UCRL-17784

cy. 2

University of California

Ernest O. Lawrence Radiation Laboratory

USE OF THE PROJECTION OPERATOR METHOD
IN NUCLEAR REACTION THEORY

W. Tobocman

August 1967

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 5545

UCRL-17784 Cy. 2

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Submitted to Phys. Rev.

UCRL-17784
Preprint

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

USE OF THE PROJECTION OPERATOR METHOD IN NUCLEAR REACTION THEORY

W. Tobocman

August 1967

USE OF THE PROJECTION OPERATOR METHOD IN NUCLEAR REACTION THEORY*

W. Tobocman†

Lawrence Radiation Laboratory
University of California
Berkeley, California

August 21, 1967

ABSTRACT

H. Feshbach has shown how the introduction of the projection operator onto the bound states of a system of nucleons can facilitate the calculation of the transition amplitude for a nuclear scattering reaction. Feshbach's method is based on the relationship of the transition amplitude to the T-matrix. In this paper we show how the projection operator method can be applied to the generalized R-matrix expression for the transition amplitude.

In order to test the validity of the approximations customarily employed in applications of the projection operator formalism, we have applied the method to a simple soluble model. We find that the method works quite well provided that all second order terms are retained. The generalized R-matrix is found to work better than the T-matrix method, but the R-matrix method depends sensitively on the choice of the value of the boundary radius.

---

*This work wad done under the auspices of the U.S. Atomic Energy Commission.
†Present address: Physics Department, Case Western Reserve University, Cleveland, Ohio 44106

I. INTRODUCTION

H. Feshbach[1] has shown how the introduction of a projection operator onto the bound states of a system of nucleons can facilitate the calculation of the transition amplitude for a nuclear reaction. This method has received several elaborations[2] and applications.[3] The Feshbach method utilizes the relationship between the T-matrix and the scattering amplitude. In this paper we show how the projection operator method can be used to evaluate the generalized R-matrix.[4] When approximations are made to carry out calculations using the projection operator formalism, the consequences of these approximations can be expected to be somewhat different for the R-matrix than for the T-matrix.

In order to test the validity of the approximations customarily employed in applications of the projection operator formalism, we have applied the method to a simple soluble model. Both the T-matrix and R-matrix approaches are tested. The model consists of two s-wave channels coupled by a zero range separable potential. In addition, there is an elastic zero range interaction in each channel. We find that the projection operator method works pretty well provided that all second order terms are retained. The R-matrix calculation gives a better result than the T-matrix calculation, but the elastic R-matrix results are quite sensitive to the choice of the boundary radius.

In Section II the scattering problem is formulated and the projection operator formalism for the T-matrix is presented. The projection operator formalism for the R-matrix is outlined in Section III. In Section IV we introduce the usual second order approximation for the reduced operators. We describe the coupled s-wave channel scattering model we wish to use to test our methods in Section V. In Sections VI and VII we apply our approximate

projected T-matrix and R-matrix methods to the scattering model. In Section VIII we describe the results of numerical evaluation of the expressions derived in Sections V, VI, and VII.

II. THE PROJECTION OPERATOR METHOD APPLIED TO THE T-MATRIX

For the sake of simplicity we will restrict ourselves to the problem of the elastic and inelastic scattering of a particle by a target capable of existing in a finite number of discrete states. The Hamiltonian will be taken to be

$$\begin{aligned} H &= H_T(\xi) + H_P(\underset{\sim}{r},\xi) + V(\underset{\sim}{r},\xi) \\ &= H_0(\underset{\sim}{r},\xi) + V(\underset{\sim}{r},\xi) \end{aligned} \tag{1}$$

where H_T is the Hamiltonian for the internal structure of the target, V is the interaction between the target and the incident particle, and H_P is the relative motion Hamiltonian. H_P will consist of a kinetic energy T and an elastic scattering interaction U.

$$H_P(\underset{\sim}{r},\xi) = T(\underset{\sim}{r}) + U(\underset{\sim}{r},\xi) \tag{2}$$

Let $\Psi_\alpha^{(+)}$ be the wave function describing the scattering process of interest. Then

$$(E - H)\Psi_\alpha^{(+)} = 0 \tag{3}$$

where E is the total energy. The subscript identifies the initial state of excitation of the target. Now let $\Phi_\alpha^{(+)}$ be the eigenstate of H_0 at the energy E,

$$(E - H_0)\Phi_\alpha^{(+)} = 0 , \tag{4}$$

which has the same incident asymptotic behavior as $\Psi_\alpha^{(+)}$. Then $\Psi_\alpha^{(+)}$ and $\Phi_\alpha^{(+)}$ are related by the Lippman-Schwinger equation[5]

$$\Psi_\alpha^{(+)} = \Phi_\alpha^{(+)} + (E - H_o + i\epsilon)^{-1} V \Psi_\alpha^{(+)} \tag{5A}$$

$$= [1 + (E - H + i\epsilon)^{-1} V] \Phi_\alpha^{(+)} \tag{5B}$$

Let Λ_β be the eigenstate of $H_T + T$ corresponding to channel β .

$$(E - H_T - T) \Lambda_\beta = 0 \tag{6}$$

The transition amplitude for scattering from channel α to channel β may now be written[5] as $2\hbar \mathcal{J}_{\beta\alpha}$ where

$$\mathcal{J}_{\beta\alpha} = \langle \Lambda_\beta | H - H_T - T | \Psi^{(+)} \rangle (2\hbar)^{-1} \tag{7A}$$

$$= (\langle \Lambda_\beta | U | \Phi_\alpha^{(+)} \rangle + \langle \Phi_\beta^{(-)} | V | \Psi_\alpha^{(+)} \rangle) (2\hbar)^{-1} \tag{7B}$$

$$= T_{\beta\alpha}^{(0)} + T_{\beta\alpha} \tag{7C}$$

The various wave functions that appear above are normalized to unit incident current. The first term on the right of Eq. (7B) is the scattering amplitude due to interaction U . The interaction U is chosen to be a simple potential well that can provide an approximate description of the average elastic scattering. U is the optical potential. Thus there is no difficulty in calculating $T_{\beta\alpha}^{(0)}$.

The remainder, $T_{\beta\alpha} = \langle \Phi_\beta^{(-)} | V | \Psi_\alpha^{(+)} \rangle$, will be the main object of our attention. This remainder we call the T-matrix. By making use of the formal solution of the Lippman-Schwinger equation, Eq. (4B), we have

$$T_{\alpha\beta} = \langle \Phi_\beta^{(-)} | V + V(E - H + i\epsilon)^{-1} V | \Phi_\alpha^{(+)} \rangle / 2\hbar \tag{8}$$

We define the transition operator, T , to be

$$T = V + V(E - H + i\epsilon)^{-1} V \tag{9}$$

Now we are prepared to introduce the projection operator onto the bound states of the system Q . Let $P = 1 - Q$ be the projection operator onto the unbound states of the system. The reduced transition operator $\hat{T}$ is defined by the Lippman-Schwinger equation

$$\hat{T} = V + V(E - H_o + i\epsilon)^{-1} P\hat{T} \quad . \tag{10}$$

$\hat{T}$ is what T would be if the bound states were eliminated as intermediate states from the perturbation expansion.

We solve Eq. (10) for V

$$V = \hat{T}[1 + (E - H_o + i\epsilon)^{-1} P\hat{T}]^{-1} \tag{11}$$

and substitute the result into Eq. (9) for T to find after a few algebraic manipulations that

$$T = \hat{T} + \hat{T}(E - H_{\odot} - Q\hat{T} + i\epsilon)^{-1} Q\hat{T} \tag{12}$$

The transformation of Eq. (9) into Eq. (12) is the essence of the projection operator method. The advantage gained is that the inversion of $E - H$ need only be performed in that part of Hilbert space spanned by the bound states included in Q. The price paid for this advantage is the replacement of the simple interaction V by the more complicated reduced transition operator $\hat{T}$. Due to the nature of P it is believed that $\hat{T}$ can be well approximated by a few terms of a perturbation expansion.

III. THE PROJECTION OPERATOR METHOD APPLIED TO THE GENERALIZED R-MATRIX

We will refer to the region of configuration space exterior to the range of V as the asymptotic region of space. In the asymptotic region of space the wave function describing the scattering process will have the form

$$\Psi_\alpha^{(+)} \rightarrow \sum_\beta X_\beta(\xi,\Omega)\,[\delta_{\beta\alpha}\,U_\beta^{(2)}(r) - \mathcal{S}_{\beta\alpha}\,U_\beta^{(1)}(r)] \quad , \tag{13}$$

where X_β is the product of an eigenstate of H_T with the spherical harmonics for the angular dependence of relative motion of the two nuclides of channel β. $U_\beta^{(2)}$ is the unit current radial incoming wave function for channel β while $U_\beta^{(1)}$ is the corresponding outgoing radial wave function. The scattering matrix $\mathcal{S}_{\beta\alpha}$ is related to the transition amplitude $2\hbar\,\mathcal{J}_{\beta\alpha}$ by

$$\mathcal{S}_{\beta\alpha} = \delta_{\beta\alpha} - 2i\,\mathcal{J}_{\beta\alpha} \quad , \tag{14}$$

where $\delta_{\beta\alpha}$ is the Kronecker delta function.

The relationship between the scattering matrix $\mathcal{S}_{\beta\alpha}$ and the generalized R-matrix $\mathcal{R}_{\beta\alpha}$ defined by

$$\mathcal{R}_{\beta\alpha}(\bar{R},R) = \frac{\hbar^2}{2m}\sqrt{\bar{R}R}\,\langle X_\beta(\xi,\Omega)\,\frac{\delta(r-\bar{R})}{r^2}\,|(E-H)^{-1}|\,X_\alpha(\xi',\Omega')\,\frac{\delta(r'-R)}{r'^2}\rangle$$

can be shown to be[4]

$$\mathcal{S}_{\beta\alpha} = \sum_\gamma (Z^{(1)-1})_{\beta\gamma} Z^{(2)}_{\gamma\alpha} \tag{16A}$$

where

$$Z_{\alpha\beta}^{(i)} = \delta_{\alpha\beta}\gamma_{\alpha}^{(i)}(\bar{R}) - \gamma_{\beta}^{(i)}(R)\, D_R \mathcal{R}_{\alpha\beta}(\bar{R},R) + \mathcal{R}_{\alpha\beta}(\bar{R},R)\, D_R \gamma_{\beta}^{(i)}(R) \quad (16B)$$

$$\gamma_{\alpha}^{(i)}(R) = \left(\frac{\hbar^2 R}{2m}\right)^{1/2} U_{\alpha}^{(i)}(R) \quad (16C)$$

$$D_R = R^{1/2} \frac{\partial}{\partial R} R^{1/2} \quad (16D)$$

Eq. (16) is derived in reference (4) for the case $R = \bar{R}$. The generalized R-matrix is seen to be made up of matrix elements of the Green's function

$$G = (E - H)^{-1} \quad (17)$$

with respect to the channel wave functions. Of course, there is a freedom of choice as to how we define the singularity in G but this ambiguity does not affect the Wronskian of $\mathcal{R}$ that occurs in Eq. (16B).

In the above expression for the R-matrix the values of R and $\bar{R}$ must be such that the matching radius $\bar{R}$ is smaller than or equal to the boundary radius R . (ξ,Ω,R) and $(\xi,\Omega,\bar{R})$ are configuration space points located in the asymptotic region.

We use the expression "generalized R-matrix" to differentiate $\mathcal{R}$ from the R-matrix of E. Wigner.[6] The Wigner R-matrix is given by Eq. (15) with $\bar{R} = R$ and a particular representation used for $(E - H)^{-1}$. We use the word "generalized" to emphasize the fact that other representations for $(E - H)^{-1}$ can be used as well. Having made this point, we will henceforth refer to $\mathcal{R}$ as simply the R-matrix.

In the T-matrix treatment we were able to use the optical potential U to reproduce the average elastic scattering and confine our attention to the remainder of the transition amplitude. The same can be done in the R-matrix treatment. To do this we introduce the Green's function G_o associated with the Hamiltonian $H_o = H_T + T + U$.

$$G_o = (E - H_o + i\epsilon)^{-1} \tag{18}$$

Here it is convenient to explicitly choose the scattering type of singularity by including the imaginary infinitesimal $i\epsilon$. Now since

$$\begin{aligned} G_o^{-1} &= (E - H_o + i\epsilon) \\ &= (E - H + i\epsilon) + V \\ &= G^{-1} + V \quad , \end{aligned} \tag{19}$$

we have the following experssion for G :

$$G = G_o + GVG_o \tag{20A}$$

$$= G_o(1 - VG_o)^{-1} \tag{20B}$$

Using the right side of Eq. (20A) in the definition of the R-matrix shown in Eq. (15), we can arrive at an expression for the R-matrix which consists of an optical model term plus a remainder.

Next we consider how the projection operator onto the bound states, $Q = 1 - P$, can be used to facilitate the operator inversion required to evaluate G. We start by defining a reduced Green's function $\hat{G}$.

$$\hat{G} = G_o + G_o V P \hat{G} \tag{21}$$

Solving this equation for G_o

$$G_o = \hat{G}(1 + VP\hat{G})^{-1} , \tag{22}$$

and using the result to eliminate G_o from Eq. (20B) gives

$$G = \hat{G} + GVQ\hat{G} \tag{23A}$$

$$= \hat{G}(1 - VQ\hat{G}) \tag{23B}$$

For our purposes it is most convenient to rewrite Eq. (23) to read

$$G = \hat{G} + \hat{G}VQ(1 - \hat{G}VQ)^{-1}\hat{G} \tag{24}$$

Eqs. (14), (15), (16), (18), (21), and (24) constitute the application of the projection operator method to the R-matrix formalism. Eqs. (14) and (16) show how to calculate the transition amplitude from the R-matrix. Eq. (15) expresses the R-matrix in terms of the Green's function. Eq. (24) gives the Green's function in terms of the reduced Green's function and the projection operator. Finally, Eq. (21) defines the reduced Green's function in terms of the conjugate projection operator and the optical model Green's function defined by Eq. (18).

Thus we have succeeded in injecting the two essential ingredients of the projection operator treatment of the T-matrix into a projection operator treatment of the R-matrix. In Eq. (24) we see that the operator inversion is limited by the projection operator Q to the portion of Hilbert space spanned by a discrete set of eigenvectors. From Eqs. (24) and (21) we see that the reduced Green's function can be expressed as an optical model Green's function plus a remainder.

IV. APPROXIMATING THE REDUCED OPERATORS

The two formalisms for calculating the transition amplitude for scattering derived above are exact. In principle, the optical potential U and the projection operator Q can be chosen in a completely arbitrary way. In applications it is necessary to use an approximate representation for the reduced operators. The usual choice is the first iteration of the integral equation.

In the T-matrix formalism we iterate Eq. (10) once and let

$$\hat{T} \approx V + VG_oPV \tag{25}$$

This is then substituted into Eq. (12).

$$T \approx T_A$$

$$T_A = V + VG_oPV + V(1+G_oPV)\,[E-H_o-QV(1+G_oPV) + i\epsilon]^{-1}\,Q(1 + VG_oP)\,V \tag{26}$$

In practice, the higher order terms in V are often neglected also.

$$T \approx T_C$$

$$T_C = V + V[E - H_o - QV(1 + G_oPV) + i\epsilon]^{-1}\,QV \tag{27}$$

We will also consider an intermediate approximation, namely

$$T \approx T_B$$

$$T_B = V + VG_oPV + V[E - H_o - QV(1 + G_oPV) + i\epsilon]^{-1}\,QV\ . \tag{28}$$

In the R-matrix formalism we iterate Eq. (21) once and let

$$G \approx G_o + G_o VPG_o \tag{29}$$

This is then substituted into Eq. (24)

$$G \approx G_x$$

$$G_x = G_o + G_o VPG_o + G_o(1 + VPG_o)\, VQ[E - H_o - (1 + VPG_o)\, VQ + i\epsilon]^{-1}(1+VPG_o) \tag{30}$$

Here also we can simplify by dropping the higher order terms,

$$G \approx G_z$$

$$G_z = G_o + G_o VQ[E - H_o - (1 + VPG_o)\, VQ + i\epsilon]^{-1} \tag{31}$$

or make the intermediate approximation,

$$G \approx G_y$$

$$G_y = G_o + G_o VPG_o + G_o VQ[E - H_o - (1 + VPG_o)\, VQ + i\epsilon]^{-1} \quad . \tag{32}$$

V. THE ZERO RANGE COUPLED CHANNEL MODEL

To compare the projected T-matrix and R-matrix scattering formalisms described above, we will apply them to a simple scattering model which is exactly soluble. We will consider the scattering of s-wave particles in two channels. The scattering will result from a zero range elastic interaction U and a separable zero range interaction V that couples the two channels. The Hamiltonian for this model is just

$$H = H_o + V \tag{33A}$$

$$H_o = H_T(\xi) + T(r) + U(r,\xi) \tag{33B}$$

$$T(r) = \frac{-\hbar^2}{2m} \frac{1}{r} \frac{d^2}{dr^2} r \tag{33C}$$

To define U and V we make use of the two eigenstates of the internal motion Hamiltonian H_T.

$$[\mathcal{E}_\alpha - H_T(\xi)]\, X_\alpha(\xi) = 0 \qquad \alpha = 1,2 \tag{34}$$

$$U(r,\xi) = \frac{-\hbar^2}{2m} \sum_{\alpha=1}^{2} |X_\alpha(\xi)\rangle\left(\frac{1}{r} + b_\alpha\right) \delta(r) \langle X_\alpha(\xi)| \tag{35}$$

$$V(r,\xi) = \frac{\hbar^2}{2m} \sum_{\alpha=1}^{2} \sum_{\beta=1}^{2} \left|\frac{\delta(r)}{r} X_\alpha(\xi)\right\rangle v_o \left\langle \frac{\delta(r)}{r} X_\beta(\xi)\right| \tag{36}$$

Whenever V and U multiply each other, it will be understood that the Dirac delta functions appearing in U are to be evaluated first. Channel 1 will be regarded as the elastic channel.

The wave function for the system, the exact wave function, will be an eigenfunction of H

$$(E - H)\, \Psi_\gamma^{(+)}(r,\xi) = 0 \quad . \tag{37}$$

We will call the eigenfunction of H_o ,

$$(E - H_o)\, \Phi_\gamma^{(+)}(r,\xi) = 0 \quad , \tag{38}$$

the approximate wave function. Let us write

$$\Psi_\gamma^{(+)}(r,\xi) = \sum_\alpha X_\alpha(\xi)\, \psi_{\gamma\alpha}^{(+)}(r)/r \tag{39A}$$

$$\Phi_\gamma^{(+)}(r,\xi) = X_\gamma(\xi)\, \phi_\gamma^{(+)}(r)/r \tag{39B}$$

Then the Schrödinger equations become

$$\left[\frac{d^2}{dr^2} + k_\alpha^2 + (\frac{1}{r} + b_\alpha)\, \delta(r)\right] \psi_{\gamma\alpha}^{(+)}(r) = \delta(r)\, v_o \sum_\beta \psi_{\gamma\beta}^{(+)}(0) \tag{40A}$$

$$\left[\frac{d^2}{dr^2} + k_\alpha^2 + (\frac{1}{r} + b_\alpha)\, \delta(r)\right] \phi_\alpha^{(+)}(r) = 0 \tag{40B}$$

$$k_\alpha^2 = \frac{2m}{\hbar^2}(E - \mathcal{E}_\alpha) \tag{40C}$$

The regular solution of Eq. (40B) can be easily shown to be

$$\phi_\alpha^{(+)}(r) = 2(\frac{m}{\hbar k_\alpha})^{1/2}\, e^{i\delta_\alpha} \sin(k_\alpha r + \delta_\alpha) \qquad k_\alpha^2 > 0 \tag{41A}$$

$$\phi_\alpha(r) = \sqrt{2b_\alpha}\ \ell^{-b_\alpha r} \qquad \frac{\hbar^2\alpha^2}{2m} = \mathcal{E}_\alpha - E > 0 \tag{41B}$$

where

$$\delta_\alpha = -\tan^{-1}(k_\alpha/b_\alpha) \tag{41C}$$

We see that there will be one bound state provided that b_α is positive. The reason for our choice of normalization in Eq. (41A) becomes clear when we rewrite it in the form

$$\frac{\phi_\alpha^{(+)}}{r}(r) = -\left(\frac{m}{\hbar k_\alpha}\right)^{1/2}\left[\frac{e^{-ik_\alpha r}}{ir} - e^{i2\delta_\alpha}\ \frac{e^{ik_\alpha r}}{ir}\right] \tag{42}$$

$$= U_\alpha^{(2)}(r) - e^{i2\delta_\alpha}\ U_\alpha^{(1)}(r)$$

where $U_\alpha^{(1)}$ is the unit current outgoing radial wave function for our problem. The "approximate" Green's function G_o is just

$$G_{o\alpha\beta}(r,r') = \langle r,X_\alpha|(E - H_o + i\epsilon)^{-1}|\ r',X_\beta\rangle \tag{43}$$

$$= -\delta_{\alpha\beta}\ \frac{2m}{\hbar^2 k_\alpha}\ \frac{\sin(k_\alpha r_< + \delta_\alpha)\ e^{i(k_\alpha r_> + \delta_\alpha)}}{r_< r_>}$$

$$= \delta_{\alpha\beta}\ \frac{2m}{\hbar^2}\ g_\alpha(r,r')/rr'$$

The exact scattering wave function can be found by solving the L-S equation for Ψ which reads

$$\psi_{\gamma\alpha}^{(+)}(r) = \delta_{\gamma\alpha}\ \phi_\alpha^{(+)}(r) + g_\alpha(r,0)\ v_o\ \Sigma\ \psi_{\gamma\beta}^{(+)}(0) \tag{44}$$

Setting $r = 0$ and summing over α gives

$$\sum_{\alpha=1}^{2} \psi_{\gamma\alpha}^{(+)}(0) = \phi_{\gamma}^{(+)}(0) \Big/ \left[1 - v_o \sum_{\alpha} g_{\alpha}(0,0)\right] \tag{45}$$

$$= \left(\frac{4m}{\hbar k_{\gamma}}\right)^{1/2} e^{i\delta_{\alpha}} \sin \delta_{\gamma} \Big/ \left[1 + v_o \sum_{\alpha} \frac{e^{i\delta_{\alpha}} \sin}{k_{\alpha}} \delta_{\alpha}\right]$$

This can now be substituted back into Eq. (44) to give

$$\psi_{\gamma\alpha}^{(+)}(r) = 2\left(\frac{m}{\hbar k_{\alpha}}\right)^{1/2} \left\{\delta_{\gamma\alpha} \sin (k_{\alpha} r + \delta_{\alpha}) e^{i\delta_{\alpha}} - \Gamma_{\gamma\alpha} e^{ik_{\alpha} r}\right\} \tag{46A}$$

$$\Gamma_{\gamma\alpha} = \frac{v_o \sin \delta_{\gamma} e^{i\delta_{\gamma}} \sin \delta_{\alpha} e^{i\delta_{\alpha}}}{(k_{\alpha} k_{\gamma})^{1/2} \left[1 + v_o \sum_{\beta=1}^{2} \frac{e^{i\delta_{\beta}} \sin}{k_{\beta}} \delta_{\beta}\right]} \tag{46B}$$

Finally, we note that the unscattered wave function Λ_{α} is given by

$$\Lambda_{\alpha} = X_{\alpha}(\xi)\, \lambda_{\alpha}(r)/r \tag{47A}$$

$$\lambda_{\alpha} = 2\left(\frac{m}{\hbar k_{\alpha}}\right)^{1/2} \sin k_{\alpha} r \tag{47B}$$

Now we are prepared to evaluate the various quantities of interest to us.

The two contributions to the exact transition amplitude are calculated from the definitions given in Eq. (7)

$$T_{\beta\alpha}^{(0)} = - \delta_{\beta\alpha} e^{i\delta_{\alpha}} \sin \delta_{\alpha} = \delta_{\beta\alpha} T_{\alpha} \tag{48A}$$

$$T_{\beta\alpha} = \frac{v_o}{(k_{\beta} k_{\alpha})^{1/2}} \frac{T_{\beta} T_{\alpha}}{(1 - v_o \sum_{\gamma} T_{\gamma} k_{\gamma}^{-1})} = \Gamma_{\beta\alpha} \tag{48B}$$

where by Eq. (42B)

$$T_\gamma = -e^{i\delta_\gamma} \sin \delta_\gamma = k_\gamma (b_\gamma + ik_\gamma)^{-1} \tag{49}$$

Eqs. (7), (48), and (49) provide us with the expressions for the exact transition amplitudes for our system.

VI. APPLICATION OF THE T-MATRIX METHOD TO THE MODEL

Our next task will be to calculate the matrix elements

$$(T_Q)_{\beta\alpha} = \langle \Phi_\beta^{(-)} | T_Q | \Phi_\alpha^{(+)} \rangle \quad , \quad Q = A,B,C \tag{50}$$

of the approximate transition operators T_Q derived from the T-matrix method in Section III. These are to be compared to the exact T-matrix. As a first step we use the definition of V given in Eq. (36) to simplify the approximate expression for $\hat{T}$.

$$V(1 + G_o PV) = Vx \tag{51A}$$

$$x = 1 + \frac{\hbar^2 v_o}{2m} \sum_{\alpha=1}^{2} \sum_{\beta=1}^{2} \langle \frac{\delta(r)}{r} X_\alpha | G_o P | \frac{\delta(r)}{r} X_\beta \rangle \tag{51B}$$

Combining Eqs. (26) and (51) and again making use of Eq. (36) we find

$$T_A = xV + x^2 V[E - H_o - xQV + i\epsilon]^{-1} QV \tag{52}$$

$$= Vx(1 + xy)$$

where

$$y = \frac{\hbar^2 v_o}{2m} \sum_{\alpha=1}^{2} \sum_{\beta=1}^{2} \langle \frac{\delta(r)}{r} X_\alpha | (E - H_o - xQV + i\epsilon)^{-1} Q | \frac{\delta(r)}{r} X_\beta \rangle \tag{53}$$

Similarly, Eqs. (27) and (28) can be written

$$T_B = V(x + y) \tag{54}$$

$$T_C = V(1 + y) \tag{55}$$

The numerical constants x and y depend on the definition of the projection operators P and Q.

The most desirable choice for the projection operator Q would appear to be a projector onto the bound states of H. These are not readily available, so we will take Q to be the projector onto the bound states of H_o.

$$Q = \sum_{\alpha=1}^{2} \left| \frac{e^{-b_\alpha r}}{r} X_\alpha \right\rangle (2b_\alpha) \left\langle \frac{e^{-b_\alpha r}}{r} X_\alpha \right| \tag{56}$$

$$= 1 - P$$

Combining Eqs. (56) and (51) we find

$$x = 1 - v_o \sum_\alpha T_\alpha^* k_\alpha^{-1} = 1 - v_o \sum_\alpha \frac{1}{b_\alpha - ik_\alpha} \tag{57}$$

Combining Eqs. (53) and (56) we find

$$y = z(1 - xz)^{-1} \tag{58A}$$

$$z = 2v_o \sum_{\alpha=1}^{2} \frac{b_\alpha}{b_\alpha^2 + k_\alpha^2} \tag{58B}$$

The last ingredient to go into our evaluation of the approximate T-matrices will be the matrix elements of V.

$$V_{\beta\alpha} = \langle \Phi_\beta^{(-)} | V | \Phi_\alpha^{(+)} \rangle / 2\hbar \tag{59}$$

$$= v_o T_\beta T_\alpha (k_\beta k_\alpha)^{-1/2}$$

Our final result is thus

$$(T_A)_{\beta\alpha} = V_{\beta\alpha}x(1 + xy) \tag{60A}$$

$$(T_B)_{\beta\alpha} = V_{\beta\alpha}(x + y) \tag{60B}$$

$$(T_C)_{\beta\alpha} = V_{\beta\alpha}(1 + y) \tag{60C}$$

This is to be compared with the exact result given in Eq. (48B).

$$T_{\beta\alpha} = V_{\beta\alpha}x^{*-1} = (T_E)_{\beta\alpha} \tag{61}$$

VII. APPLICATION OF THE R-MATRIX METHOD TO THE MODEL

Using the results derived in Section VI we may immediately simplify somewhat Eqs. (30), (31), and (32) for the approximate Green's functions.

$$G_x = G_o + G_o VPG_o(1 + xy) + xG_o VQ[E - H_o - xVQ + i\epsilon]^{-1} \tag{62}$$

$$G_y = G_o + G_o VPG_o + G_o VQ[E - H_o - xVQ + i\epsilon]^{-1} \tag{63}$$

$$G_z = G_o + G_o VQ[E - H_o - xVQ + i\epsilon]^{-1} \tag{64}$$

These expressions are substituted for $(E-H)^{-1}$ in Eq. (15) and the results are used to evaluate the expressions in Eqs. (16), (14), and (7). The calculation is straightforward but somewhat lengthy. We will merely display the results in terms of the resulting T-matrices.

$$(T_x)_{\beta\alpha} = V_{\beta\alpha}(1 - (1 - x)J_\alpha)(1 - xz - (1 - x)K)^{-1} \tag{65A}$$

$$(T_y)_{\beta\alpha} = V_{\beta\alpha}(1 - xz + xzJ_\alpha)(1 - xz + xzK)^{-1} \tag{65B}$$

$$(T_z)_{\beta\alpha} = V_{\beta\alpha}xJ_\alpha(1 - xz + xK)^{-1} \tag{65C}$$

where

$$J_\alpha = 2b_\alpha k_\alpha^{-1} e^{-b_\alpha R} \sin k_\alpha R \tag{66}$$

$$K = 2v_o \sum_{\alpha=1}^{2} \frac{-b_\alpha}{b_\alpha^2 + k_\alpha^2} e^{(ik_\alpha - b_\alpha)R} \tag{67}$$

We see that the dependence on the boundary radius R is contained in J_α and K. For this simple model all dependence on the matching radius $\overline{R}$ cancels out.

VIII. NUMERICAL CALCULATIONS AND COMPARISONS

The cross section σ_{11} for elastic scattering and the cross section σ_{12} for inelastic scattering were calculated from the definition

$$\sigma_{Q\alpha\beta} = \frac{4\pi}{k_\alpha^2} \left| T_{\alpha\beta}^{(0)} + (T_Q)_{\alpha\beta} \right|^2 \tag{68A}$$

$$Q = E, A, B, C, X, Y, Z, V \tag{68B}$$

The subscript E identifies the exact result as shown in Eq. (48B) or Eq. (61). The approximate T-matrix theory results corresponding to subscripts A,B,C are shwon in Eqs. (60A),(60B), and (60C). The subscripts X,Y,Z identify the R-matrix theory results corresponding to Eqs. (65A),(65B), and (65C). The subscript V serves to identify the simple distorted wave Born approximation prediction.

$$(T_V)_{\beta\alpha} = V_{\beta\alpha} \tag{69}$$

It is clear that in the limit as V becomes very small all the approximate results, with one exception, become exact. In this limit

$$V \to 0, \quad x \to 1, \quad y \to 0, \quad K \to 0, \quad z \to 0 \tag{70}$$

Then to first order in V

$$(T_Q)_{\alpha\beta} \to V_{\alpha\beta} \qquad Q = A, B, C, E, X, Y, V \tag{71A}$$

$$(T_Z)_{\alpha\beta} \to V_{\alpha\beta} J_\beta \tag{71B}$$

Aside from this, comparison to the various expressions is not very illuminating. We note that the R-matrix approximate results for T are not symmetric. From the explicit forms it is hard to see just how well the approximate expressions reproduce the exact results. Thus it is necessary to compare the results of numerical evaluation.

The numerical calculations were performed using the following parameters

$$m = 1.0 \text{ AMU}$$
$$\mathcal{E}_1 = 0.0 \text{ MeV}$$
$$\mathcal{E}_2 = 4.0 \text{ MeV}$$
$$B_1 = \hbar^2 b_1^2/2m = 3.0 \text{ MeV}$$
$$B_2 = \hbar^2 b_2^2/2m = 2.0 \text{ MeV}$$

The interaction strength v_o and the boundary radius R were each assigned a range of values. With this choice of parameters we can expect a resonance to occur in the elastic cross section at about 2 MeV. The width of the resonance and the magnitude of the inelastic cross section increase with increasing interaction strength v_o.

In Figs. (1a), (1b), (1c), and (1d) we see a comparison of how well the various approximate treatments reproduce the elastic cross section in the neighborhood of the resonance as a function of the interaction strength v_o. By choosing the values $0.14F^{-1}$, $0.09F^{-1}$, $0.05F^{-1}$, and $0.02F^{-1}$ for v_o, we find the resulting resonance widths to be about 1 MeV, 0.5 MeV, 0.25 MeV, and 0.05 MeV.

The projected T-matrix results are seen to improve as the width is reduced. The approximation T_X is a definite improvement over T_Y and T_Z wherein certain second order terms are neglected. The projected R-matrix result T_A is seen to do very well in the large width case but surprisingly the fit to the exact result deteriorates as the resonance width is reduced. It is also surprising that the projected R-matrix approximations to the T-matrix T_B and T_C give uniformly poor results.

The fact that the fit T_A provides to the exact elastic cross section deteriorates with decreasing resonance width is due to the fact that the optimum choice of the boundary radius R seems to vary with the width. In Figs. (2a) and (2b) we see the v_o=.05 case performed for R = 2.0 F and 3.8 F . The Fig. (1) calculation used R = 2.6 F . The R = 3.8 F result for T_A is an excellent fit to the elastic cross section in the vicinity of the resonance.

We conclude that the second order projected T-matrix formalism can give a good fit to the resonant elastic cross section if the width is less than 0.25 MeV. Retention of all the second order terms gives a noticeable improvement. The second order projected R-matrix formalism can yield a near perfect fit to the resonant elastic cross section provided the boundary radius R is tuned to the appropriate value. For this calculation the retention of all second order terms appears vital.

In Figs. (3a) and (3b) we have plotted the elastic cross sections in the energy range 0-20 MeV for v_o=0.14 F^{-1} and v_o=0.09 F^{-1} . For smaller values of v_o the curves are very nearly coincident. The fits for T_A and T_X are again seen to be pretty good. For some reason, at high energy T_B seems to be the best.

The inelastic cross sections are plotted in Figs. (4a),(4b),(4c), and (4d). As the interaction strength v_o is decreased, the various approximate cross sections, except for that resulting from T_Y, approach the exact result.

The projected R-matrix result, calculated from T_X, does better than the projected T-matrix result, calculated from T_A. It is surprising that T_Y, which is an approximation to T_X, leads to a better result for the inelastic cross section. Similarly, T_B, an approximation to T_A, does better than T_A. This is just the reverse of what we found for the elastic transition probabilities.

It is interesting that the projected T-matrix and R-matrix methods give better inelastic cross sections than does the distorted wave Born approximation given by T_V.

In Figs. (5a) and (5b) are shown inelastic cross sections for interaction strength $v_o=0.05$. In Fig. (5a) the projected R-matrix results were calculated with a boundary radius of $R=3.8$ F, while for the projected R-matrix results shown in Fig. (5b) $R=2.0$ F was used. The inelastic transition probabilities appear to be relatively insensitive to the value of the boundary radius.

IX. DISCUSSION

Our study has revealed several interesting facts. We find that a consistent treatment of second order terms is important in a projected T-matrix formalism and is vital in a projected R-matrix formalism. When all the second order terms are included, then the R-matrix formalism is capable of yielding a result superior to the T-matrix formalism result. Proponents of the T-matrix method have emphasized that their calculations contain no adjustable parameters.

Our results suggest that the presence of the adjustable boundary radius R in the R-matrix method may in fact be advantageous.

In all applications of R-matrix theory one must face the problem of truncating the eigenfunction expansion used to represent the R-matrix. How is one to recover the coherent contribution of the infinite number of distant levels discarded by truncation? Presumably, the introduction of the optical potential through the replacement of G by $G_o + GVG_o$ should go a long way toward ameliorating the injury resulting from truncating an eigenfunction expansion of G. However, the projection operator formalism carries us further still. Herein the truncation is done exactly and the result is the replacement of the interaction V by the effective interaction

$$\hat{T} = (1 - VPG_o)^{-1}V \approx V + VPG_oV .$$

We have seen that if we do truncate drastically but retain the second order contribution to $\hat{T}$ we can do very well. We conclude that unless very many terms are included in the eigenfunction expansion of the R-matrix, it is advisable to replace the interaction V by the (complex) effective interaction $\hat{T}$.

REFERENCES

1. H. Feshbach, Ann. Phys. (N.Y.) 5 (1958) 357, and 19 (1962) 257.
2. W. M. MacDonald, Nuc. Phys. 54 (1964) 393, and 56 (1964) 636.
3. C. Bloch and V. Gillet, Phys. Lett. 16 (1965) 62.
   W. Glöckle, J. Hüfner, and H. A. Wiedenmüller, Nuc. Phys. A90 (1967) 481.
4. R. H. Lemmer and C. M. Shakin, Ann. Phys. 27 (1964) 13.
   L. Garside and W. M. MacDonald, Phys. Rev. 138 (1965) B582.
5. W. Tobocman and M. A. Nagarajan, Phys. Rev. 138 (1965) B1351.
6. R. G. Newton, "Scattering Theory of Waves and Particles" (McGraw-Hill, 1966).
7. A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30 (1958) 257.

FIGURE CAPTIONS

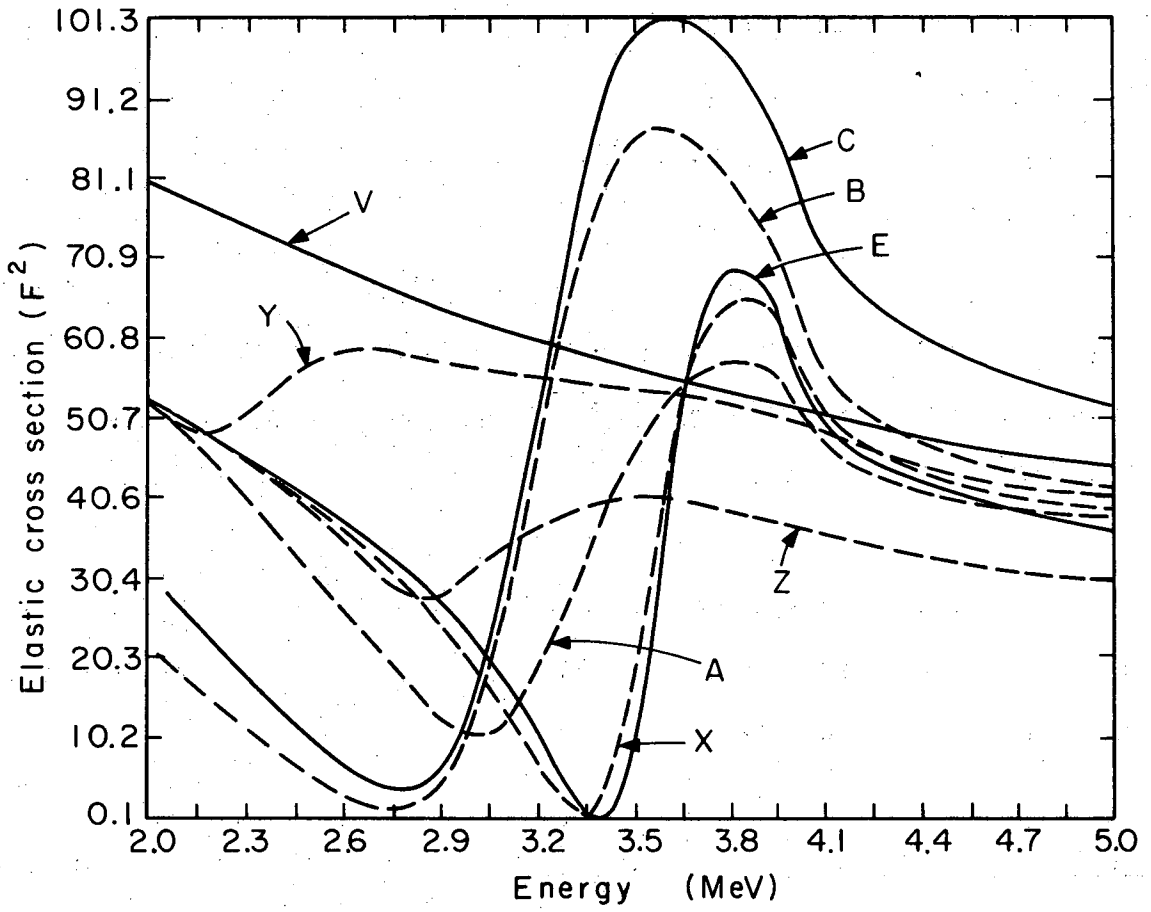
Fig. (1) Elastic scattering cross section calculated from the T-matrix shown in A: Eq. (60A), B: Eq. (60B), C: Eq. (60C), E: Eq. (61), V: Eq. (69), X: Eq. (65A), Y: Eq. (65B), and Z: Eq. (65C). The boundary radius used for curves X,Y, and Z was $R = 2.6$ F . The interaction strength was a: $v_o = 0.14\ F^{-1}$, b: $v_o = 0.09\ F^{-1}$, c: $v_o = 0.05\ F^{-1}$, and d: $v_o = 0.02\ F^{-1}$.

Fig. (2) Elastic scattering cross section calculated as in Fig. (1). The interaction strength was $v_o = 0.05\ F^{-1}$, and the boundary radius was a: $R = 2.0$ F , b: $R = 3.8$ F .

Fig. (3) Elastic scattering cross section calculated as in Fig. (1). The boundary radius used for curves X,Y and Z was $R = 2.6$ F . The interaction strength was a: $v_o = 0.14\ F^{-1}$ and b: $v_o = 0.09\ F^{-1}$.

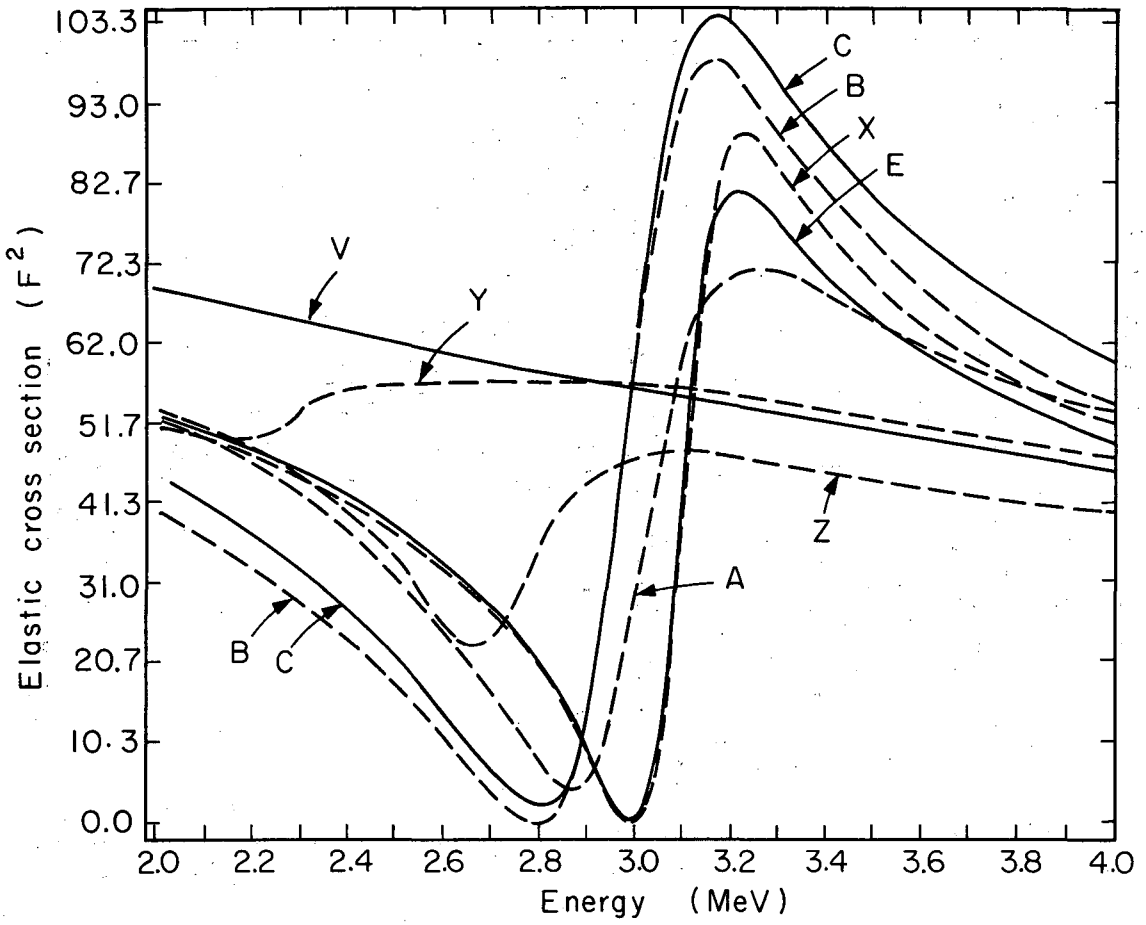
Fig. (4) Inelastic scattering cross section calculated from the T-matrix shown in A: Eq. (60A), B: Eq. (60B), C: Eq. (60C), E: Eq. (61), V: Eq. (69), X: Eq. (65A), Y: Eq. (65B), Z: Eq. (65C). The boundary radius used for curves X,Y, and Z was $R = 2.6$ F . The interaction strength was a: $v_o = 0.14\ F^{-1}$, b: $v_o = 0.09\ F^{-1}$, c: $v_o = 0.05\ F^{-1}$, and d: $v_o = 0.02\ F^{-1}$.

Fig. (5) Inelastic scattering cross section calculated as in Fig. (4). The interaction strength was $v_o = 0.05$, and the boundary radius was a: $R = 3.8$ F and b: $R = 2.0$ F .



XBL678-3996

Fig. 1(a)



XBL678-3995

Fig. 1(b)

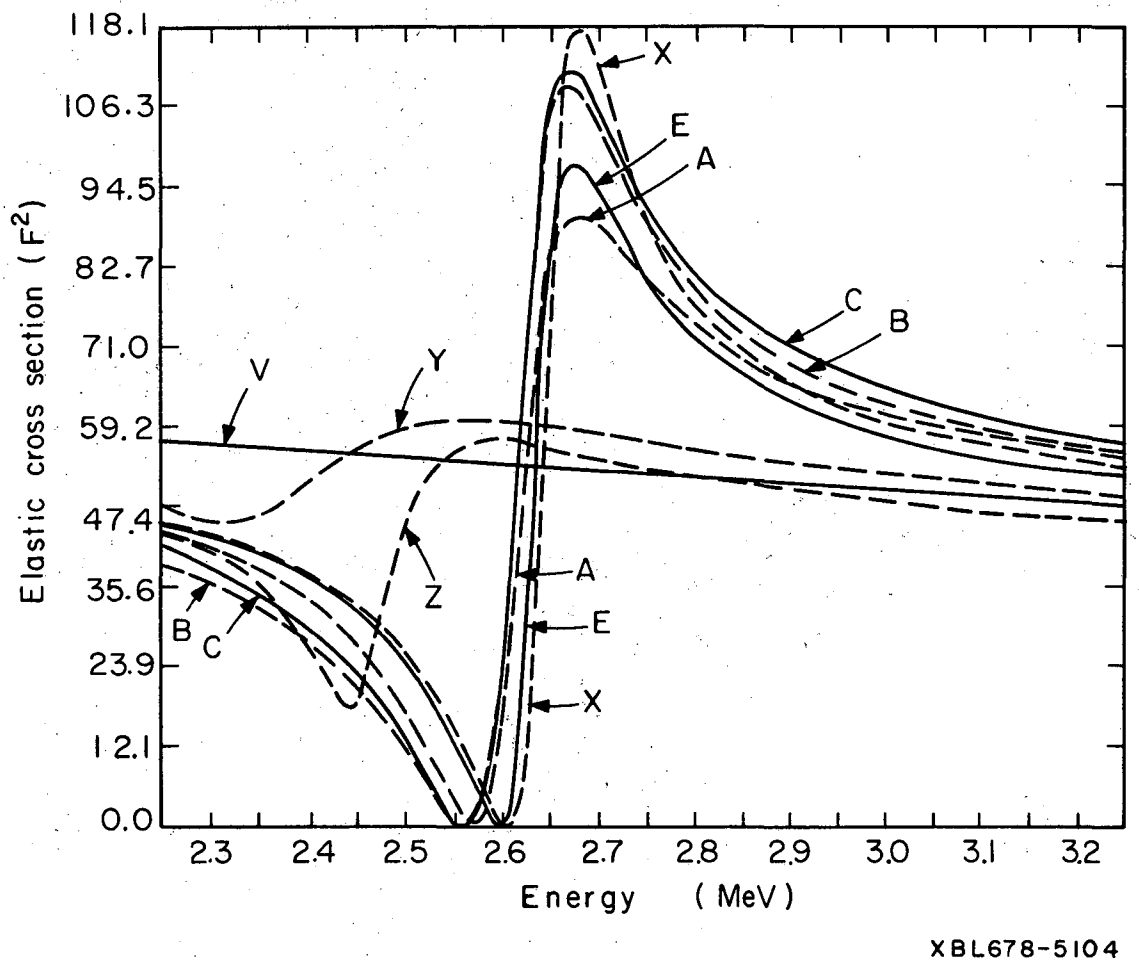

118.1
106.3
94.5
82.7
71.0
59.2
47.4
35.6
23.9
12.1
0.0
Elastic cross section (F^2)
2.3
2.4
2.5
2.6
2.7
2.8
2.9
3.0
3.1
3.2
Energy (MeV)
X
E
A
C
B
V
Y
Z
A
E
X
B
C
XBL678-5104

Fig. 1(c)

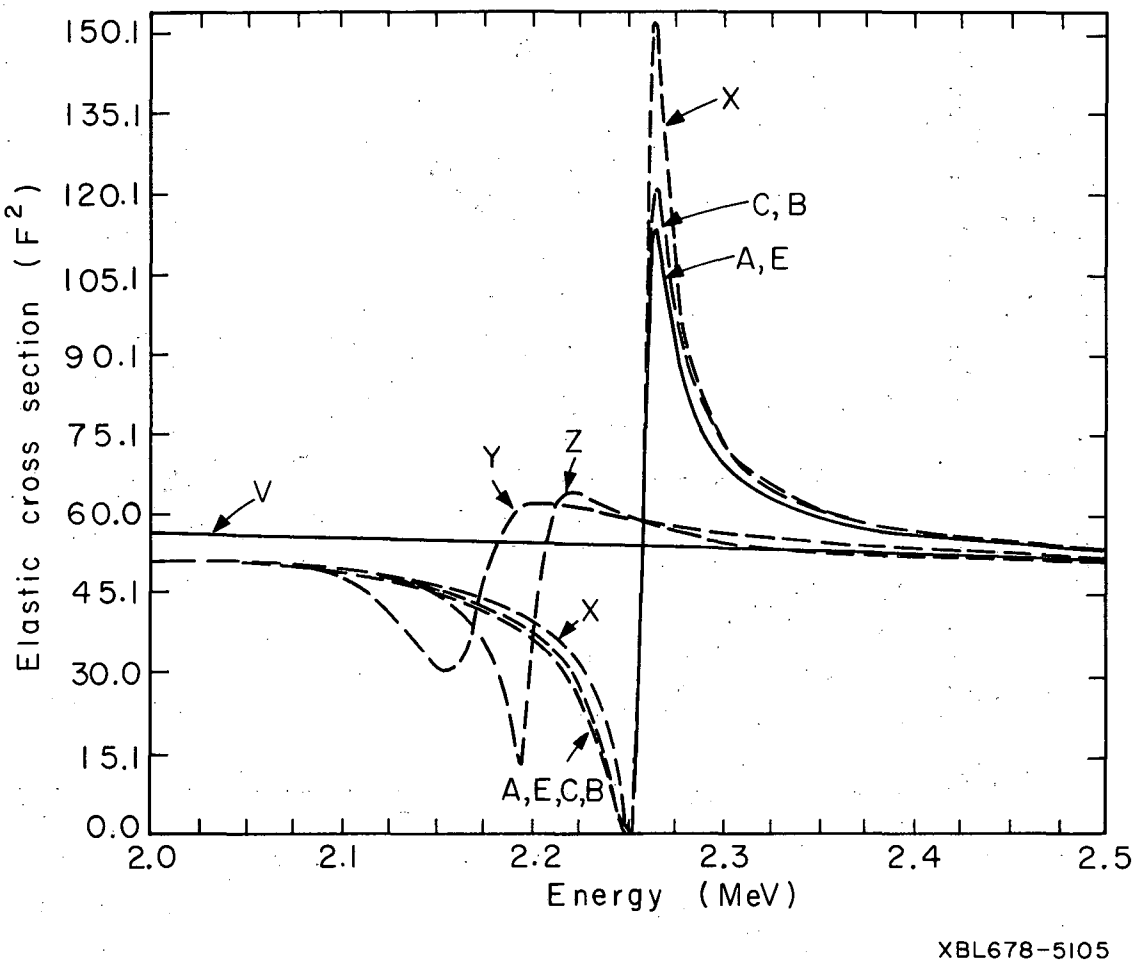

150.1
135.1
120.1
105.1
90.1
75.1
60.0
45.1
30.0
15.1
0.0
Elastic cross section (F^2)
2.0
2.1
2.2
2.3
2.4
2.5
Energy (MeV)
X
C, B
A, E
Y
Z
V
X
A,E,C,B
XBL678-5105

Fig. 1(d)

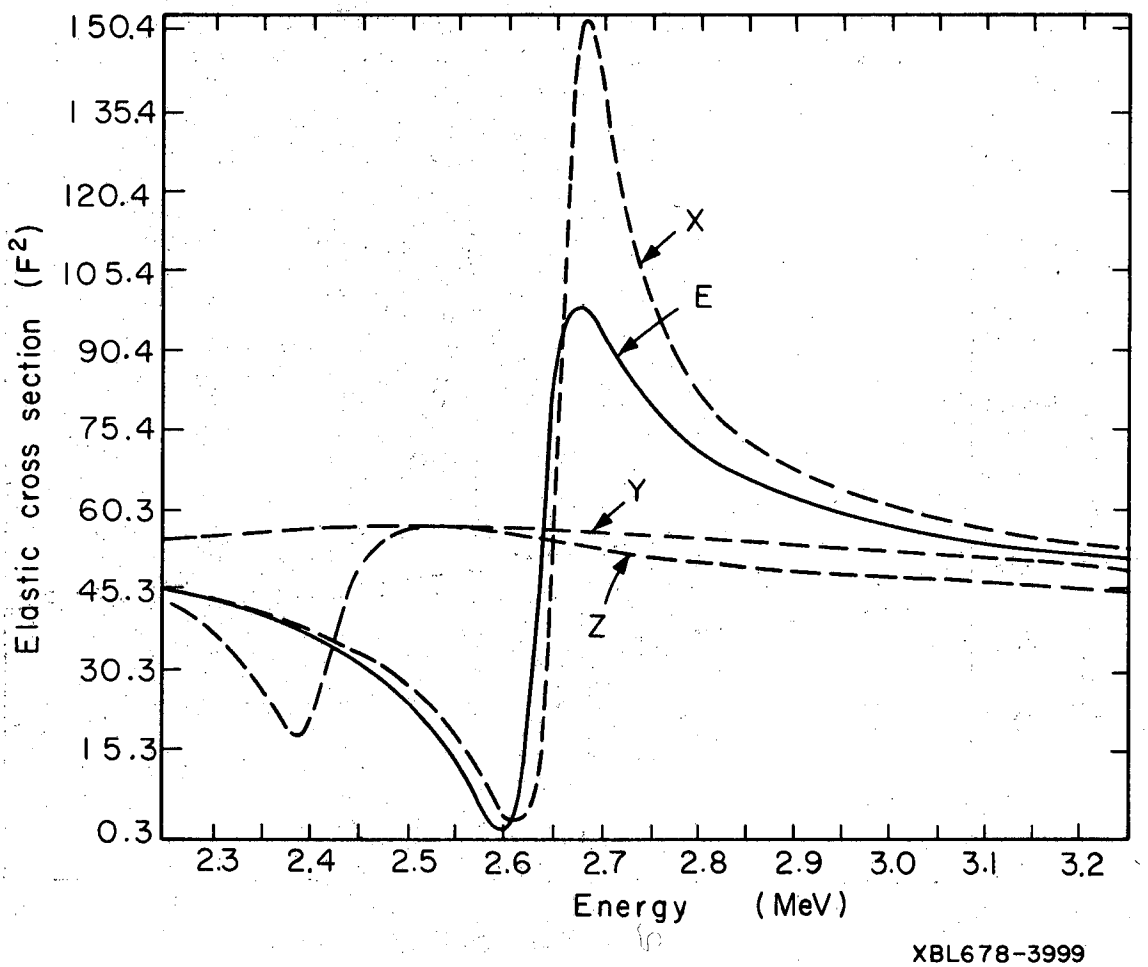
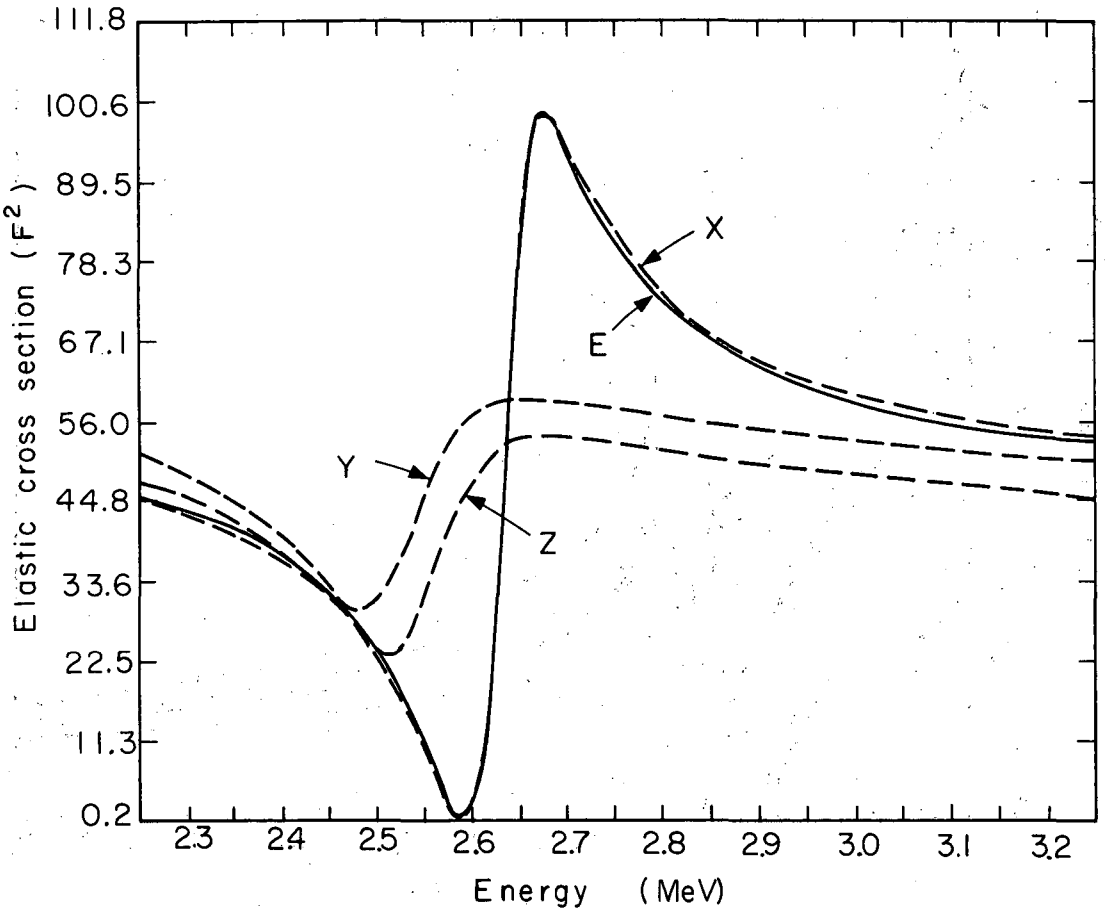

150.4
135.4
120.4
105.4
90.4
75.4
60.3
45.3
30.3
15.3
0.3
Elastic cross section (F^2)
2.3
2.4
2.5
2.6
2.7
2.8
2.9
3.0
3.1
3.2
Energy (MeV)
X
E
Y
Z
XBL678-3999

Fig. 2(a)



XBL678-5103

Fig. 2(b)

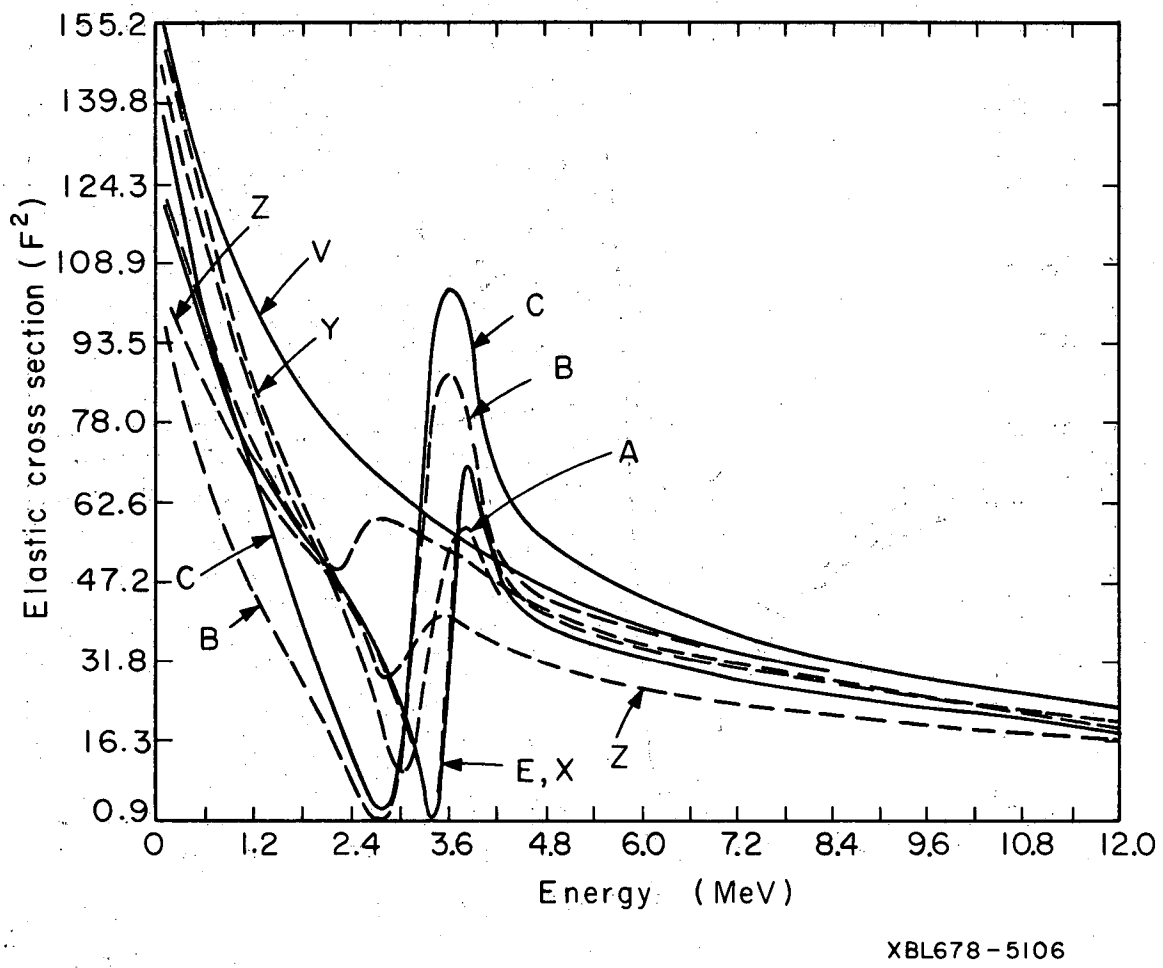
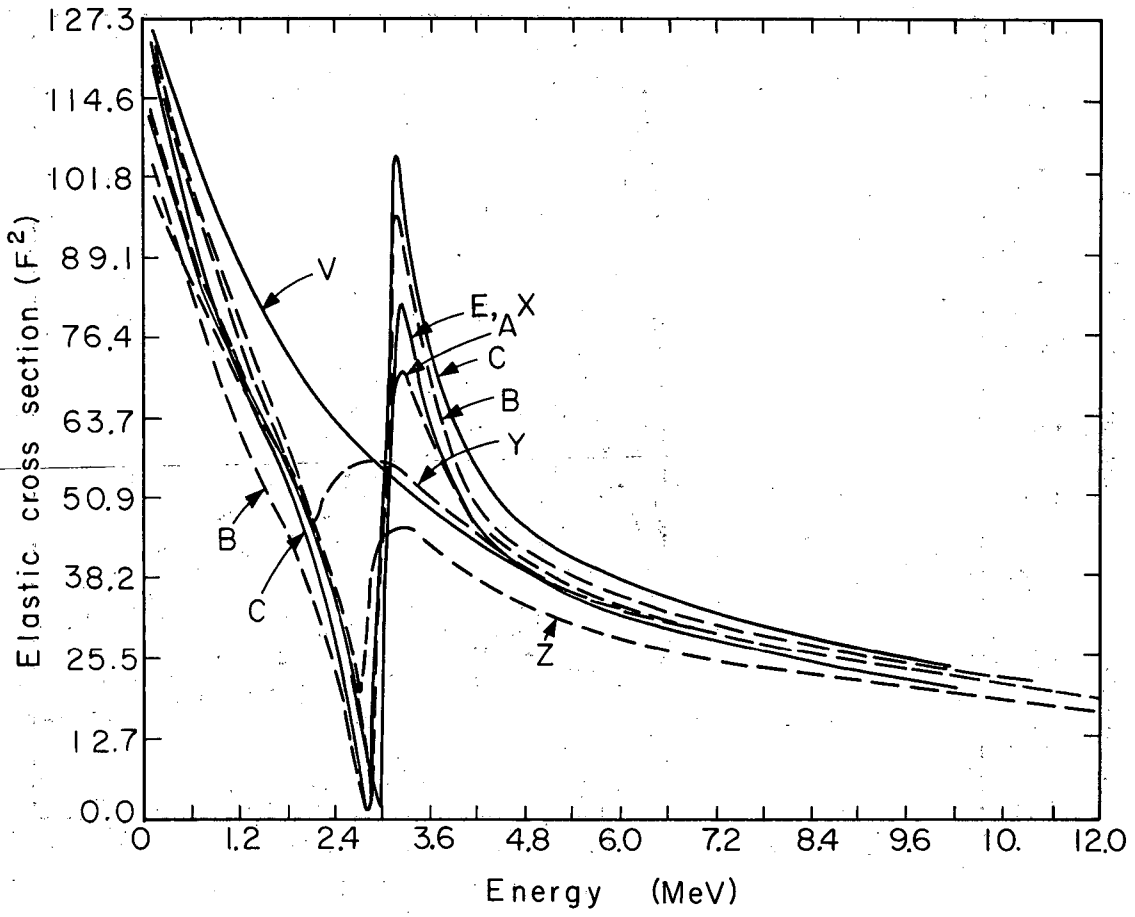
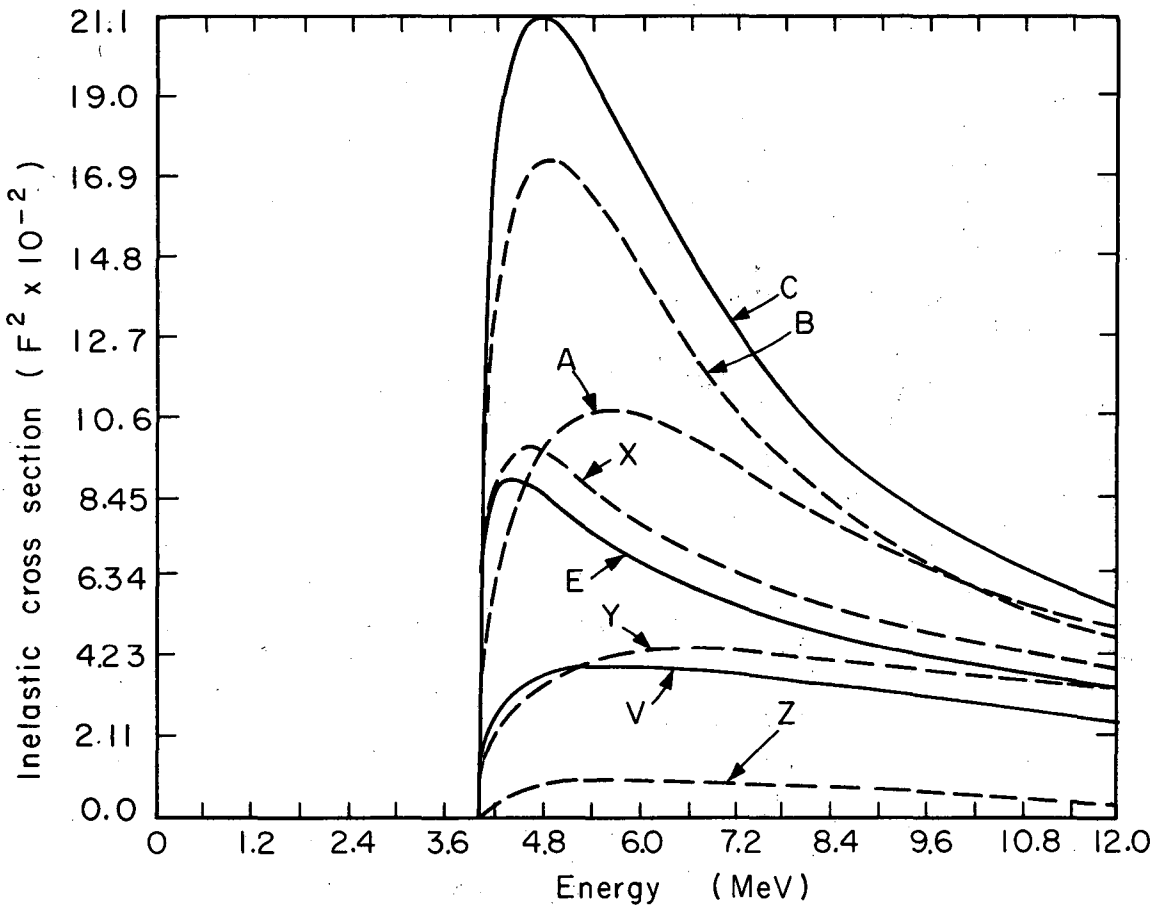

155.2
139.8
124.3
108.9
93.5
78.0
62.6
47.2
31.8
16.3
0.9
Elastic cross section (F^2)
0
1.2
2.4
3.6
4.8
6.0
7.2
8.4
9.6
10.8
12.0
Energy (MeV)
Z
V
Y
C
B
A
C
B
E, X
Z
XBL678-5106

Fig. 3(a)



XBL678-5107

Fig. 3(b)



XBL678-3997

Fig. 4(a)

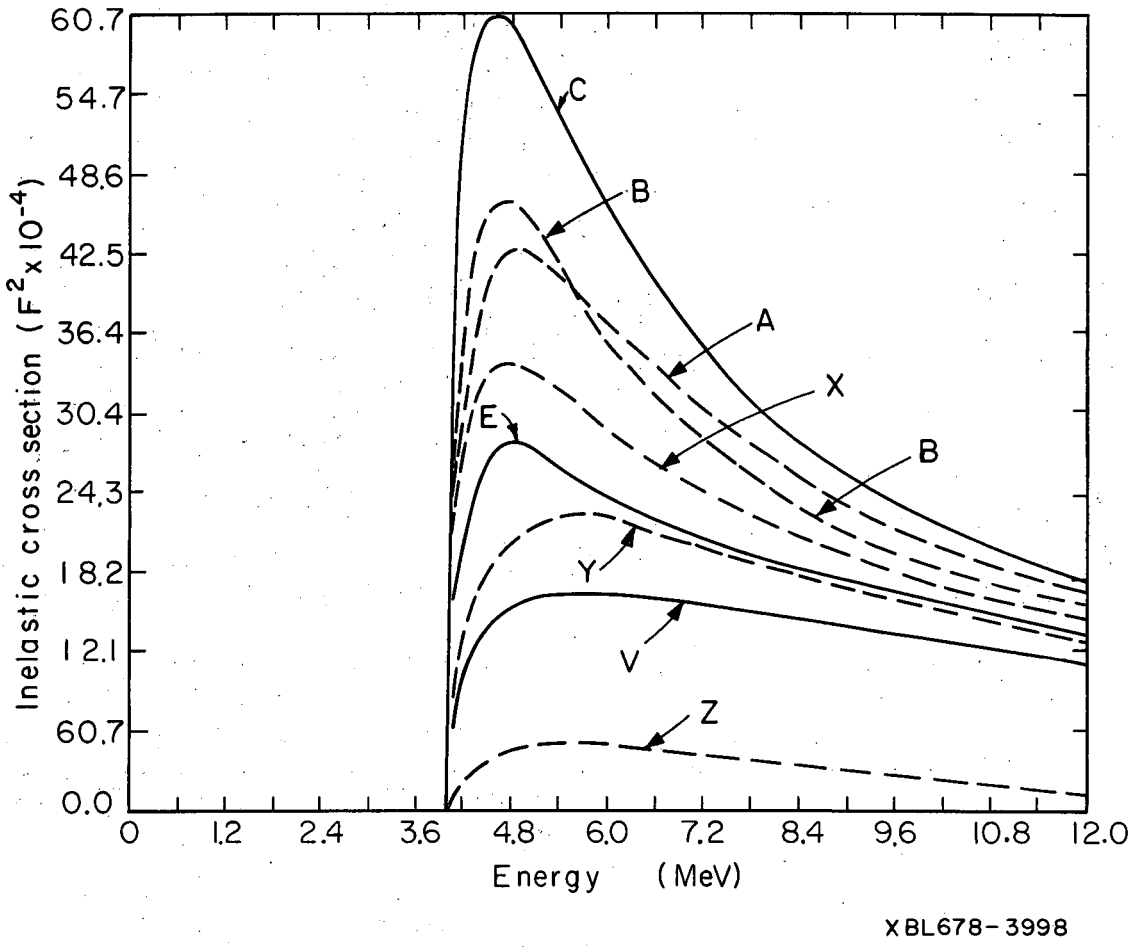

60.7
54.7
48.6
42.5
36.4
30.4
24.3
18.2
12.1
60.7
0.0
Inelastic cross section ($F^2 \times 10^{-4}$)
0
1.2
2.4
3.6
4.8
6.0
7.2
8.4
9.6
10.8
12.0
Energy (MeV)
C
B
A
X
B
E
Y
V
Z
XBL678-3998

Fig. 4(b)

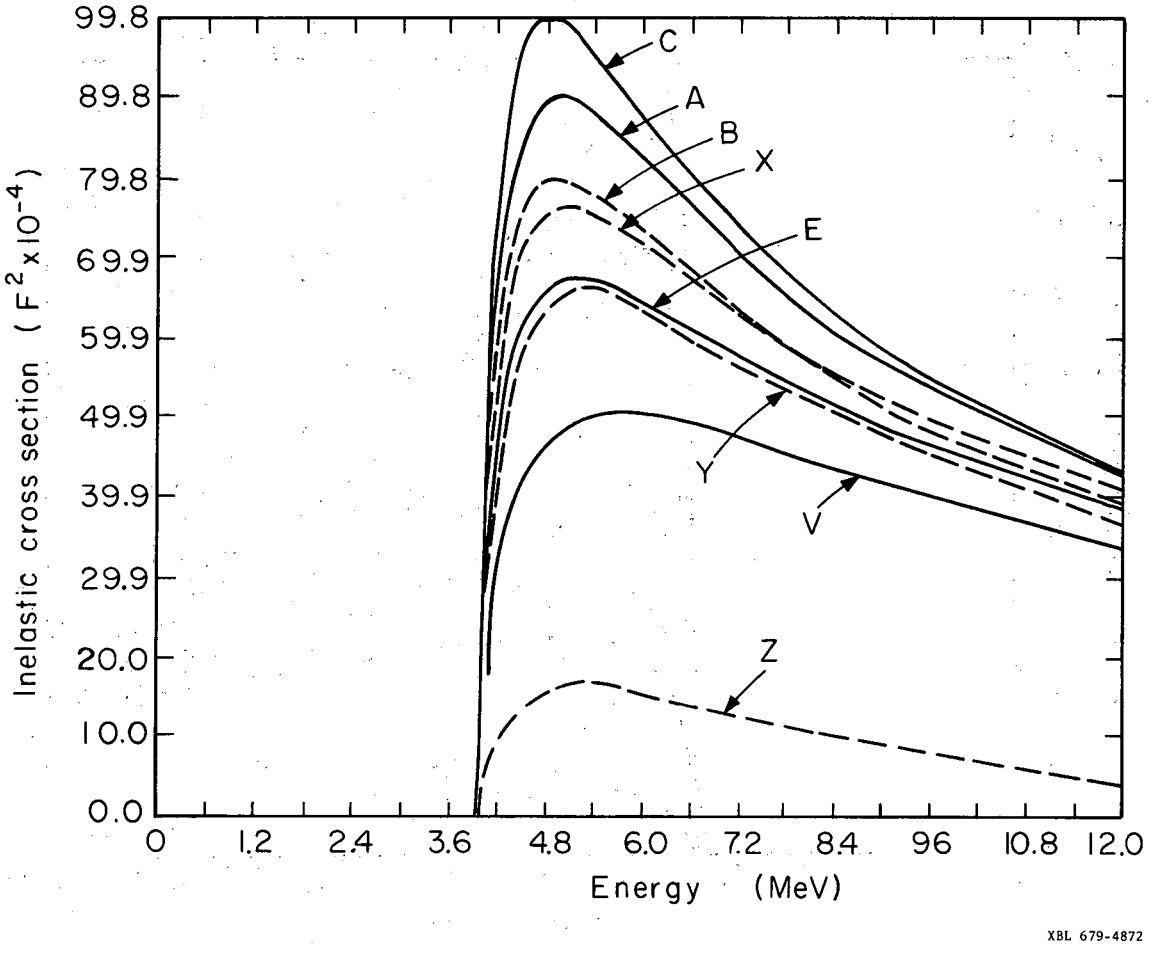

99.8
89.8
79.8
69.9
59.9
49.9
39.9
29.9
20.0
10.0
0.0
Inelastic cross section (F² x 10⁻⁴)
0
1.2
2.4
3.6
4.8
6.0
7.2
8.4
9.6
10.8
12.0
Energy (MeV)
C
A
B
X
E
Y
V
Z
XBL 679-4872

Fig. 4(c)

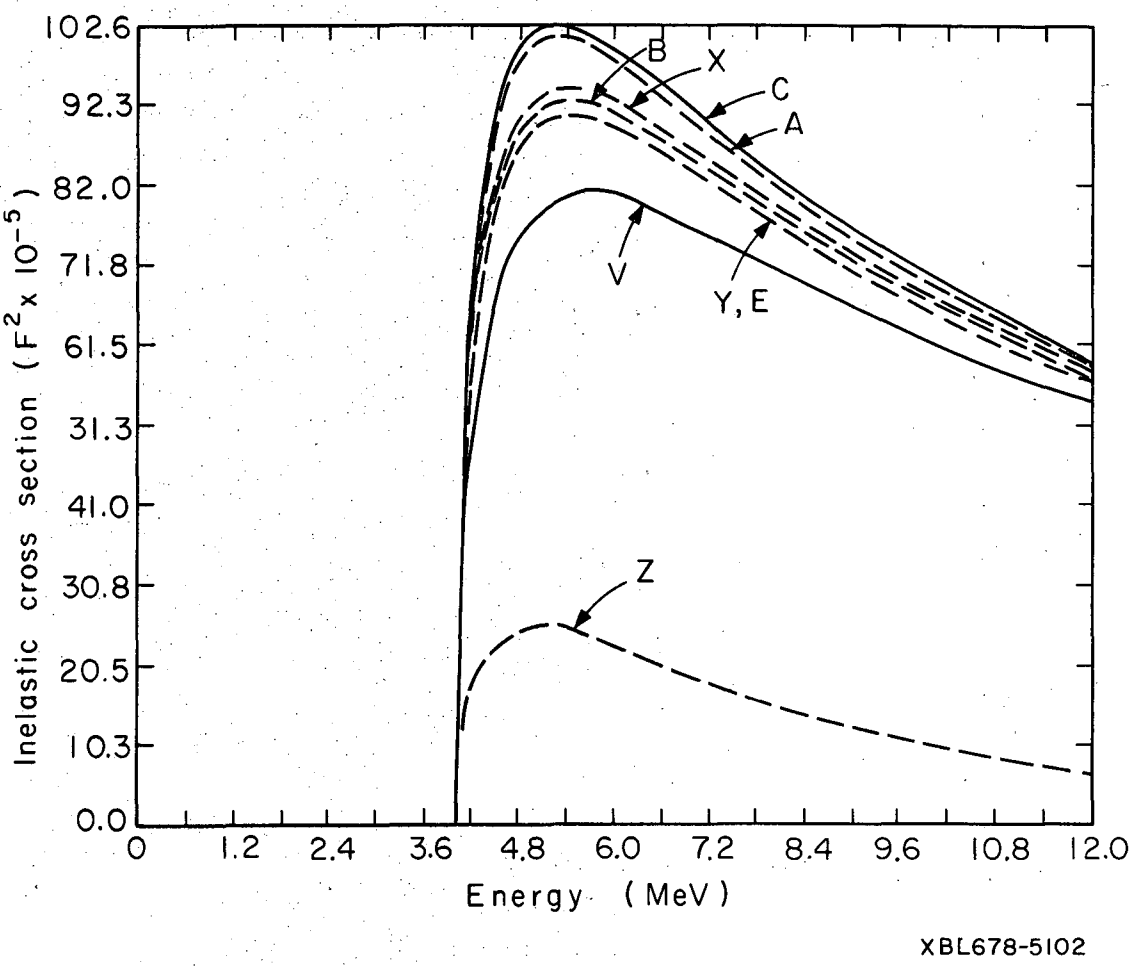
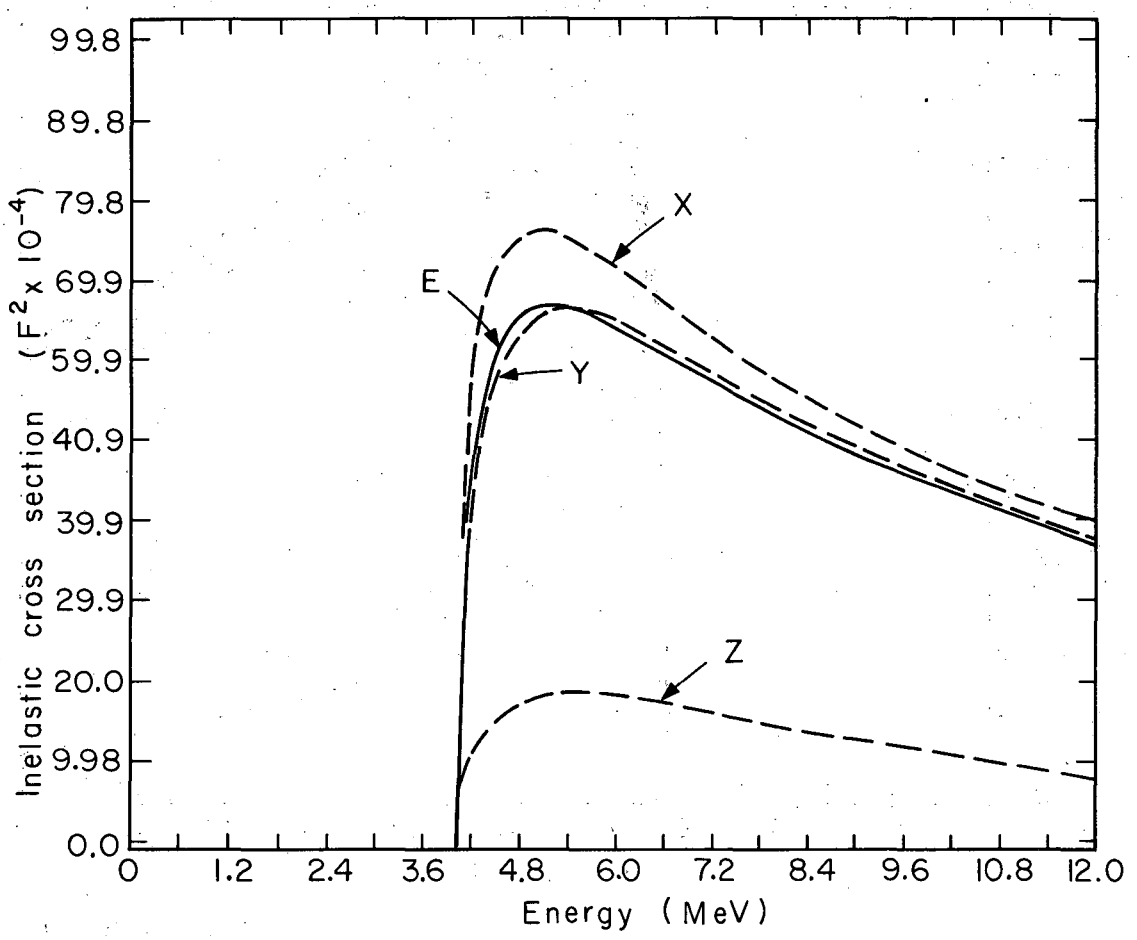

102.6
92.3
82.0
71.8
61.5
31.3
41.0
30.8
20.5
10.3
0.0
Inelastic cross section (F² x 10⁻⁵)
0
1.2
2.4
3.6
4.8
6.0
7.2
8.4
9.6
10.8
12.0
Energy (MeV)
B
X
C
A
V
Y, E
Z
XBL678-5102

Fig. 4(d)



XBL678-5108

Fig. 5(a)

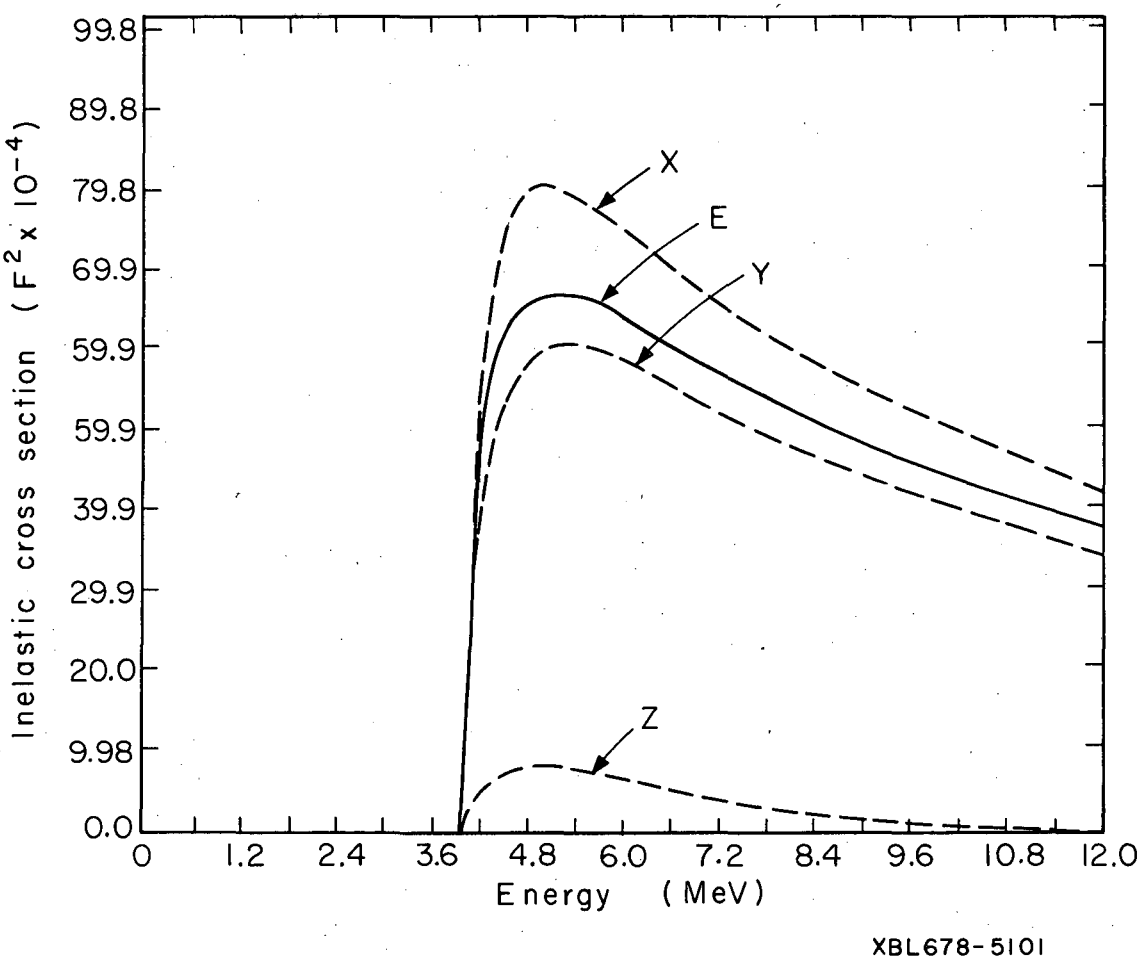

99.8
89.8
79.8
69.9
59.9
59.9
39.9
29.9
20.0
9.98
0.0
Inelastic cross section (F² x 10⁻⁴)
X
E
Y
Z
0
1.2
2.4
3.6
4.8
6.0
7.2
8.4
9.6
10.8
12.0
Energy (MeV)
XBL678-5101

Fig. 5(b)

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.