

ISTITUTO NAZIONALE DI FISICA NUCLEARE

Laboratori Nazionali di
Legnaro

INFN/BE-79/5
14 Maggio 1979

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S. S. Ahmad: ON A ONE-PARTICLE IN CONTINUUM APPROACH FOR THE PHOTOREACTION CROSS SECTIONS^(*).

SUMMARY.

A formalism for calculating the photonuclear reaction cross sections has been developed by extending a natural boundary condition method employed so far for the accurate description of the nucleon induced reactions from a definite nuclear model. The comparison of the present approach with some coupled-channels type methods for one-particle continuum treatment is also discussed.

RIASSUNTO.

E' stato sviluppato un formalismo per il calcolo delle sezioni d'urto di reazione fotonucleare; partendo dal metodo della condizione al contorno naturale, fino ad ora impiegato sulla base di un prefissato modello nucleare per la descrizione accurata delle reazioni indotte da nucleoni. Il presente approccio viene confrontato con alcuni metodi di canali accoppiati per il trattamento di una particella nel continuo.

INTRODUCTION.

The continuum shell model ideology has been regarded as a convenient framework for carrying out the dynamical calculations of typical reaction processes. It has been used mainly to interpret the origin of the resonances observed in the elastic, inelastic and photodisintegration reactions by analysing the corresponding reaction cross section over a wide energy range by taking into account the appropriate model potentials. PHILPOTT⁽¹⁾, however, has recently pointed out that apart from its remarkable success, the presently available continuum shell model calculations are still quite primitive in comparison with the standard nuclear structure calculations and there is much scope for advancement through the development of valid approximation techniques and more automated calculational approach.

(*) Work supported in part by INFN under the contract No. 720: 6/10/78

In this spirit, the present work deals with the extension of a natural boundary condition method for studying the photonuclear reactions within the framework of a one-particle in continuum formalism. The underlying methodology of this approach is essentially the one employed by B. A. ROBSON and coworkers⁽²⁻⁵⁾ in the iterative R-matrix method for calculating the cross sections as one of the alternative approaches to the standard coupled-channels calculations⁽⁶⁾. Since the observed photonuclear reactions can be regarded as a proper nuclear reaction phenomenon, the main motivation behind the present approach is the belief that a method formulated for the direct calculation of the nuclear reaction cross sections may also be appropriate for studying the photonuclear reactions including those involving the giant resonance excitations.

As well-known⁽⁷⁻⁹⁾, the central idea is to construct a total nuclear wave function of the A-particles system in terms of reactions initiated by a nucleon incident on the target containing (A-1) particles. Of course, in practice, only the components of predominant importance in the treatment of the photonuclear resonances - for example the channels with total quantum numbers $J^{\pi} = 1^{-}$, corresponding to the excited A-particles system - will be of major concern. This can be utilized in evaluating the probability amplitude for the decay into a ground state through the photon emission. Consequently, one may calculate the radiative capture cross section which in turn enables one to calculate the photodisintegration cross section through the employment of standard techniques.

The present work emphasizes upon an alternative approach for handling the construction of the total wave function incorporating the discrete and continuum effects in the A-particles system appearing in the methodology mentioned above. This is of considerable importance since the conventional calculating techniques are very time consuming owing to the fact that in the resonance region the continuum seems to vary so rapidly that a satisfactory numerical integration requires a very dense mesh and hence the inversion of extremely large matrices. Thus, because of the necessity of saving computer time and storage requirements, either many useful ingredients are sometimes left out of the model⁽¹⁰⁾ or, in some cases, the numerical solution becomes quite impracticable⁽¹¹⁾. Hence it seems worthwhile tackling the same problem from alternative viewpoints which may not be only merely efficient but also help in accumulating rather refined information and, perhaps, a wider understanding of the otherwise relatively less satisfactory interpretations and calculated results.

The plan of the paper is as follows. Section 2 describes the present approach for the one-particle in continuum treatment of photonuclear resonance reactions together with the necessary ingredients for calculating the corresponding cross section. A detailed discussion on the comparison of this approach with some of the contemporary coupled-channels type methods is given in Section 3.

2. - FORMULATION OF THE METHOD.

In order to present the overall formulation in a transparent form, this section is subdivided into three parts. Starting from a brief description of the necessary ingredients and an unambiguous definition of the various notations for the formulation (Subsect. 2.1), the actual method for constructing the total nuclear wave function is given in Subsect. 2.2. Finally the formulas for calculating the photodisintegration cross sections are recalled in subsection 2.3; for the sake of completeness.

2.1. - The basic ingredients.

Consider a reaction initiated by a single nucleon with the (A-1) nucleons target such that all the nuclear interactions occur in the internal region of the configuration space where the surfaces of the boundaries are defined by the channel radii a_c ; as in the reaction formulation of LANE and D. ROBSON⁽¹²⁾. Let ψ be the complete wave function corresponding to the A-nucleons system and may be expanded in the eigenstates of total angular momentum J such that

$$\psi = \sum_c u_c(r_c) |c\rangle \quad (1)$$

where the antisymmetrized channel surface functions $|c\rangle$ incorporate the target-nucleon angular momentum coupling in the standard fashion, viz.

$$|c\rangle = \mathcal{A} \left[\sum_{m M_\nu} C(j I_\nu J | m M_\nu M) Y_{\ell(1/2)j}^{m_\ell}(\hat{r}_A) \Phi_{I_\nu M_\nu}(r_1, r_2, \dots, r_{A-1}) \right] \quad (2)$$

and the operator \mathcal{A} antisymmetrizes the particle states (with space and spin coordinates denoted by \underline{r}_A) with that of target $\Phi_{I_\nu M_\nu}(r_1, r_2, \dots, r_{A-1}) \equiv |\Phi_\nu\rangle$.

The antisymmetrized target wave functions satisfy the orthogonality relation $\langle \Phi_\mu | \Phi_\nu \rangle = \delta_{\mu\nu}$ and the channel radii are chosen such that the wave function and its first radial derivative vanish at the corresponding surface; as described in detail by BARRETT and B. A. ROBSON⁽⁴⁾. Although the excitation energies ω_ν of the target spectrum can be calculated satisfactorily by adopting an appropriate procedure for the spherical or deformed nuclei⁽¹³⁾ with a suitable target Hamiltonian through the relation

$$(H_\Gamma - \omega_\nu) |\Phi_\nu\rangle = 0, \quad (3)$$

the quantities ω_ν may be taken from the observed data so that a correct threshold behaviour may be ensured.

The single-particle wave functions

$$\varphi_i(r_i) = \sum_{m_\ell m_s} C(\ell \frac{1}{2} j | m_\ell m_s m) i^\ell Y_{\ell m_\ell}(\hat{r}_i) \chi_{(1/2)m_s}(r_i) u_i(r_i) \quad (4)$$

satisfy the orthogonality relation $\langle \varphi_i | \varphi_j \rangle = \delta_{ij}$ over the internal region and are such that their logarithmic derivative are independent of the radial quantum number (which is amalgamated in the subscript i with the spin and angular momentum quantum numbers) at the matching boundary. The single-particle Hamiltonian ($H_{s.p.}$) is assumed to incorporate the potential

$$V_{s.p.}(r_i) = -v_o f(r_i) + v_{s.o.} \frac{1}{r_i} \frac{df(r_i)}{dr_i} \underline{\sigma} \cdot \underline{\ell} + v_{Coul}(r_i) \quad (5)$$

where $1/2\underline{\sigma}$ and $\underline{\ell}$ denote the spin and orbital angular momentum operators of the nucleon and $v_o, v_{s.o.}$ are the strengths of the central and spin-orbit potentials with a suitable form factor $f(r_i)$ and the Coulomb potential $v_{Coul}(r_i)$ for the incident proton. The employment of a suitable nuclear form factor - for example the Saxon-Woods type - generates the corresponding energy spectrum with a discrete and a continuum part through the equation

$$(H_{s.p.} - \epsilon_i) |\varphi_i(r_i)\rangle = 0 \quad (6)$$

At this stage it may be convenient to introduce the total Hamiltonian of the system, viz.

$$H = H_{s.p.} + H_T + V_R \quad (7)$$

where $H_0 (= H_{s.p.} + H_T)$ is assumed to be diagonal in the channel space and generates the antisymmetric basic states $\xi_i(\underline{r}_1, \underline{r}_2, \dots, \underline{r}_A)$ which will be assumed⁽¹⁴⁾ to form an orthonormal set. Moreover, one may note that

$$\langle c' | c \rangle = \delta_{cc'}, \quad \text{and} \quad \langle c' | \xi_i \rangle = u_i(r_{c'}) \delta_{ic'}. \quad (8)$$

Finally, as is customary^(7-10, 15-17), the residual interaction may be taken of the form of a zero-range force with a Soper mixture, e. g.

$$V_R(\underline{r}_i, \underline{r}_j) = V_o \delta(\underline{r}_i - \underline{r}_j) (a_o + a_\sigma \underline{\sigma}_i \cdot \underline{\sigma}_j) \quad (9)$$

where the parameters V_o, a_o and a_σ are to be taken according to the specific reaction.

2. 2. - The Method.

Consider the Bloch-Schrödinger equation corresponding to the Hamiltonian H of eq. (7) in the form

$$\left[H - \mathcal{L}(\underline{b}) - E \right] |\psi_k\rangle = \mathcal{L}(\underline{b}) |\psi_k\rangle \quad (10)$$

where the A-particles Bloch operator⁽¹⁸⁾ is given by⁽⁴⁾

$$\begin{aligned} \mathcal{L}(\underline{b}) &= \sum_c \left| c \right\rangle \bar{\mathcal{L}}(b_c) \left\langle c \right| \\ &= \sum_c \left| c \right\rangle \frac{\hbar^2}{2m_c} \sum_{i=1}^A \delta(r_i - a_c) \left[\frac{\partial}{\partial r_i} - \frac{(b_c - 1)}{a_c} \right] \left\langle c \right| \end{aligned} \quad (11)$$

and the boundary condition parameters $b_c \in \{\underline{b}\}$ will be specified later.

As well known, the differential equation (10) assumes as many linearly independent degenerate solutions, $|\psi_k\rangle$, as the number of open channels in the reaction under consideration; say M. Following the standard techniques^(2-5, 12), one may write in the internal region⁽¹⁹⁾

$$\begin{aligned} |\psi_k\rangle &= \sum_j a_{kj} |\xi_j\rangle \\ &= \sum_{pq} |\xi_p\rangle \mathcal{G}_{pq} \langle \xi_q | \mathcal{L}(0) | \psi_k \rangle \end{aligned} \quad (12)$$

where a_{kj} are the expansion coefficients and the states $|\xi_i\rangle$ are the solution of the equation

$$(H_0 - \epsilon_i^{(o)}) |\xi_i\rangle = 0 \quad (13)$$

satisfying the boundary conditions

$$\mathcal{L}(\tilde{\underline{b}}) |\xi_i\rangle = 0 \quad (14)$$

and the parameters $\tilde{b}_c \in \{\tilde{\underline{b}}\}$ are yet unspecified. Moreover, the propagator \mathcal{G} is introduced through the matrix elements⁽²⁰⁾

$$\begin{aligned} \mathcal{G}_{ij} &= \langle \xi_i | \mathcal{G} | \xi_j \rangle \\ &= \langle \xi_i | (H_0 + V_R + \mathcal{L}(0) - E)^{-1} | \xi_j \rangle, \end{aligned} \quad (15)$$

where the boundary condition parameters b_c are chosen to be zero for the sake of simplicity⁽²⁻⁵⁾.

In the external region the wave function can be expressed in terms of the antisymmetric unit flux incoming (\mathcal{J}_c^-) and outgoing (\mathcal{O}_c^-) nucleon waves and the target/residual nucleus through the relation

$$|\psi_\mu\rangle = \sum_{\tilde{c}} \left[\mathcal{J}_c^- \delta_{\mu\tilde{c}} - S_{\mu\tilde{c}} \mathcal{O}_{\tilde{c}}^- \right] - \sum_{\bar{c}} S_{\mu\bar{c}} \mathcal{O}_{\bar{c}}^-, \quad \mu = 1, 2, \dots, M \quad (16)$$

where, in the notation of BARRETT and B. A. ROBSON⁽⁴⁾, \tilde{c} (\bar{c}) denotes open (closed) channels, $S_{\mu\tilde{c}}$ are the usual S-matrix elements, $\mathcal{O}_{\tilde{c}}^-$ describes a fully antisymmetric exponentially decaying outgoing nucleon wave and the residual nucleus, viz.

$$\mathcal{O}_{\tilde{c}}^- = W_{\tilde{c}}^-(q_{\tilde{c}}^-) | \tilde{c} \rangle \quad (17)$$

with $q_{\tilde{c}}^- = k_{\tilde{c}}^- r_{\tilde{c}}^-$, $k_{\tilde{c}}^- = (2m_{\tilde{c}}E)^{1/2}/\hbar$ such that $E = E_x - Q_{\tilde{c}}^-$; E_x being the excitation energy and $Q_{\tilde{c}}^-$ the channel threshold and $W_{\tilde{c}}^-(q_{\tilde{c}}^-)$ represent the usual Whittaker functions for the case of protons and the modified spherical Bessel functions for neutrons⁽²⁴⁻²⁵⁾. On the other hand,

$$\mathcal{J}_{\tilde{c}}^- = I_{\tilde{c}}^- v_{\tilde{c}}^{-1/2} | \tilde{c} \rangle = \mathcal{O}_{\tilde{c}}^{\ast} \quad (18)$$

where $v_{\check{c}}$ is the relative velocity in channel \check{c} and the radial wave functions $I_{\check{c}}$ and $O_{\check{c}}$ are such that

$$I_{\check{c}} = O_{\check{c}}^* = \left[G_{\check{c}}(\varrho_{\check{c}}) - i F_{\check{c}}(\varrho_{\check{c}}) \right] \exp(i\omega_{\check{c}}), \quad (19)$$

with $\omega_{\check{c}}$ being the Coulomb phase in channel \check{c} (zero for neutrons) and $F_{\check{c}}(G_{\check{c}})$ representing the regular (irregular) Coulomb function with the well defined asymptotic behaviour for protons and spherical Bessel (Neumann) function for neutrons^(24, 25).

The states $|\psi_{\mu}\rangle$ may now be transformed into the corresponding antisymmetric standing-wave solutions for the open channels; viz.

$$\begin{aligned} |\bar{\psi}_{\nu}\rangle &= \sum_{\mu} (\Omega^{-})_{\nu\mu} |\psi_{\mu}\rangle \\ &= \sum_{\check{c}} \left[(\Omega^{-})_{\nu\check{c}} \mathcal{I}_{\check{c}} - (\Omega^{+})_{\nu\check{c}} \mathcal{O}_{\check{c}} \right] + \sum_{\check{e}} (A)_{\nu\check{e}} \mathcal{O}_{\check{e}} \end{aligned} \quad (20)$$

where

$$\begin{aligned} (\Omega^{\pm})_{\mu\nu} &= v_{\mu\nu} \exp(\pm i\delta_{\mu\nu}), \\ (A)_{\nu\check{e}} &= -\sum_{\mu} (\Omega^{-})_{\nu\mu} S_{\mu\check{e}}, \quad S_{\mu\check{e}} = \sum_{\nu} \left[(\Omega^{-})^{-1} \right]_{\mu\nu} \left[\begin{array}{c} + \\ \nu\check{e} \end{array} \right], \end{aligned} \quad (21)$$

and $v_{\mu\nu}$ and $\delta_{\mu\nu}$ refer to the corresponding (real) amplitudes and phases.

By using the equations (12) and (20) it is straightforward to see that the wave function of the system under consideration can be derived from

$$|\bar{\psi}_{\nu}\rangle = \sum_{ij} (\Omega^{-})_{\nu i} \alpha_{ij} |\xi_j\rangle \quad (22)$$

and the expansion coefficients may be evaluated in the standard way^(26, 27). However, the operator Ω^{-} remains to be determined. This is done by matching of the wave functions in the external and internal regions through the employment of the natural boundary conditions which ensure a smooth matching⁽²⁻⁵⁾. In fact eqs. (12) and (20) give the following set of coupled equations:

$$\begin{aligned} \left[(\Omega^{-})_{\nu\check{d}} I'_{\check{d}} - (\Omega^{+})_{\nu\check{d}} O'_{\check{d}} \right] &= \sum_{\check{e}} R_{\check{d}\check{e}} \left[(\Omega^{-})_{\nu\check{e}} \tilde{I}'_{\check{e}} - (\Omega^{+})_{\nu\check{e}} \tilde{O}'_{\check{e}} \right] + \sum_{\check{e}} R_{\check{d}\check{e}} (A)_{\nu\check{e}} \tilde{O}'_{\check{e}}, \\ (A)_{\nu\check{d}} O'_{\check{d}} &= \sum_{\check{e}} R_{\check{d}\check{e}} \left[(\Omega^{-})_{\nu\check{e}} \tilde{I}'_{\check{e}} - (\Omega^{+})_{\nu\check{e}} \tilde{O}'_{\check{e}} \right] + \sum_{\check{e}} R_{\check{d}\check{e}} (A)_{\nu\check{e}} \tilde{O}'_{\check{e}}, \end{aligned} \quad (23)$$

where the primes denote the radial derivatives and $\tilde{O}_{\check{c}} \equiv r_{\check{c}} O_{\check{c}}$, $\tilde{I}_{\check{c}} \equiv r_{\check{c}} I_{\check{c}}$. Finally the R-matrix elements are given by

$$R_{\check{d}\check{e}} = \left(\frac{\hbar^2 a_{\check{d}}}{2m_{\check{d}}} \right)^{1/2} \sum_{\mu\nu} \langle \xi_{\nu} | \mathcal{G}_{\nu\mu} | \xi_{\mu} | \check{e} \rangle \left(\frac{\hbar^2 a_{\check{e}}}{2m_{\check{e}}} \right)^{1/2}. \quad (24)$$

and it is understood that the reduced width amplitudes are evaluated at the surface.

The operators Ω^{\pm} may now be determined in the following manner:

- start with the arbitrary values of the parameters $b_{\check{c}}^{(\nu)}$ for all except one of the open channels ν , known values of the n. b. c. parameters for the closed channel (cf. through the eq. (11) of ref. (2)) and an initial guess for the value $b_{\nu}^{(\nu)}$.
- construct a finite set of basis states by solving the inverse Schrödinger equation satisfying appropriate boundary conditions.
- calculate the matrix elements of eq. (24) in the above basis and solve the set of coupled equations (23) to obtain the phases $\delta_{\nu\nu}$ and the relative amplitudes $(v_{\nu\check{e}} / v_{\nu\nu})$.
- use this derived value of $\delta_{\nu\nu}$ to calculate a new value of $b_{\nu}^{(\nu)}$ by using the eq. (12) of ref. (2) and repeat the calculations with the new basis set.

In this way an iteration procedure is developed for a particular open channel which needs to be repeated at each energy for all the open channels separately. The knowledge of all the phases and rela-

tive amplitudes thus obtained enables one to calculate the transformation operators in eq. (21).

Alternatively, since the operators Ω^\pm are known, instead of introducing the expansion coefficients in eq. (22) and the basis states corresponding to the natural boundary conditions, one may directly calculate the state $|\psi_\mu\rangle$ and hence $|\psi_\nu\rangle$ through the equation (20) by the knowledge of $I_{\hat{c}}$, $O_{\hat{c}}$ and $O_{\hat{c}}^-$ in the external region⁽²⁸⁾.

2.3. - The Photodisintegration Cross Section.

Assuming that the first order perturbation theory can be used to calculate various electromagnetic processes, we start from the electric dipole operator $D(1, \mu)$ for the emission of an E1 photon (angular momentum 1, Z-projection μ) to obtain the electric dipole matrix element for the capture of a nucleon of spin s and Z-projection m_s incident along the direction \hat{k} on to a target (spin I and projection M_I) in the form

$$Q_{1\mu}(\hat{k}; sm_s IM_I) = \langle g, s. | D(1, \mu) | \tilde{\psi}(\hat{k}; sm_s IM_I) \rangle \quad (25)$$

where the total state vector for the system under consideration is given by

$$| \tilde{\psi}(\hat{k}; sm_s IM_I) \rangle = \frac{4\pi}{k} \sum_{J M \ell m_\ell j m} \exp(i\omega_\ell) Y_{\ell m_\ell}^*(\hat{k}) \times C(\ell sj | m_\ell m_s m) C(jIJ | m M_I M) \bar{\psi}_\nu^{JM} \rangle \quad (26)$$

The dipole photoemission cross section for the capture of a nucleon incident on the target may be written as⁽³³⁾

$$\frac{d\sigma_1^{\text{Capt}}}{d\Omega}(\hat{k}, \hat{k}_\gamma) = \frac{16}{9} \pi (E_\gamma / \hbar c)^3 \frac{1}{\hbar v} \left[(2s+1)(2I+1) \right]^{-1} \left| Q_{10}(\hat{k}, sm_s IM_I) \right|^2 \quad (27)$$

where v is the velocity of the incident nucleon and E_γ is the energy of the emitted photon. It is now straightforward to obtain the total cross section for E1 capture γ -rays by integrating the last equation over all directions which in turn gives the total integrated cross section for the absorption of the γ -rays of energy E_γ with the emission of the nucleon and the residual nucleus in the standard way⁽⁷⁾.

Alternatively, one may adopt the prescription given in the work of BARRET and DELSANTO⁽²⁹⁾ for determining the total photoabsorption cross section from a knowledge of the dipole matrix element in eq. (25).

3. - COMPARISON AND DISCUSSION.

Various methods have been proposed so far for the calculation of photonuclear reaction cross section within the domain of the one-particle in continuum version of the continuum shell model ideology. Amongst these methods, a number of calculations^(7, 14, 34) - carried out for different nuclei from the Tamm-Dancoff approximation, Eigenchannel method and the coupled-channels reaction theory - revealed that although the degree of accuracy in reproducing the photodisintegration cross section together with the incorporation of more sophisticated nuclear models seems to increase respectively, neither of these methods is completely satisfactory and require considerably long time for computation⁽²⁹⁾. Consequently, the main efforts during the last few years for the further improvement of the continuum shell model calculations were in the direction of extracting the new methods from the previously established conventional theories by substantially simplifying the numerical procedure; e. g. the separable expansion method due to BIRKHOLZ^(8, 35), the BARRETT and DELSANTO method^(2-4, 10, 29) and the modified continuum treatment of MICKLINGHOFF^(11, 35, 36, 37).

Whereas a detailed numerical calculation regarding the convergence of these methods together with their comparison with the present approach for the realistic photonuclear reactions will be the subject of a subsequent work; it may be of some interest to outline here a formal comparison which may reflect the inherent difference and/or the formal resemblance among the various techniques.

In this respect we may start the BARRET and DELSANTO (BD) method which is based on the hypothesis that an optimum choice of the boundary condition parameters and the employment of the most realistic physical model should minimize the number of basis states for achieving a desirable accuracy; especially in cases where the number of reaction channels is large. The formalism presented here for the photonuclear reactions resembles the BD approach in the sense that both employ the basis states which satisfy the natural boundary conditions. The main difference is in the numerical techniques and the fact that the BD method employs a "matrix diagonalisation" technique - similar to that of the Eigenchannel theory without requiring, however, the S-matrix to be obtained in a diagonal form. Consequently the overall calculation of the cross section takes remarkably less time for computation.

Since the results of the application of the BD method for the realistic and simulated elastic and inelastic reactions were identical to those of the Iterative R-matrix method and both results were in very good agreement with the experiments^(2, 3), it is expected that the present approach may also retain the same standard. In addition, the results of DELSANTO et al.⁽¹⁰⁾ for the continuum calculations⁽³⁸⁾ of photonuclear reaction cross sections in ^4He may also be reproduced by the present approach if one incorporates appropriately in the formulation of section 2 the method of PHILPOTT (see refs. (40), (41)) for the elimination of the centre-of-mass spuriousities.

Recently, MICKLINGHOFF⁽³⁵⁾ has presented a very interesting formal and numerical comparison of his perturbative continuum treatment (PCT) with the separable expansion (SEP) method of BIRKHOLZ⁽⁸⁾. Transforming the Schrödinger type description of the continuum shell model treatment into the Lippmann-Schwinger type approach, the underlying idea involved in these methods is to separate the corresponding Lippmann-Schwinger Kernel into a separable and a residual kernel and treat the later as a perturbation. In addition, the model space corresponding to the unperturbed system is separated into a finite number of square integrable functions (e. g. the harmonic oscillator functions) and a modified continuum. In the present approach, on the other hand, this distinction is not mentioned explicitly but the continuum states are discretized within the internal region by using the Bloch operator and, of course, no residual kernel - which may give to continuum-continuum coupling - is involved⁽³⁶⁾. This type of coupling, however, is often neglected in the other methods as well. Moreover, in the present approach, the bound-continuum coupling is introduced through the Bloch operator which guarantees that the total wave function is smooth at the boundary. Since the SEP method neglects the bound-continuum coupling and deals only with the bound-bound coupling, one may be inclined to think that the present approach may give slightly better results for a given number of basis states. In the PCT, on the other hand, the neglect of the bound-continuum coupling is optional since for light nuclei - provided one uses a sufficiently large number of oscillator functions - only bound-bound coupling may yield very good results⁽³⁵⁾.

The reason why the natural boundary condition methods give a rapid convergence to the corresponding coupled-channel calculations may also emerge from the last remark; e. g. although the bound-continuum coupling is minimized through $\Delta\mathcal{L} \rightarrow 0$, the resulting basis states are modified in such a way that a small number of them is sufficient to introduce an appropriate bound-bound coupling in the overall formulation. These points will be elaborated mathematically in a subsequent work.

In conclusion we may remark here that in view of its remarkable success for the particle induced reactions, the present formulation can offer an alternative approach for analysing the photoreaction cross sections and may be applied to the photoionization of atoms with appropriate modifications.

ACKNOWLEDGEMENTS.

The author is grateful to Professors R. A. RICCI and G. MOSHINI for the hospitality at LNL. He would like to thank Professor A. M. SARUIS (Centro di Calcolo del CNEN, Bologna) for many illuminating discussions. He would also like to express his gratitude to Professors C. VILLI, G. PISENT and V. VANZANI for the encouragement and hospitality at the Istituto di Fisica dell'Università, Padova. Thanks are also due to Professor F. ZARDI for a critical reading of the manuscript and many useful comments.

The INFN grant for partial financial support is also acknowledged.

APPENDIX

Consider the Lippmann-Schwinger equation corresponding to the physical solution at energy E, viz.

$$| \psi_k^E \rangle = | \varphi \rangle + \mathcal{G}_0 V_R | \psi_k^E \rangle \tag{A.1}$$

where $|\varphi\rangle$ is an eigenstate of the Hamiltonian H_0 to which is associated the propagator \mathcal{G}_0 . The standing-wave solution, on the other hand, satisfies a similar equation⁽³⁰⁾

$$| \bar{\psi}_\nu^E \rangle = | \varphi \rangle + \bar{\mathcal{G}}_0 V_R | \bar{\psi}_\nu^E \rangle, \tag{A.2}$$

where $\bar{\mathcal{G}}_0$ represents the principal value Green's function.

From now on the superscript E will be dropped for simplicity. Since the transition operator T is related to the solution $|\psi_k\rangle$ through the relation: $V_R | \psi_k \rangle = T | \varphi \rangle$, one can write

$$\left[1 - \bar{\mathcal{G}}_0 V_R \right] | \psi_k \rangle = (1 + i\pi T) \left[1 - \bar{\mathcal{G}}_0 V_R \right] | \bar{\psi}_\nu \rangle, \tag{A.3}$$

where use has been made of the identity

$$\lim_{\eta \rightarrow 0^+} \left(\frac{1}{q \pm i\eta} \right) = P \left(\frac{1}{q} \right) \mp i\pi \delta(q) \tag{A.4}$$

in the standard notation⁽³¹⁾. Finally, one can write

$$| \bar{\psi}_\nu \rangle = \left[1 - \bar{\mathcal{G}}_0 V_R \right]^{-1} (1 + i\pi T)^{-1} \left[1 - \bar{\mathcal{G}}_0 V_R \right] | \psi_k \rangle. \tag{A.5}$$

A comparison of the above equation with eq. (20) shows that the operator Ω^- may be written as

$$\Omega^- = \left[1 - \bar{\mathcal{G}}_0 V_R \right]^{-1} (1 + i\pi T)^{-1} \left[1 - \bar{\mathcal{G}}_0 V_R \right] \tag{A.6}$$

which shows the involvement of the principal value Green's function and the residual interaction together with the transition operator in the transformation of a physical solution into a standing wave solution. Finally, one may note that the substitution

$$\left[1 - \bar{\mathcal{G}}_0 V_R \right]^{-1} (T) \left[1 - \bar{\mathcal{G}}_0 V_R \right] \equiv K \tag{A.7}$$

enables one to rewrite (A.6) in the well known form

$$\Omega^- = \left[1 + i\pi K \right]^{-1}, \tag{A.8}$$

where K may be regarded as the reactance matrix and may be written in a form similar to that of VITTURI and ZARDI⁽³²⁾ by the employment of the natural boundary conditions.

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- (19) It should be remarked here that the present form appears as the result of considering the orthonormal basis states within the internal region. This in turn implies that the single particle states $\varphi_i(\underline{r}_A)$ are orthogonal to the states of the (A-1) particles constituting the target. This assertion holds, however, so long as all the single particle wave functions in the A-particles system are treated on the equal footing. In case, for example, the target wave function results from the Slater determinant of the (A-1) single particle wave functions in the Hartree - Fock basis and $\varphi_i(\underline{r}_A)$ results from the Saxon-Woods or some other basis; the basis states become non-orthogonal. Consequently the closure relation used in the derivation of eq. (12) needs to be replaced by $\sum_i |\xi_i\rangle \langle \xi_i| \left[\frac{N-1}{N} \right]_{ij} \langle \xi_j| = 1$ with $\left[\frac{N-1}{N} \right]_{ij} = \langle \xi_i | \xi_j \rangle \neq \delta_{ij}$. However, since the single particle potential of eq. (5) may be assumed to simulate the Hartree-Fock potential to a certain extent⁽¹⁷⁾, we shall deal throughout with the orthonormal basis sets.
- (20) At this stage it seems worthwhile to remark that the propagator \mathcal{G} may also be expressed in terms of the free propagators \mathcal{G}_0 corresponding to the Hamiltonian H in the standard fashion⁽²¹⁻²³⁾, viz.

$$\mathcal{G} = \mathcal{G}_0 (1 + h \mathcal{G}_0)^{-1} = (1 + \mathcal{G}_0 h)^{-1} \mathcal{G}_0, \quad (3a)$$

where $h = V_R + \Delta\mathcal{L}$ and $\Delta\mathcal{L} = \mathcal{L}(\underline{b}) - \mathcal{L}(\underline{\tilde{b}})$. The involvement of the boundary condition mixing and the residual interaction may be made explicit through the relation⁽²³⁾

$$\mathcal{G} = \mathcal{G}_0 \left[1 - \left\{ 1 + V_R \mathcal{G}_0 + \Delta\mathcal{L} \mathcal{G}_0 \right\}^{-1} V_R \mathcal{G}_0 \right] \left[1 + \Delta\mathcal{L} \mathcal{G}_0 \right]^{-1}. \quad (3b)$$

As emphasized by D. Robson and Lane⁽²¹⁾ and Vitturi and Zardi⁽²²⁾, this approach enables one to introduce eventually the concept of the intermediate structure (fine structure) occurring in the formation of, say, a giant resonance. In fact, the spectral representation of the free propagator may be used to write

$$\mathcal{G}_0 = \frac{|\xi_i\rangle \langle \xi_i|}{\epsilon_i^{(0)} - E} + \sum_{j \neq i} \frac{|\xi_j\rangle \langle \xi_j|}{\epsilon_j^{(0)} - E} \equiv \mathcal{G}_0^{(i)} + \mathcal{G}_0^{(j)} \quad (3c)$$

which leads to the interpretation that the formation of a typically large resonance may be due to the partial dissolution of a special state, $|\xi_i\rangle$, by V_R and $\Delta\mathcal{L}$ in the presence of the neighbouring ordinary states $|\xi_j\rangle$. In the present approach, however, this distinction is no longer retained and the line shape of the resonance is forced to emerge into the photodisintegration cross section by the employment of the minimum number of basis states which automatically adjust the mixing of the special and ordinary states. This resembles in some extent the alternative of the methodology adopted by Birkholz⁽⁸⁾ within the spirit of Buck and Hill's formulation⁽⁷⁾ and will be discussed further in the next section.

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 (28) That the two approaches are identical at the matching boundary may be shown in the following way. From eq. (12) one can write for the standing wave solution of eq. (22)

$$\begin{aligned} |\bar{\psi}_\nu\rangle &= \sum_i (\bar{Q}^-)_{\nu i} \sum_{pq} |\xi_p\rangle \mathcal{G}_{pq} \langle \xi_q | \mathcal{L}(b) | \psi_i \rangle \\ &= \sum_i (\bar{Q}^-)_{\nu i} \left[H + \mathcal{L}(b) - E \right]^{-1} \left[H + \mathcal{L}(b) - E \right] | \psi_i \rangle \\ &= \sum_i (\bar{Q}^-)_{\nu i} | \psi_i \rangle \end{aligned} \quad (4a)$$

where use has been made of eqs. (10) and (15) together with the fact that $|\psi_i\rangle$ are degenerate solutions of the nuclear Hamiltonian in the internal as well as the external region. Substitution of eq. (16) in eq. (4a) yields

$$|\bar{\psi}_\nu\rangle = \sum_{\bar{c}} \left[(\bar{Q}^-)_{\nu \bar{c}} \mathcal{G}_{\bar{c}} - (\bar{Q}^+)_{\nu \bar{c}} \mathcal{O}_{\bar{c}} \right] + \bar{c} (A)_{\nu \bar{c}} \mathcal{O}_{\bar{c}} \quad (4b)$$

which is same as eq. (20). Thus, so long as the matching radius is chosen large enough such that all nuclear interactions can be assumed to occur in the internal region, the expansion (22) is a good approximation to represent the state $|\bar{\psi}_\nu\rangle$ which may be employed for calculating the photodisintegration cross section (cf. the subsection 2.3). This is in agreement with the method of Barrett and Delsanto⁽²⁹⁾ and will be discussed further in the following section. In order to have an idea about the physical information contained in the operator \bar{Q}^- , an explicit form of this operator in terms of the Green's function and the transition operator is given in the appendix.

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