7. Symposium on interoctions of fast neutrons with nuclei. Gaussic, Germany, D.D., 21-25 November 1977
CEA-CONF--4199

ON USEFULLNESS OF MATRIX METHODS IN OPTICAL MODEL CALCULATIONS

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Some advantages of using matrix methods in optical model are pointed out in connection with evaluation problems and microscopic aspects.

1. Introduction

Conventional optical model codes generally use numerical integration methods to solve the Schrödinger equation describing neutron scattering from a complex potential. In principle any potential shape can be dealt with. However, from a practical viewpoint, such methods are not very suitable for treating directly non local potentials because iteration procedures involving tabulations of approximate wave functions have to be used to solve integro-differential equations [2]. Moreover almost all the calculation is usually performed again when any parameter or the neutron energy change. In view of evaluation purposes, coherent and accurate enough calculations of various neutron cross-sections for a given target over a wide energy range generally involve a specific optimization of optical parameters [2], given to start either some standard or adapted to neighbouring nuclei parametrisation. Thus computer time problems arise. It may also be desirable to try and limit the number of free parameters or understand physical aspects by using potentials, generally non local, suggested by microscopic models of nuclear structure. In this study we point out some advantages brought by matrix methods, instead of numerical one's, for treating generalized spherical neutron optical potentials.

2. Summary of the formalism

In the frame of the so-called "calculable R-matrix" method [3], variational forms of wave functions and phase-shifts can be obtained [4] that involve the inversion, at a c. of m. energy E, of the A matrix whose elements are :

$$A_{\alpha c} = \langle a | T + U + \mathcal{L} - E | c \rangle \qquad (1)$$

T, U and $\mathcal{L}$ are, respectively, the c. of m. kinetic energy, the nuclear potential, and the boundary condition operator of Bloch [5,3] making the matrix $T + \mathcal{L}$ symmetric and here chosen as

$$\mathcal{L}(o) = \sum_{\alpha \equiv (\ell, j)} |\alpha\rangle \frac{\hbar^2}{2mR} \delta(r-R) \frac{d}{dr} r \langle \alpha |$$

(m = reduced mass). In (1), space-coordinate integrations are to be performed within a sphere of radius R ≡ RMAX. In this internal region, the "a" projected radial wave functions ψ_α can be connected to their usual asymptotic forms $[I_\ell + S_\alpha O_\ell]$, that define the corresponding S-matrix elements, as it follows :

$$\psi_\alpha(r) = \mathcal{R}_\alpha(r;E) \cdot \left[\frac{d}{dr} r (I_\ell + S_\alpha O_\ell) \right]_R \qquad (r < R) \qquad (2)$$

where

$$\mathcal{R}_\alpha(r;E) = \frac{\hbar^2 R}{2m} \, \Phi_\ell(r) \cdot \widetilde{A^{-1}} \cdot \Phi_\ell(R) \qquad (3)$$

In (3) Φ_ℓ is the one-column matrix consisting of the N ≡ NMAX independent radial basis functions $\Phi_{n\ell}$ (n=1,2,--,N) chosen to calculate the A matrix (1). The only quantity $S_\alpha \equiv \exp(2i\delta_\alpha)$ necessary to obtain any required observable at energy E is deduced from (2) when written at the matching radius R, that is, letting $\mathcal{R}_\alpha \equiv \mathcal{R}_\alpha(R;E)$:

$$[I_\ell + S_\alpha O_\ell]_R = \mathcal{R}_\alpha [(r I_\ell)' + S_\alpha (r O_\ell)'] \qquad (4)$$

Practical constraints of such a matrix method consist of :

i/ carrying out easy procedures to calculate the matrix elements (1), especially for every term of U. As in matrix Hartree-Fock methods, the basis states are chosen to be the spherical harmonic oscillator functions

$$\Phi_{n\ell}(r) \sim r^\ell \cdot \exp(-\beta r^2/2) \cdot L_{n-1}^{\ell+1/2}(\beta r^2)$$

because of their remarkable properties.

ii/ obtaining quick enough convergence of the quantities of interest as a function of successive values of the order NMAX of the A matrix.

3. Some applications

3.1. Concerning the calculation of the matrix elements of T, $\mathcal{L}$, E or any local potential U(r) in (1), recurrence formulas for Laguerre polynomials are useful. For example $\langle n_\alpha, \ell | U(r) | n_c, \ell \rangle$ can be easily deduced from the only quantities of the form $\langle 1, o | V(r) | n_c, o \rangle$.

3.2. Matrix method lends itself to the treatment of non local folding potentials derived from the following local form [2] consisting of the usual real (R), surface derivative absorption (D) and spin-orbit (So) terms :

$$U(r) = -V_R \vartheta_R(r) + i W_D \frac{d\vartheta_D(r)}{dr} + 2\left(\frac{\hbar}{\pi}\right)^2 V_{So} \frac{1}{r} \frac{d}{dr} \vartheta_{So}(r) \, \vec{\ell} \cdot \vec{J} \qquad (5)$$

Here, the different functions $\vartheta_i(r)$ are of the folding form :

$$\vartheta_i(r) = \int \tilde{v}_{\mu_i}(|r - r_1|) \, \rho(r_1) \, d^3 r_1 \qquad (i = R, D, So) \qquad (6)$$

When a normalized gaussian function $\tilde{v}_\mu(x) \sim \exp(-x^2/\mu^2)$ and the nonlocalisation procedure of Perey et al. [1] are used, the method described in ref. [6] leads to practical expressions for the matrix elements of the different terms in (5). For example we obtain the following factorized form of the real term :

$$\langle a|V_R\left(\frac{r+r'}{2}\right).\tilde{v}_\Delta(|r-r'|)|c\rangle = \sum_{n=1}^{n_a+n_c+\ell-1} \left(1-\beta\Delta^2/4\right)^{-1}\left(1+\beta\Delta^2/4\right)^{-n-1/2} . f(M,n_a,n_c,\ell) . P_R(M) \qquad (7)$$

where Δ is the nonlocality range, $M = n_a + n_c + \ell - n$, f a geometrical factor, and :

$$P_R(M) = \sum_{k=1}^{M} (-2)^{k-1} \frac{\Gamma(M+1/2)}{\Gamma(k).\Gamma(M+1-k)} . m_k(R_R) \qquad (8)$$

$$m_k(R_R) = \frac{\beta^{3/2}}{2\pi} \frac{\Gamma(k)}{\Gamma(k+1/2)} G^{-k-1/2} \int \exp(-\beta r_1^2/G).L_{k-1}^{1/2}(\beta r_1^2/G).\rho(r_1)\,d^3r_1 \qquad (9)$$
$$(G = 1+\beta\mu^2)$$

For each term in (5) the "density" functions ρ and the "diffuseness" parameters μ are only in a limited number of these m_k coefficients. When ρ is constant inside a sphere of radius $R_i = t_i A^{1/3}$ ($i = R, D, So$) and zero outside, all the dependence on R_i is included in the m_k whose very simple expressions are given in ref. [6]. Fig. 1 illustrates what sort of convergence can be expected from the use of such a realistic folding potential as a function of β and NMAX. Calculated quantities, associated to the low energy n-^{93}Nb interaction are : s and p-wave strength functions (S_0,S_1), elastic scattering radius (R'), elastic scattering (σ_{el}) reaction (σ_R) and total (σ_T) cross sections at 10 keV and 1 MeV. Convergence is obtained at N = 8 for R = 10 fm and $\beta = 0.123$ fm^{-2}. For the same β or $\beta = 0.175$ fm^{-2} and R = 11 fm, calculations performed for ^{208}Pb have shown that N = 9 is sufficient.

3.3. In the frame of systematic search for optimised parameters, partial matrices in (1) can be calculated once for all and then reused when multiplicative parameters (E, V_R, W_D, V_{SO}) are changed. In particular the sensitivity to such parameters γ of any calculated quantity can be easily obtained, in a single computer run, by means of the corresponding derivative of $\mathcal{R}_\alpha$. Following (3):

$$\frac{d\mathcal{R}_\alpha}{d\gamma} = -\frac{\hbar^2 R}{2m} \tilde{\phi}_\alpha(R).\tilde{A}^{-1}.\frac{d\tilde{\Lambda}}{d\gamma}.\tilde{A}^{-1}.\phi_\alpha(R) \qquad (10)$$

In order to deduce sensitivities to Δ or to geometry optical parameters, (10) can be used too with $\frac{d\Lambda}{d\rho}$ matrices given by (7) where proper derivatives are taken. In the case of a square density function ρ, the derivatives of the m_k with respect to μ_i or R_i have very simple expressions. As illustrative results, a number of so calculated sensitivities are shown in Table 1 for various physical quantities associated to the interaction n-^{93}Nb in the energy range 10 keV $\leq E_n \leq$ 1 MeV. A local but energy dependent folding potential has been employed with the following parameters (energies in MeV, lengths in fm) :

$V_R = 54.51 - 0.3\,E_n$, $\mu_R = 1.882$, $r_R = 1.21$
$W_D = 2.118 + 0,3\,E_n$, $\mu_D = 1.76$, $r_D = 1.26$
$V_{SO} = 6.73$, $\mu_{SO} = 1.43$, $r_{SO} = 1.12$

In fig.2 the corresponding total cross-section is compared to experimental data [7]. Given sensitivities, fitting limitations or improvements can be easily inferred. The fit of low energy data is very close to that obtained by Ch. Lagrange from a Saxon-Woods potential [8]. Fig.3 shows how satisfactory can be the prediction of elastic scattering angular distributions [8] as compared to experimental data at 8.05 MeV [9].

3.4. Other general types of potentials, suggested by microscopic models of nuclear structure, can be conveniently treated by matrix methods. For example, explicit and simple forms for the different local and non local terms of a Hartree-Fock potential can be given [10] in terms of the parameters of an effective density-dependent two-body force and of density matrices. Such microscopic fields can be easily tested as the main real part of an optical potential by using matrix methods. We have found it very practical to construct their matrix elements in (1) by choosing as β value the one used in the Hartree-Fock procedure, for example 0.175 for ^{208}Pb and 0.214 (cf fig.1) for ^{93}Nb. In the already studied cases, convergence is obtained for NMAX = 9.

Another example consists of the non local optical potential calculated in the intermediate structure model with weak particle-vibration coupling as detailed for example in ref.11). We have found that matrix methods are well suited for handling such a type of potential. In particular, its construction is facilitated by the representation (2) of wave functions and by practical procedures to determine the required continuum resonances.

4. In conclusion it appears that much work remains to be done to explore the possible advantages of matrix methods. However the various aspects briefly described above show that such techniques may be of practical interest in applications of the optical model and especially in connection with microscopic theories.

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	$S_0 \times 10^4$	$S_1 \times 10^4$	R'	$\sigma_T(0.01)$	$\sigma_T(0.2)$	$\sigma_T(1)$
	(a)	(a)	(a)	(b)	(b)	(b)
exp.val.	0.36±0.06	5.16±0.24	7.±0.2	7800	9430	6500
calc.val.	0.39	5.01	6.82	8377	9064	6483
d/dE	-0.29	9.09	-4.74	-48201	2073	-3005
d/dV_R	-0.019	1.645	-0.159	-66.61	992.7	599.7
d/dR_R	-0.328	30.6	-2.2	532	21127	12367
d/da_R	0.222	3.635	0.67	2724	4107	1673
d/dW_D	0.175	1.097	-0.028	881.2	167	-136.1
d/dR_D	0.008	1.765	0.016	370	474.7	19.63
d/da_D	0.214	2.347	0.004	1320	674.9	33.26

TABLE 1

Sensitivities of the interaction n-^{93}Nb (energies in MeV, lengths in fm)
(a) BNL-325, vol.I (1973) - (b) BNL-325, suppl. n° 2, vol.IIB (1966)

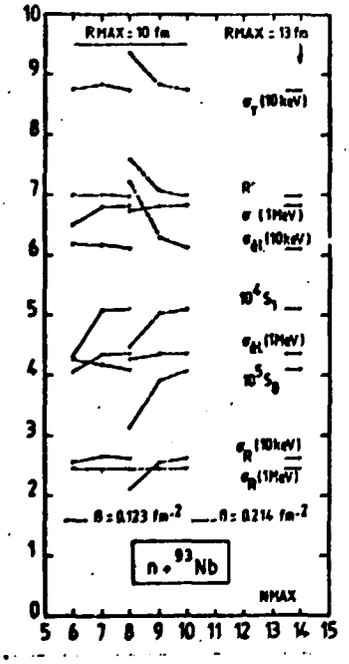

Fig. 1

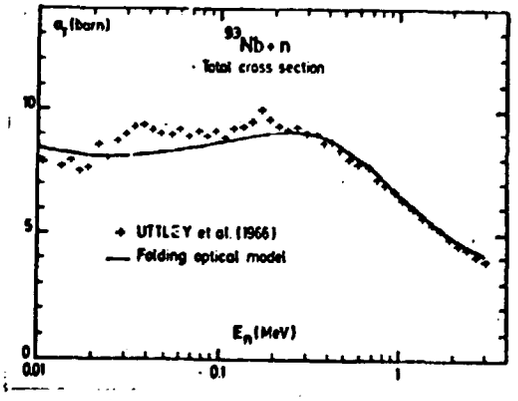

Fig. 2

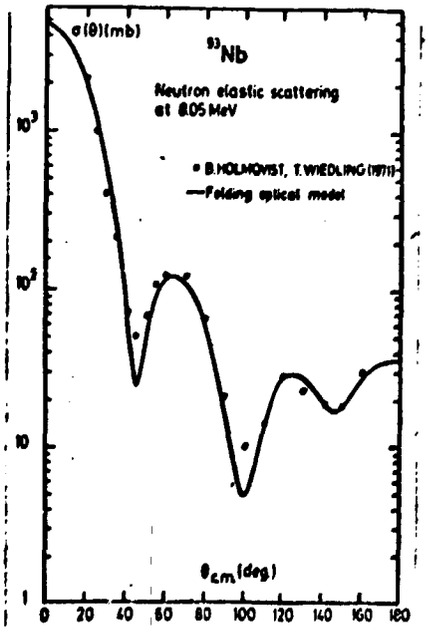

Fig. 3

Fig.1 : Convergence properties of calculated quantities for n-^{93}Nb interaction.

Fig.2 : Adjustment theory-experiment [7] for neutron total cross-section of ^{93}Nb.

Fig.3 : Comparison theory-experiment [9] for neutron elastic scattering from ^{93}Nb at 8.05 MeV.