METHODS IN COMPUTATIONAL PHYSICS

Advances in Research and Applications

Edited by

Berni Alder

Sidney Fernbach

Manuel Rotenberg

Volume 6: Nuclear Physics
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Preface

The Schroedinger equation can be solved analytically in only a few special cases. For this reason, it has been necessary to construct models which approximate the energy spectra and the first few moments of the density distribution in nuclei. It is here that the digital computer has had a great effect; the theoretician is allowed to develop complex models with the knowledge that a quantitative check with experiment will be possible. The first four chapters of this volume describe the computational aspects of four models of the nucleus: the optical model; the Brueckner-Watson model; the Hartree-Fock model; and the shell model.

In the case of a few-particle system, the Rayleigh-Ritz method can be used to obtain results as accurately as desired. It is applied here to the description of light nuclei and hypernuclei, with Monte Carlo techniques being used to carry out the higher dimension integrals.

Computer studies of experimental phase shifts have yielded phenomenological nucleon–nucleon forces which are reliable over a large range of energies. We have devoted the final chapter to a description of a phase-shift analysis.

September, 1966

Berni Alder
Sidney Fernbach
Manuel Rotenberg

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Introduction

OPTICAL MODEL CALCULATIONS ARE now considered, as standard methods of analysis for elastic scattering data which are becoming available at an increasing rate and with increasing accuracy. A complete compendium of such analyses may be found in a recent book by Hodgson (1963). A number of optical model programs are available and are often used with low efficiency at the cost of considerable computer time. The purpose of this article is to give a review of the methods used in optical model calculations including automatic search techniques, and to indicate how to speed up the computations while retaining desired accuracy in the results.

We shall present all the formulas required to compute the final quantities of interest, i.e., the differential elastic scattering cross sections, polarizations, and total reaction cross section for particles of spin 0, $\frac{1}{2}$, and 1 incident against 0-spin targets. The numerical solutions of the radial Schroedinger differential equations will be discussed in some detail as these calculations represent an important part of the total computation. The equations are usually solved by the Runge-Kutta, Cowell, or Noumerov methods which are subject to a local truncation error of order $\lesssim h^5$ and can be programmed quite easily. We shall compare these methods with respect to speed and accuracy. The final errors in the coefficients of the scattering matrix which we call the C coefficients will be discussed and illustrated for a typical test case. We shall also discuss and compare several methods for automatically searching over the parameter space for the best fit to the experimental data, and we shall present a recommended search program for which we give estimated computing times and storage requirements on an IBM 7094 Mod I computer.

I. General Description of the Problem and the Program

A. Physical Description and Formulation

The Schroedinger equation for the system is given by

$$[-(\hbar^2/2\mu)\nabla^2 + \mathscr{V}]\Psi = E\Psi \tag{1-1}$$

where

$$\mu = m_i \cdot m_t/(m_i + m_t) \tag{1-2}$$

is the reduced mass, m_i and m_t being, respectively, the masses of the incident and target particles, while

$$E = E_{\text{LAB}} \cdot m_t/(m_i + m_t) \tag{1-3}$$

is the energy in the center of mass system, E_{LAB} being the lab energy of the incident particle.

The optical potential is generally given by

$$\mathscr{V} = \mathscr{V}_{coul}(r) + \mathscr{V}_{CR}(r) + i\mathscr{V}_{CI}(r) + \{\mathscr{V}_{SR}(r) + i\mathscr{V}_{SI}(r)\}\hbar^2(\mathbf{S}\cdot\mathbf{L}) \tag{1-4}$$

where the various terms in Eq. (1-4), which depend only on the distance r between the incident and the target particles, represent, respectively, the coulomb, central real, central imaginary, spin-orbit real, and spin-orbit imaginary potentials. The operators **S** and **L** represent, respectively, the spin and orbital angular momentum operators of the incident particle in units of $\hbar$, while the total angular momentum **J** is given by $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Other terms which have also been considered include:

(a) a coulomb spin-orbit potential for spin $\frac{1}{2}$ particles (Melkanoff *et al.*, 1961);

(b) a quadratic spin-orbit potential for spin 1 particles (Raynal, 1963a,b);

(c) a tensor potential for spin 1 particles (Raynal, 1963a,b) which leads to systems of two coupled equations.

We shall ignore these various terms as they seem to play a minor part in the interaction.

Separation of the variables appearing in the complete Schroedinger equation leads to the usual radial equation for each value of the orbital and total angular momenta l and j:

$$\{d^2/dr^2 - l(l+1)/r^2 + (k^2/E)[E - (\mathscr{V}_{coul}(r) + \mathscr{V}_{CR}(r) + i\mathscr{V}_{CI}(r)) - (\mathscr{V}_{SR}(r) + i\mathscr{V}_{SI}(r))\hbar^2(j(j+1) - l(l+1) - s(s+1))/2]\}\psi_l^j(r) = 0 \tag{1-5}$$

where

$$k = (2\mu E/\hbar^2)^{1/2}$$

and $\psi_l^j(r)$ is the radial wave function which must satisfy the following boundary conditions: (a) it must vanish at the origin; and (b) the asymptotic form of the solution should in principle be matched to a plane wave plus an outgoing wave. In the actual case the solution is matched to a linear combination of regular and outgoing coulomb wave functions at the point r_m beyond which the nuclear potential is sufficiently small:

$$\psi_l^j(r_m) = F_l(\eta, kr_m) + C_l^j[G_l(\eta, kr_m) + iF_l(\eta, kr_m)] \tag{1-6}$$

where F_l and G_l are, respectively, the regular and irregular normalized coulomb wave functions,

$$\eta = \mu ZZ'e^2/(\hbar^2 k),$$

Z and Z' being the incident and target particle charge numbers, and the coefficients C_l^j are related to the nuclear phase shifts, δ_l^j, and to the absorption coefficients, $|\eta_l^j|^2$, as follows:

$$C_l^j = (-i/2)[\exp(2i\,\delta_l^j) - 1] = (-i/2)[\eta_l^j - 1]. \tag{1-7}$$

All the physically measurable quantities are expressed in terms of the C_l^j coefficients. The total reaction cross section may be written as follows:

$$\sigma_R = [4\pi/((2s+1)k^2)] \sum_{l=0}^{\infty} \sum_{j=|l-s|}^{l+s} (2j+1)\{\mathrm{Im}\, C_l^j - |C_l^j|^2\}. \tag{1-8}$$

The angular distributions are more easily given for specific values of s.

1. $s = 0$

The scattering amplitude is given by

$$A(\theta) = f_c(\theta) + k^{-1} \sum_{l=0}^{\infty} \exp(2i\sigma_l)(2l+1)C_l^l P_l(\cos\theta) \tag{1-9}$$

where $f_c(\theta)$ is the coulomb scattering amplitude,

$$f_c(\theta) = -\eta \exp[-i\eta \ln(\sin^2(\theta/2)) + 2i\sigma_0]/[2k \sin^2(\theta/2)], \tag{1-10}$$

and the coulomb phase shifts are given by

$$\sigma_l = \arg \Gamma(l + 1 + i\eta). \tag{1-11}$$

The differential scattering cross section is then

$$\sigma(\theta) = |A(\theta)|^2. \tag{1-12}$$

2. $s = \frac{1}{2}$

The two independent scattering amplitudes are

$$A(\theta) = f_c(\theta) + k^{-1} \sum_{l=0}^{\infty} \exp(2i\sigma_l)[(l+1)C_l^{l+\frac{1}{2}} + lC_l^{l-\frac{1}{2}}]P_l(\cos\theta)$$

$$B(\theta) = ik^{-1} \sum_{l=0}^{\infty} \exp(2i\sigma_l)[C_l^{l+\frac{1}{2}} - C_l^{l-\frac{1}{2}}]P_l^1(\cos\theta). \tag{1-13}$$

The differential cross section and the polarization for an unpolarized incident beam are given by

$$\sigma(\theta) = |A(\theta)|^2 + |B(\theta)|^2, \tag{1-14}$$

$$P(\theta) = [A^*(\theta)B(\theta) + A(\theta)B^*(\theta)]/\sigma(\theta). \tag{1-15}$$

3. $s = 1$

In this case there are four independent scattering amplitudes and various authors have used different sets of them. We present here the results obtained from the use of the helicity formalism (Raynal, 1963b, 1964):

$$\left.\begin{aligned}
A(\theta) &= f_c(\theta)(1+\cos\theta)/2 + (2k)^{-1}\sum_{J=1}^{\infty}\{(J+1)\exp(2i\sigma_{J-1})C^J_{J-1} \\
&\quad + J\exp(2i\sigma_{J+1})C^J_{J+1} + (2J+1)\exp(2i\sigma_J)C^J_J\} \\
&\quad \cdot\{(1-\cos\theta)P_J^1(\cos\theta)/[J(J+1)\sin\theta] + P_J(\cos\theta)\} \\
B(\theta) &= -f_c(\theta)\sin\theta/\sqrt{2} + (\sqrt{2}k)^{-1}\sum_{J=1}^{\infty}\{\exp(2i\sigma_{J-1})C^J_{J-1} \\
&\quad - \exp(2i\sigma_{J+1})C^J_{J+1}\}P_J^1(\cos\theta) \\
C(\theta) &= f_c(\theta)(1-\cos\theta)/2 + (2k)^{-1}\sum_{J=1}^{\infty}\{(J+1)\exp(2i\sigma_{J-1})C^J_{J-1} \\
&\quad + J\exp(2i\sigma_{J+1})C^J_{J+1} - (2J+1)\exp(2i\sigma_J)C^J_J\} \\
&\quad \cdot\{(1+\cos\theta)P_J^1(\cos\theta)/[J(J+1)\sin\theta] - P_J(\cos\theta)\} \\
D(\theta) &= f_c(\theta)\cos\theta + k^{-1}\sum_{J=1}^{\infty}\{J\exp(2i\sigma_{J-1})C^J_{J-1} \\
&\quad + (J+1)\exp(2i\sigma_{J+1})C^J_{J+1}\}P_J(\cos\theta).
\end{aligned}\right\} \tag{1-16}$$

For an unpolarized incident beam, the differential cross section is now given by

$$\sigma(\theta) = (1/3)\{2|A(\theta)|^2 + 4|B(\theta)|^2 + 2|C(\theta)|^2 + |D(\theta)|^2\} \tag{1-17}$$