approach one can use different reference potentials $V_0(r)$ and generate quite different final potentials in the process, all of which reproduce the initial phase shift data quite well. Working with only a finite number of phase shifts does not enable one to derive a unique potential. There is also the question of error in the phase shifts themselves. This has not been taken into account in our analysis.

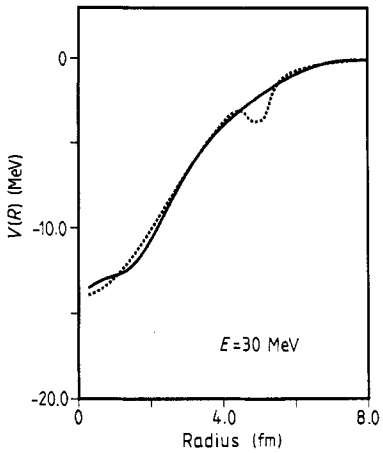

Figure 4. Original (dotted curve) and generated (full curve) potentials for the perturbed Gaussian at $E = 30$ MeV.

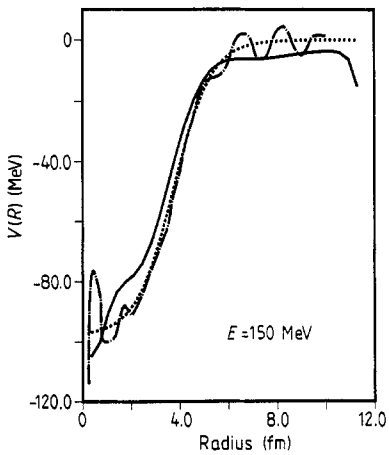

Figure 5. Original (dotted curve) and generated (full curve) potential for the Woods-Saxon potential at 150 MeV.

4. Conclusions

We have carried out an evaluation of the perturbative iterative scheme for generating phase equivalent potentials, as introduced by Ioannides and MacKintosh. The procedure has been applied to real potentials, using a very accurate method for computing the phase shifts, and employing modified Laguerre polynomials as basis functions in the iteration. The potentials generated are quite different from those obtained by Coudray (1977), using Fredholm determinants based on the Newton-Sabatier equations. Our results display much larger variations from the goal potential in the case of the square well, but are free of the oscillating behaviour for the smoother potentials. For smooth potentials such as the Gaussian or the Woods-Saxon, reproduction of the phase shifts and the potential form is quite good even at low energies, where the determinantal approach of Coudray resulted in considerable oscillation.

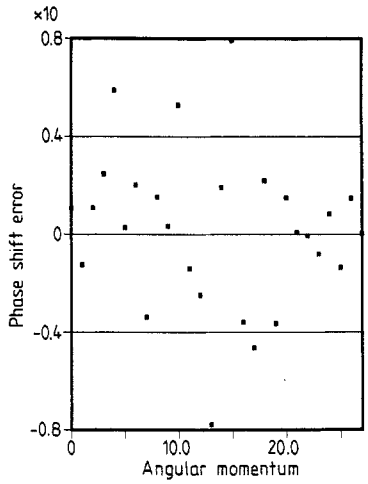

Figure 6. Difference between the goal and computed phase shifts for the Woods-Saxon potential at 150 MeV.

This technique includes a method for generating smooth potentials based on an expansion in terms of associated Laguerre polynomials, from which phase shifts can be computed without numerical integration. This enables one to adjust the coefficients in the potential expansion to fit a particular form, and compute the associated phase shifts, or alternatively, adjust the expansion coefficients to reproduce a given set of phase shift data as well as possible. We are currently proceeding with calculations along these lines.

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