New treatment of the one-particle continuum in nuclear reaction theory

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A new method is proposed for the treatment of the one-particle continuum in nuclear reaction theory. The method comprises a matrix diagonalisation technique similar to that used in the eigenchannel theory. However, in contrast to the eigenchannel theory, this method does not require the S matrix to be obtained in a diagonal form. It is shown that by a relaxation of this requirement, a numerically much faster method of treating the one-particle continuum can be developed.

1. INTRODUCTION

After an initial period of optimism due to its success in explaining the photonuclear giant dipole resonance microscopically, the Tamm-Dancoff approximation (i.e., the one particle-one hole approximation with only $1\hbar\omega$ transitions considered) has since revealed its inadequacies. The hope of reproducing all the basic features of the photo cross sections through continuum calculations based on this approximation has not been fulfilled. A number of continuum calculations[1-3] performed for different nuclei have shown that only the gross structure of the cross sections can be reproduced, and that the peaks obtained are too high and narrow compared with experiment. It has therefore become clear that although the Tamm-Dancoff scheme of configurations can still be used as a starting point, higher order configurations, collective correlations, or in general, more complicated features must be introduced in order to achieve a better agreement with experimental results.

However, most of the attempts for a better understanding of the structure of the photonuclear cross sections have been made through bound-state calculations. While these calculations can certainly give a clue to the validity and usefulness of the assumption made, it is clear that their interpretation is not totally unambiguous. They are clearly unsuitable if one wants to explain the finer details of the reaction, such as the (γ, p) or (γ, n) cross sections, separately, or the angular distribution of the reaction products.

Several methods of treating the one-particle continuum have now been developed (see, e.g., Refs. 1 and 4), and of these the eigenchannel (EC) method[1] and the coupled channel method have been widely applied.[2,3,5] Both of these methods, however, suffer from disadvantages. The EC method requires a search procedure for the eigenphases of the S matrix, resulting in many diagonalisations of large matrices for each excitation energy at which the cross sections are to be calculated. It therefore proves to be a time-consuming process. On the other hand, the EC method, because of its utilisation of a matrix diagonalisation technique, is easily extended to approximations more sophisticated than the simple Tamm-Dancoff approximation. The coupled channel method, although rather quicker numerically than the EC method for simple cases, is much more difficult to extend to complicated models unless further simplifying approximations are made. Both of these methods have been recently discussed in detail.[1,4]

In this paper we present a new method which retains the flexibility of the EC diagonalisation technique but which is numerically much faster. In fact is it shown in Sec. 3 that only a very small number of diagonalisations are required. This method should therefore be particularly useful in investigations aimed at extending into the continuum region calculations based on the more sophisticated nuclear models. Because of the size of the matrices to be diagonalised in any such model, a treatment of these problems with the EC method is often not practicable. On the other hand, a treatment with the coupled channels technique usually involves severe formal difficulties.

Although so far only photonuclear reactions have been mentioned, the new method involves the calculation of the scattering matrix and so can be applied to other types of nuclear reactions. In fact, in the following, no hypothesis is made about the nature of the particular reaction treated, except for Sec. 5 which is devoted to the explicit derivation of the formulas for the photoreaction cross sections. The method is also general with regard to the complexity of the shell model ap-

proximation treated, except in so far as it is restricted to the case where only one particle at a time is in the continuum.

In Sec. 2 we discuss the discretization of the continuum and the boundary conditions used to this end. Section 3 describes the solution of the nuclear Hamiltonian in the internal region. In Sec. 4 it is shown how the S matrix can be calculated and in Sec. 5 how the formulas for photoreaction cross sections are obtained. Section 6 discusses the treatment of the closed channels, and Sec. 7 contains a summary of the conclusions reached.

2. DISCRETIZATION OF THE CONTINUUM AND BOUNDARY CONDITIONS

We consider the reaction

$$a + X \rightarrow b + Y , \tag{2.1}$$

where a can be any incoming particle and b any outgoing particle. Let Ψ be the wave function describing the compound nucleus system. The nuclear Hamiltonian H can be considered to be composed of two parts,

$$H = H_0 + V , \tag{2.2}$$

where H_0 is a shell model Hamiltonian and V is the residual interaction. H_0 is a sum of single particle operators

$$H_0 = \sum_{i=1}^{A} h_0(i) = \sum_{i=1}^{A} [t(i) + v_0(i)] , \tag{2.3}$$

where $t(i)$ is the kinetic energy operator and $v_0(i)$ is the shell model potential. In the so-called bound state calculations where v_0 is assumed to be a potential of infinite depth we have a denumerably infinite set of discrete energy levels ϵ_j and therefore of wave functions φ_j where

$$H_0 \varphi_j = \epsilon_j \varphi_j . \tag{2.4}$$

The use of a more realistic finite potential introduces the difficulty of a continuous infinite set of basis wave functions which may be discretized by an appropriate choice of boundary conditions, as will be shown later. In the following we denote this discretized set of wave functions by $\{\varphi_j\}$. We may now apply the usual formalism of the bound-state calculations.

The nuclear Schrödinger equation may be written as

$$H \psi_i = E_i \psi_i . \tag{2.5}$$

The nuclear wave function ψ_i can be expanded in terms of the discretized basis $\{\varphi_j\}$, i.e.,

$$\psi_i = \sum_j a_{ij} \varphi_j . \tag{2.6}$$

Substituting Eq. (2.6) into Eq. (2.5), we obtain, as in a bound-state calculation, a system of infinite homogeneous equations

$$\sum_j a_{ij} [(\epsilon_j - E_i)\delta_{jk} + V_{kj}] = 0 , \tag{2.7}$$

where V_{kj} is the matrix element $\langle \varphi_k | V | \varphi_j \rangle$. In order to solve this system of infinite equations, we truncate the basis such that only ν basis functions are considered. The number ν must be sufficiently large so that the basis is reasonably complete. The condition for the system of equations (2.7) to be soluble is the secular equation

$$\det[(\epsilon_j - E_i)\delta_{jk} + V_{kj}] = 0 . \tag{2.8}$$

The solutions of Eq. (2.8) are the eigenvalues E_i of the nuclear Schrödinger equation. We require that one of the eigenvalues E_i be equal to the excitation energy E_x. Clearly with an arbitrary choice of boundary conditions this requirement cannot in general be fulfilled. A particular choice of the basis functions as obtained by a suitable selection of the boundary conditions is necessary.

We divide the configuration space into an external and an internal region, the boundary being a sphere of radius a. The matching radius a is chosen large enough such that all nuclear interactions may be assumed to occur in the inner region, as in the R-matrix theory. In general, the wave function in the asymptotic region can be expressed as

$$\psi_k = \sum_c i v_c^{-1/2} [A_{kc} I_c + B_{kc} O_c] \bar{\psi}_c . \tag{2.9}$$

Here I_c and O_c are the radial parts of the incoming and outgoing particle wave functions in the channel c and $\bar{\psi}_c$ is the wave function of the target or residual nucleus together with the angular parts of the incoming or outgoing particle divided by its radius; the summation is over all open channels. A normalisation factor $v_c^{-1/2}$, where v_c is the relative velocity in channel c, has been introduced so that if A_{kc} or B_{kc} have unit value then the corresponding incoming or outgoing spherical wave has unit flux. The S matrix is then defined by

$$B_{kc} = - \sum_{c'} S_{cc'} A_{kc'} . \tag{2.10}$$

It is possible to choose the A_{kc} such that we obtain a stationary wave solution, i.e., the amplitudes of incoming and outgoing waves in all channels are equal, but there is a phase shift between them. We then obtain for the wave function of the

kth combination in the asymptotic region

$$\psi_k = \sum_c i v_c^{-1/2} V_{kc}[e^{-i\delta_{kc}} I_c - e^{+i\delta_{kc}} O_c]\tilde{\psi}_c . \quad (2.11)$$

The ingoing and outgoing radial wave functions I_c and O_c are defined by

$$I_c^* = O_c = [G_{l_c}(k_c r) + iF_{l_c}(k_c r)]\, e^{-i\omega_c} , \quad (2.12)$$

where

$$k_c = \frac{[2\mu_c(E_x - Q_c)]^{1/2}}{\hbar} .$$

Here F_l and G_l are the regular and irregular solutions of the radial differential equation (i.e., Coulomb functions for protons and spherical Bessel functions and Neumann functions multiplied by $k_c r$ for neutrons). l_c is the orbital angular momentum of the particle in channel c, and ω_c is the Coulomb phase. Finally E_x, μ_c, and Q_c are the excitation energy, reduced mass, and threshold in channel c, respectively.

Substituting Eq. (2.12) into Eq. (2.11) we obtain

$$\psi_k = \sum_c \xi_{kc}(k_c r)\tilde{\psi}_c , \quad (2.13)$$

where

$$\xi_{kc}(k_c r) = 2 v_c^{-1/2} V_{kc}[G_{l_c}(k_c r)\sin(\delta_{kc} - \omega_c) + F_{l_c}(k_c r)\cos(\delta_{kc} - \omega_c)] . \quad (2.14)$$

At this point the difference between the present method and the eigenchannel theory becomes apparent. In the eigenchannel theory it is required that

$$\delta_{k1} = \delta_{k2} = \delta_{k3} = \cdots = \delta_{kn} . \quad (2.15)$$

Condition (2.15) is equivalent to requiring that the S matrix is in a diagonal form. Therefore the wave functions are eigenfunctions of the S matrix, or, as they are called in the eigenchannel theory, eigenchannels. Here no such restriction is required. Therefore the S matrix is no longer diagonal and the wave functions are no longer eigenchannels.

We now proceed to calculate the logarithmic derivative of the asymptotic radial wave function $\xi_{kc}(k_c r)$ at the matching radius a, and impose for the internal radial wave functions u_{cn} the requirement that

$$b_{\text{in}} = b_{\text{out}} , \quad (2.16)$$

where

$$b_{\text{in}} \equiv \left[\frac{r u'_{cn}(\kappa_{cn} r)}{u_{cn}(\kappa_{cn} r)}\right]_{r=a} \quad (2.17)$$

and

$$b_{\text{out}} \equiv \left[\frac{r \xi'_{kc}(k_c r)}{\xi_{kc}(k_c r)}\right]_{r=a} . \quad (2.18)$$

κ_{cn} is the wave number in the internal region; n refers to the radial quantum number.

As mentioned before, a complete basis of single particle wave functions $\{\varphi_i\}$ would require an infinite number of radial quantum numbers, but in order to restrict the dimension of the basis to an acceptable level, only a few radial quantum numbers are kept for every channel. The number of radial quantum numbers kept for each channel c is denoted by ν_c where

$$\nu = \sum_c \nu_c .$$

Usually a value for ν_c of four to six suffices.[6]

Besides requiring that the logarithmic derivatives of the inside and outside wave functions match, we also require that their amplitudes match. We thus write the matching condition for the magnitudes of the outside and inside wave functions as follows:

$$\xi_{kc}(k_c a) = \sum_{n=1}^{\nu_c} a_{k,cn} u_{cn}(\kappa_{cn} a) . \quad (2.19)$$

In the following, for convenience of notation, we substitute a single index i for the two indices c and n. We also refer to the set $\{\varphi_i\}$ connected to the radial parts of the single particle wave functions u_{cn} through the relation

$$\varphi_i = u_{cn}\tilde{\psi}_c . \quad (2.20)$$

From the single particle Schrödinger equation (2.4) and the boundary condition (2.16), we can then obtain the single particle energies ϵ_i and wave functions φ_i and proceed to compute the matrix elements of the total Hamiltonian H [Eq. (2.2)]. The nuclear Hamiltonian in the internal region [Eq. (2.5)] can then be diagonalised [i.e., the secular equation (2.7) may be solved] and the energy eigenvalues E_i obtained. Of course, in general none of the eigenvalues E_i will be equal to the excitation energy E_x.

As we require that one of the eigenvalues

$$E_i = E_x , \quad (2.21)$$

we must vary the set of phases δ_{kc} and repeat the whole procedure until the consistency requirement (2.21) is fulfilled. There are of course a large number of ways of setting up an iteration procedure which eventually leads to the condition (2.21). The EC method is one of these. Due to the restriction (2.15) on the phases in the asymptotic region, the EC method is numerically very waste-

ful, because a large number of time-consuming diagonalisations are needed. In fact the whole procedure must be repeated for every excitation energy E_x because the boundary conditions b_{out} are also a function of the excitation energy. In practice it is found that in a typical one particle-one hole calculation using the EC method (for instance, in ^{16}O; see Ref. 1), about 50 to 100 diagonalisations are required at each energy E_x for which the cross sections are to be calculated.

By relaxing the restriction (2.15), a more efficient search procedure leading to the satisfaction of the consistency condition (2.21) has been developed. Many diagonalisations of large matrices are no longer required at each excitation energy E_x. The new procedure is discussed in detail in the next sections. To illustrate the method we discuss in Secs. 3, 4, and 5 the simple situation when all channels are open. In Sec. 6 the treatment when some channels are closed is discussed.

3. SOLUTION OF THE NUCLEAR HAMILTONIAN IN THE INTERNAL REGION

In the situation where all N channels are open there are N independent degenerate solutions of the nuclear Schrödinger equation (2.5) with an eigenvalue $E_i = E_x$. Therefore we need to find N independent sets of δ_{kc}. This can be achieved by fixing arbitrarily for every $k = k'$, $N-1$ phases $\delta_{k'c}$ and varying the remaining phase $\delta_{k'c'}$ until consistency is achieved. Of course c' is chosen to be different for every different k'. To be more specific, a possible although arbitrary choice can be to assume some fixed boundary conditions for $c \neq k$ and to vary the phase δ_{kc} when $c = k$ for all values of k. Adopting this choice we illustrate now in the case $k = 1$ the search procedure for the phase δ_{11} that leads to a solution of the nuclear Schrödinger equation satisfying the condition (2.21).

For the sake of notational simplicity we rewrite Eq. (2.7) in the following way:

$$\begin{pmatrix} P & V \\ V^\dagger & Q \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = E_x \begin{pmatrix} X \\ Y \end{pmatrix}, \tag{3.1}$$

where

$$P \equiv \begin{pmatrix} \epsilon_1 + V_{11} & V_{12} & \cdots & V_{1\nu_1} \\ V_{21} & \epsilon_2 + V_{22} & \cdots & V_{2\nu_1} \\ \vdots & \vdots & & \vdots \\ V_{\nu_1 1} & V_{\nu_1 2} & \cdots & V_{\nu_1\nu_1} \end{pmatrix}, \tag{3.2}$$

$$Q \equiv \begin{pmatrix} \epsilon_{\nu_1+1} + V_{\nu_1+1\,\nu_1+1} & V_{\nu_1+1\,\nu_1+2} & \cdots & V_{\nu_1+1\,\nu} \\ V_{\nu_1+2\,\nu_1+1} & \epsilon_{\nu_1+2} + V_{\nu_1+2\,\nu_1+2} & \cdots & V_{\nu_1+2\,\nu} \\ \vdots & \vdots & & \vdots \\ V_{\nu_1\,\nu_1+1} & V_{\nu_1\,\nu_1+2} & \cdots & \epsilon_{\nu\nu} + V_{\nu\nu} \end{pmatrix}, \tag{3.3}$$

$$V \equiv \begin{pmatrix} V_{1\,\nu_1+1} & V_{1\,\nu_1+2} & \cdots & V_{1\nu} \\ V_{2\,\nu_1+1} & V_{2\,\nu_1+2} & \cdots & V_{2\nu} \\ \vdots & \vdots & & \vdots \\ V_{\nu_1\,\nu_1+1} & V_{\nu_1\nu_1+2} & \cdots & V_{\nu_1\nu} \end{pmatrix}, \tag{3.4}$$

$$X \equiv \begin{pmatrix} a_{11} \\ a_{12} \\ \vdots \\ a_{1\nu_1} \end{pmatrix}, \tag{3.5}$$

$$Y \equiv \begin{pmatrix} a_{1\,\nu_1+1} \\ a_{1\,\nu_1+2} \\ \vdots \\ a_{1\nu} \end{pmatrix}. \tag{3.6}$$

In Eq. (3.1) we have separated the first ν_1 equations corresponding to the boundary conditions specified by the phase δ_{11} from the other $\nu - \nu_1$ equations that correspond to fixed boundary conditions. To make this separation evident block matrices have been used.

We now proceed to "prediagonalise" the matrix Q making use of the transformation

$$Y = CZ. \tag{3.7}$$

C is a unitary matrix such that the Hermitean matrix Q can be diagonalised with the unitary transformation $C^\dagger QC$, i.e.,

$$C^\dagger QC = \Lambda, \tag{3.8}$$

where Λ is a diagonal matrix, i.e.,

$$\Lambda_{ij} = \lambda_i \delta_{ij}. \tag{3.9}$$

Applying (3.7) and multiplying on the left by the matrix

$$\begin{pmatrix} 1 & 0 \\ 0 & C^\dagger \end{pmatrix},$$

Eq. (3.1) becomes

$$\begin{pmatrix} P & W \\ W^\dagger & \Lambda \end{pmatrix}\begin{pmatrix} X \\ Z \end{pmatrix} = E_x \begin{pmatrix} X \\ Z \end{pmatrix}, \tag{3.10}$$

where

$$W = VC\,. \tag{3.11}$$

The system of equations (3.10) can be rewritten as

$$PX + WZ = E_x X\,, \tag{3.12a}$$

$$W^\dagger X + \Lambda Z = E_x Z\,. \tag{3.12b}$$

We define now a matrix U such that

$$U_{ij} = \prod_{k \neq i} (E_x - \lambda_k)\delta_{ij} \equiv \frac{f\delta_{ij}}{E_x - \lambda_i}, \tag{3.13}$$

where the factor

$$f = \prod_k (E_x - \lambda_k) \tag{3.14}$$

has been introduced to take care of the possibility that one of the λ_k be equal to E_x. In this case the term has to be interpreted here and in the following, not as a division, but as a product of all the factors $(E_x - \lambda_k)$ with $(E_x - \lambda_i)$ excluded.

Making use of the matrix U, Eq. (3.12b) becomes

$$fZ = UW^\dagger X\,. \tag{3.15}$$

Multiplying both sides of Eq. (3.12a) by f and applying Eq. (3.15), Eq. (3.12a) becomes

$$[f(P - \tilde{E}_x) + WUW^\dagger]X = 0\,. \tag{3.16}$$

In Eq. (3.16) $\tilde{E}_x$ denotes the unit matrix (of dimension ν_1) multiplied by E_x. The system of equations (3.16) admits non-zero solutions only if

$$\det[f(P - \tilde{E}_x) + WUW^\dagger] = 0\,. \tag{3.17}$$

The matrix in Eqs. (3.16) and (3.17) is a $\nu_1 \times \nu_1$ matrix whose element i,j is given explicitly by

$$\prod_k (E_x - \lambda_R)\left\{(\epsilon_i - E_x)\delta_{ij} + V_{ij} + \sum_l \frac{(VC)_{il}(VC)^\dagger_{lj}}{E_x - \lambda_l}\right\}. \tag{3.18}$$

As mentioned before, the factor $\prod_k (E_x - \lambda_k)$, introduced to take care of the possibility that one of the λ_k be equal to E_x, can be omitted when this does not happen.

Equation (3.17) is equivalent to Eq. (2.8) but is of course much more convenient in practice since it involves only the calculation of a very small determinant of dimension $\nu_1 = 4 - 6$. Therefore, as we had previously stated, the diagonalisation of a large matrix must be performed only once [Eq. (3.8)] for each desired independent solution of the nuclear Schrödinger equation, and need not be repeated each time for different excitation energies E_x.

The search procedure for the fulfillment of the consistency requirement (2.21) is done by varying only one phase, for instance δ_{11}, and calculating the determinants [Eq. (3.17)] of only the part of the matrix directly connected with the phase δ_{11}. When Eq. (3.17) is satisfied, the eigenvectors are then directly given by Eqs. (3.7) and (3.15), i.e.,

$$Y = \frac{1}{f} CU(VC)^\dagger X\,. \tag{3.19}$$

The eigenvectors X and Y are the coefficients a_{ki} of the expansion (2.6). From them, through Eqs. (2.19) and (2.14), one can easily derive the amplitudes V_{kc} of the wave function in the asymptotic region. As will be apparent later [Eqs. (4.8) and (5.2)], the normalisation of the amplitudes V_{kc} is arbitrary. From the amplitudes V_{kc} and the sets of "consistent" phases δ_{kc}, it is then possible to calculate the S matrix and hence the reaction cross sections. This is shown in the next section.

4. CALCULATION OF THE S MATRIX AND REACTION CROSS SECTIONS

For the purpose of computing the S matrix, it is convenient to rewrite Eq. (2.11) in a matrix form:

$$\psi = T^- \tilde{I} - T^+ \tilde{O}\,, \tag{4.1}$$

where ψ is the column vector of element ψ_k, $\tilde{I}$ and $\tilde{O}$ are, respectively, the column vectors of elements

$$\tilde{I}_c = i v_c^{-1/2} I_c \tilde{\psi}_c \tag{4.2}$$

and

$$\tilde{O}_c = i v_c^{-1/2} O_c \tilde{\psi}_c\,, \tag{4.3}$$

and where $T^\pm$ is the square matrix whose elements are

$$T^\pm_{kc} = V_{kc} e^{\pm i \delta_{kc}}\,. \tag{4.4}$$

Let us consider the following linear combination of ψ_k:

$$\chi = G\psi\,, \tag{4.5}$$

where G is a not yet specified complex matrix. As in the internal region the ψ_k are degenerate solutions of the nuclear Hamiltonian with the common eigenvalue E_x; any linear combination of them will still be a solution of the Hamiltonian with the same eigenvalue E_x. If we now choose

$$G = (T^-)^{-1}\,, \tag{4.6}$$

Eq. (4.5) becomes

$$\chi = \tilde{I} - (T^-)^{-1}T^+\tilde{O}\,. \tag{4.7}$$

Therefore in this basis χ comprising unit flux in one entrance channel only, the S matrix is given by:

$$S = (T^-)^{-1}T^+, \tag{4.8}$$

as may be seen by comparing Eq. (4.7) with Eqs. (2.9) and (2.10).

Once the S matrix has been calculated by means of Eq. (4.8), the calculation of the reaction cross sections for particle-particle reactions is straightforward (see, for instance, Sec. 16.4 of Preston[7]).

5. CALCULATION OF PHOTONUCLEAR CROSS SECTIONS

In the particular case of the photonuclear cross sections it is more convenient to adopt an alternative definition of G:

$$G = (T^+)^{-1} \tag{5.1}$$

so that

$$\chi = (T^+)^{-1}T^-\tilde{I} - \tilde{O}\,. \tag{5.2}$$

This corresponds to the case where for the wave function χ_k unit flux exists in the kth exit channel and zero flux in the other exit channels. The photon channels are then treated perturbatively (see, e.g. Ref. 8).

The multipole matrix element between the ground state $|\text{g.s.}\rangle$ and the transformed state $|\chi_k\rangle$ may be written simply as

$$\langle\chi_k|D^{J\pi}|\text{g.s.}\rangle = \sum_j G_{kj}\langle\psi_j|D^{J\pi}|\text{g.s.}\rangle \tag{5.3}$$

$$= \sum_{ij} G_{kj}\,a_{ji}\langle\varphi_i|D^{J\pi}|\text{g.s.}\rangle\,, \tag{5.4}$$

where $D^{J\pi}$ is the electromagnetic transition operator of multipolarity J and parity π. The partial cross section for a particle leaving the nucleus via channel k following absorption of a photon of energy E_x and spin and parity $J\pi$ is then proportional to the square of the multipole matrix element, i.e.,

$$\sigma_k \propto \left|\sum_{ij} G_{kj}\,a_{ji}\langle\varphi_i|D^{J\pi}|\text{g.s.}\rangle\right|^2, \tag{5.5}$$

the proportionality constant being determined as in Ref. 8. The total photoabsorption cross section σ is then given by the sum of the partial cross sections, i.e.,

$$\sigma = \sum_{i=1}^{N}\sigma_i\,. \tag{5.6}$$

6. TREATMENT OF CLOSED CHANNELS

In Secs. 2–5 we have implicitly assumed that all N channels are open. In the case when some channels are closed some modifications are in order. In fact, when $E_x - Q_c$ is negative the general solution of the asymptotic radial Schrödinger equation is a linear combination of increasing and decreasing exponential functions. To be specific, in the case of N_{op} open channels and $N - N_{\text{op}}$ closed channels Eqs. (2.11) and (4.1) become

$$\psi_k = \sum_{c=1}^{N_{\text{op}}}(T^-_{kc}\tilde{I}_c - T^+_{kc}\tilde{O}_c) + \sum_{c=N_{\text{op}}+1}^{N}(F^-_{kc}\tilde{E}^-_c - F^+_{kc}\tilde{E}^+_c) \tag{6.1}$$

where

$$\tilde{E}^\pm_c = E^\pm_c(\bar{k}_c r)\tilde{\psi}_c \tag{6.2}$$

with

$$\bar{k}_c = \frac{[-2\mu_c(E_x - Q_c)]^{1/2}}{\hbar}\,. \tag{6.3}$$

Here $E^\pm_c(\bar{k}_c r)$ are two independent solutions of the radial differential equation with $E_x - Q_c < 0$, whose asymptotic behaviour is that of $e^{\pm\bar{k}_c r}$, respectively, for neutrons and $\exp[\pm(\bar{k}_c r - \eta\ln 2\bar{k}_c r)]$ for protons. In the case of neutron channels $E^\pm_c$ are the modified spherical Bessel functions multiplied by ρ:

$$\begin{aligned} E^+_c(\rho) &= (\tfrac{1}{2}\pi\rho)^{1/2}I_{l_c+1/2}(\rho)\\ E^-_c(\rho) &= (\tfrac{1}{2}\pi\rho)^{1/2}K_{l_c+1/2}(\rho)\,, \end{aligned} \tag{6.4}$$

where $\rho = \bar{k}_c r$, and I_ν and K_ν are the spherical Bessel functions of the first and third kind, respectively. In the case of proton channels $E^\pm_c$ are Whittaker's functions given by

$$\begin{aligned} E^+_c(\rho) &= e^{-\rho}\rho^{l_c+1}M(l_c+1-\eta_c, 2l_c+2, 2\rho)\,,\\ E^-_c(\rho) &= e^{-\rho}\rho^{l_c+1}U(l_c+1-\eta_c, 2l_c+2, 2\rho)\,, \end{aligned} \tag{6.5}$$

where $M(a,b,z)$ and $U(a,b,z)$ are Kummer's functions. Finally $F^\pm_{kc}$ are arbitrary constants that can be used, just as the δ_{kc} in the case of open channels, to obtain a matching of the inside and outside wave functions and logarithmic derivatives, according to the arbitrary boundary conditions prefixed as explained in Sec. 3.

In the block matrices notation of Sec. 3, Eq. (6.1) becomes

$$\begin{pmatrix}\psi\\ \bar{\psi}\end{pmatrix} = \begin{pmatrix}T^- & F^-\\ \bar{T}^- & \bar{F}^-\end{pmatrix}\begin{pmatrix}\tilde{I}\\ \tilde{E}^-\end{pmatrix} - \begin{pmatrix}T^+ & F^+\\ \bar{T}^+ & \bar{F}^+\end{pmatrix}\begin{pmatrix}\tilde{O}\\ \tilde{E}^+\end{pmatrix}, \tag{6.6}$$

where ψ, $T^\pm$, $F^\pm$ have the same meaning as ψ, $T^\pm$, $F^\pm$ in Eq (6.1) except that they refer here only to values of the index k between 1 and N_{op}, while $\bar{\psi}$, $\bar{T}^\pm$, $\bar{F}^\pm$ also have the same meaning as ψ, $T^\pm$, $F^\pm$

in Eq. (6.1), but they refer to values of k between $N_{op}+1$ and N. Since we need only N_{op} independent solutions for the calculation of the S matrix and of the cross sections we consider only the following N_{op} linear combinations of ψ_k:

$$\chi = G\psi + \bar{G}\bar{\psi}\,, \tag{6.7}$$

where G and $\bar{G}$ are two not yet specified complex matrices of dimensions $N_{op}\times N_{op}$ and $(N-N_{op})\times N_{op}$, respectively, and χ is a column vector with N_{op} elements. From Eq. (6.6) it follows

$$\chi = (GT^- + \bar{G}\bar{T}^-)\tilde{I} - (GT^+ + \bar{G}\bar{T}^+)\tilde{O} + (GF^- + \bar{G}\bar{F}^-)\tilde{E}^- - (GF^+ + \bar{G}\bar{F}^+)\tilde{E}^+. \tag{6.8}$$

In order to achieve the right asymptotic behaviour for all χ_k we require that the coefficient of $\tilde{E}^+$ disappears, i.e.,

$$GF^+ + \bar{G}\bar{F}^+ = 0\,. \tag{6.9}$$

Also the term with $\tilde{E}^-$ can be neglected in the asymptotic region, so that asymptotically we have

$$\chi = (GT^- + \bar{G}\bar{T}^-)\tilde{I} - (GT^+ + \bar{G}\bar{T}^+)\tilde{O}\,. \tag{6.10}$$

Now when we want to calculate the S matrix we require unit flux in the entrance channel, as in Eq. (4.7), and this can be achieved by imposing the condition

$$GT^- + \bar{G}\bar{T}^- = 1\,. \tag{6.11}$$

Conditions (6.9) and (6.11) can be simultaneously satisfied if we select

$$G = (T^- - f\bar{T}^-)^{-1}, \qquad \bar{G} = -Gf\,, \tag{6.12}$$

where

$$f = F^+(\bar{F}^+)^{-1}\,. \tag{6.13}$$

Under these conditions the S matrix becomes

$$S = GT^+ + \bar{G}\bar{T}^+ = (T^- - f\bar{T}^-)^{-1}(T^+ - f\bar{T}^+)\,. \tag{6.14}$$

If, however, one wants to calculate photonuclear cross sections, it is more convenient to have unit flux in the outgoing channels as in Eq. (5.2). This can be obtained by imposing the condition

$$GT^+ + \bar{G}\bar{T}^+ = 1\,. \tag{6.15}$$

Conditions (6.9) and (6.15) can be simultaneously satisfied if we select

$$G = (T^+ - f\bar{T}^+)^{-1}, \qquad \bar{G} = -Gf\,, \tag{6.16}$$

where f is given by Eq. (6.13). Under these conditions Eq. (6.10) becomes

$$\chi = (GT^- + \bar{G}\bar{T}^-)\tilde{I} - \tilde{O} = (T^+ - f\bar{T}^+)^{-1}(T^- - f\bar{T}^-)\tilde{I} - \tilde{O}\,. \tag{6.17}$$

One can then proceed exactly as in Sec. 5.

7. CONCLUSION

Although different methods of treating the one-particle continuum in the theory of nuclear reactions have been proposed in the literature, and two of them (the coupled channel and EC methods) have been extensively used, neither of these methods is completely satisfactory. The method described here retains the diagonalisation technique of the EC theory which has proved to be particularly convenient for the extension of the nuclear model beyond the simple Tamm-Dancoff approximation usually considered. At the same time the computation time required has been drastically reduced with respect to the normal eigenchannel calculation by releasing the condition that the S matrix be obtained in a diagonal form.

The method proposed here is not intended to give in itself better results than the previous theories when applied to the same nuclear model. However, because of the ease with which it can be extended to more sophisticated models and its short computation time, it is hoped that it will enable the investigation of more realistic nuclear models than have so far been treated, and thus aid in the search of a better understanding of the nuclear physics involved in the process of nuclear reactions.

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