Chapter II

Formalism of the Method of Coupled Discretized Continuum Channels

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(Received October 22, 1986)

Basic ideas and assumptions of CDCC as a phenomenological theory of multi-step direct reactions are reviewed in such a way as to clarify the formal structure of the method. In particular, truncation and discretization of the continuum of breakup channels, choice of the model Hamiltonian, boundary condition for the model wave function, and procedure of calculation of transition matrix elements are discussed in detail.

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§ 1. Introduction

The Method of Coupled Discretized Continuum Channels, abbreviated as CDCC, is a phenomenological method of analyzing direct nuclear reactions which involve breakup of loosely bound particles, such as deuteron, ^{6,7}Li, ^{12}C, etc. It is an extension of the conventional Method of Coupled Channels (CC) for bound clusters.[1] As such, its aim and basic assumptions are much the same as those of conventional CC. Its primary purpose is to analyze the mechanism of a specific multi-step direct nuclear reaction through calculation of some specific experimentally observable quantities, e.g., cross sections, analyzing powers, etc., and comparison with experimental data. It is not designed to be a method

of approximately solving the Schroedinger equation

$$H\Psi = E\Psi \tag{1·1}$$

with a given total Hamiltonian of the system, H, for a wave function Ψ in the entire configuration space under a given set of boundary conditions. In fact, knowledge of the wave function over the entire configuration space is not even needed sometimes, depending on the particular quantities to be calculated and the procedure of the calculation, as discussed in § 5.

A CDCC calculation starts with adopting a model of the multi-step direct process, specifying a set of internal states of the system, or channels, through which the reaction is assumed to proceed, and the way the channels are coupled to each other. In the present paper, we assume that the model includes only two-cluster channels consisting of two independent clusters, each in either a bound or an unbound state. We assume that only one of the clusters may be in an unbound state which can be well approximated by a state of interacting *two* nucleons or *two* fragments each in a definite bound state.

We use greek letters, α, β, γ, etc., to denote such channels, and roman letters, a and A, b and B, c and C, etc., to denote corresponding constituent clusters. We use the notations rather loosely for specifying sometimes only the kind of the clusters, and sometimes also various quantum numbers. We work in a representation in which the total angular momentum, J, and its z-component, μ, are diagonal.

Suppose γ is a channel in the model with clusters c and C which are in eigen-states, ϕ_c and ϕ_C, of respective internal Hamiltonians, h_c and h_C, with eigen-energies ε_c and ε_C

$$h_c\phi_c = \varepsilon_c\phi_c \quad \text{and} \quad h_C\phi_C = \varepsilon_C\phi_C. \tag{1·2}$$

The internal wave function of the channel, $\phi_\gamma(\xi_\gamma)$, is given by

$$\phi_\gamma(\xi_\gamma) = [\phi_c(\xi_c),\ \phi_C(\xi_C)]_{\Lambda_\gamma\mu_\gamma}, \tag{1·3}$$

where the ξ are the internal coordinates, and the square bracket indicates the angular momentum coupling to form a channel spin Λ_γ, with a z-component, μ_γ. It satisfies

$$h_\gamma\phi_\gamma = \varepsilon_\gamma\phi_\gamma, \tag{1·4}$$

where $h_\gamma = h_c + h_C$ and $\varepsilon_\gamma = \varepsilon_c + \varepsilon_C$ are the internal Hamiltonian and the internal energy of channel γ, respectively. The clusters are either in a bound or in an unbound state as already mentioned. Bound states are discrete and are labeled by a set of discrete quantum numbers. Unbound states are continuous and labeled by a set of continuous quantum numbers, in addition to discrete ones. We normalize the internal wave functions to a Kronecker delta for every discrete quantum number and a delta function for every continuous quantum number.

The model of a CDCC calculation is defined by a set of discrete and continuous channels with a corresponding set of internal wave functions $\{\phi_\gamma\}$ defined above which span a functional space, F, for the wave function of the model. Setting up the model must be done on a sound physical basis supported by experimental evidences, theoretical plausibility, etc. Its validity is eventually tested by comparison of the calculated result with experimental data. Another condition for the model, which is very important for the

feasibility of actual calculations, is that space F be minimal, including only channels which are important for the particular calculation at hand. Hence, F depends in general on the type of the reaction, the quantities, $\{Q\}$, to be calculated, the procedure of the calculation of $\{Q\}$, the incident energy, angle, etc., of observation, and also the desired accuracy of the calculation.

Let us denote the projection operator onto F by p, and its complement, $1-p$, by q:

$$p^2=p, \quad q^2=q, \quad pq=qp=0. \tag{1·5}$$

The projection of Ψ onto F, $p\Psi$, can, by definition, be expanded as

$$p\Psi=\sum_{\gamma}\Phi_{\gamma}(\xi_{\gamma}, \hat{R}_{\gamma})\chi_{\gamma}(R_{\gamma}), \tag{1·6}$$

where R_{γ} and $\hat{R}_{\gamma}$ are the magnitude and the direction of the relative coordinate, $\boldsymbol{R}_{\gamma}$, conjugate to ξ_{γ}, $\Phi_{\gamma}(\xi_{\gamma}, \hat{R}_{\gamma})$ is a so-called spin-angle function of channel γ defined by

$$\Phi_{\gamma}(\xi_{\gamma}, \hat{R}_{\gamma})\equiv[\phi_{\gamma}(\xi_{\gamma}), \quad i^{L_{\gamma}}Y_{L_{\gamma}}(\hat{R}_{\gamma})]_{J\mu}, \tag{1·7}$$

$\chi_{\gamma}(R_{\gamma})$ is the radial part of the wave function of relative motion, and $\sum_{\gamma}$ stands for summation over discrete channels and integration over continuous channels. $p\Psi$ satisfies the Schroedinger equation within F

$$H_{\text{eff}}p\Psi=Ep\Psi, \tag{1·8}$$

where H_{eff} is the Feshbach effective Hamiltonian

$$H_{\text{eff}}=p\left(H+H\frac{q}{e_q}H\right)p \tag{1·9}$$

with $e_q=E-qHq-i\varepsilon$. It has a general form

$$H_{\text{eff}}=p\,(K+V_{\text{eff}})p, \tag{1·10}$$

where K is the total kinetic energy and V_{eff} is the effective interaction potential given by

$$V_{\text{eff}}=p\left(V+H\frac{q}{e_q}H\right)p, \tag{1·11}$$

where V is the interaction potential in the original Hamiltonian, H, so that

$$H=K+V. \tag{1·12}$$

Now, it is obvious from (1·6) and (1·9) that (1·8) is equivalent to

$$(\Phi_{\delta}|H_{\text{eff}}-E|\sum_{\gamma}\Phi_{\gamma}\chi_{\gamma}\rangle=0 \tag{1·13}$$

for all the δ in F, where the left parenthesis signifies the integration over the arguments of Φ_{δ}. Equations (1·13) constitute a set of coupled equations for the unknown wave functions χ of relative motion.

Now, a CDCC calculation with an F as described above is unfeasible in practice,

because it would involve calculations of the exact internal wave functions of F, $\{\Phi_\gamma\}$, and the exact effective Hamiltonian, H_{eff}, and solving a coupled equations of the form of (1·13) for a continuous set of the χ. It is a basic assumption of CDCC that one can substitute F and H_{eff} by a finite dimensional model space, M, and a corresponding phenomenological model Hamiltonian, H_M, respectively in such a way that the desired quantities $\{Q\}$ can be calculated in good approximation with M and H_M by the procedure specified by the model. The quantities $\{Q\}$ thus calculated are compared with experimental data. The reality of the model is judged by the quality of agreement between them.

Thus, a CDCC calculation proceeds in rather distinct steps. In the subsequent sections, we sketch the formalism of CDCC following those steps. In § 2, the transition from F to M is discussed, including truncation and discretization of the continuous breakup channels. In § 3, a general prescription of constructing phenomenological Hamiltonians is given, and its application to some special cases of practical interest are discussed. In § 4, the model Schroedinger equation and the boundary condition for model wave functions are discussed in detail. In § 5, procedures of calculation of transition matrix elements are discussed. In § 6, a summary and the conclusion of the paper are given.

§ 2. Model space

Let us assume that a reasonable model of the reaction mechanism has been set, and the space F with the effective Hamiltonian H_{eff} have been defined as discussed in the previous section. As already mentioned, F and H_{eff} are virtually impossible to be calculated numerically in most cases, and have to be replaced by some phenomenological substitutes. In the present section we deal with the replacement of F by a model space, M.

2.1. *Model internal wave functions*

The first step of the replacement concerns with the internal wave functions in F. They are themselves solutions of many-body problems: (1·2). In practice, they can be calculated only approximately with some models, except in the case of the deuteron for which exact calculations are feasible. One, therefore, replaces them with eigen-functions of certain model internal Hamiltonians. We denote quantities in the model with a bar. Thus, for channel γ with clusters c and C, ϕ_{c} and ϕ_{C} are replaced by $\bar{\phi}_{\text{c}}$ and $\bar{\phi}_{\text{C}}$, respectively, which satisfy

$$\bar{h}_{\text{c}}\bar{\phi}_{\text{c}}=\bar{\varepsilon}_{\text{c}}\bar{\phi}_{\text{c}}, \quad \bar{h}_{\text{C}}\bar{\phi}_{\text{C}}=\bar{\varepsilon}_{\text{C}}\bar{\phi}_{\text{C}}, \tag{2·1}$$

and ϕ_γ is replaced by $\bar{\phi}_\gamma$ given by

$$\bar{\phi}_\gamma(\xi_\gamma)=[\bar{\phi}_{\text{c}}(\xi_{\text{c}}),\ \bar{\phi}_{\text{C}}(\xi_{\text{C}})]_{\Lambda_\gamma\mu_\gamma}, \tag{2·2}$$

which satisfies

$$\bar{h}_\gamma\bar{\phi}_\gamma=\bar{\varepsilon}_\gamma\bar{\phi}_\gamma, \tag{2·3}$$

where the $\bar{h}$ are the model Hamiltonians which are assumed to be so chosen that the $\bar{\varepsilon}$ and the $\bar{\phi}$ well approximate the corresponding ε and ϕ in F. In particular, discrete channels

in F should be replaced by discrete channels, and continuous channels by continuous channels. We assume that the $\bar{\phi}$ are normalized in the same way as the ϕ. Thus, F is replaced by a space $\bar{F}$ spanned by $\{\bar{\phi}_\gamma\}$.

Now, $p\Psi$ of (1·6) is replaced by

$$\bar{p}\Psi=\sum_\gamma \bar{\Phi}_\gamma(\xi_\gamma, \hat{R}_\gamma)\bar{\chi}_\gamma(R_\gamma), \tag{2·4}$$

where $\bar{p}$ is the projector onto $\bar{F}$, and $\bar{\Phi}_\gamma$ is given by

$$\bar{\Phi}_\gamma(\xi_\gamma, \hat{R}_\gamma)\equiv[\bar{\Phi}_\gamma(\xi_\gamma), i^{L_\gamma}Y_{L_\gamma}(\hat{R}_\gamma)]_{J\mu}. \tag{2·5}$$

2.2. *Discretization of three-body continuum channels*

The next step of the replacement deals with continuous channels in $\bar{F}$. Each of those channels consist of a bound cluster and an unbound pair of fragments as mentioned in § 1. In CDCC, a continuum of such states is truncated and discretized into a finite number of "states". The reason for this is, again, the feasibility of calculation: coupled-channel calculations can be carried through numerically only with finite number of coupled channels. Another point is that if one assumes a three-body model Hamiltonian, discussed later, for such a channel, the Lippmann-Schwinger equation has a Hilbert-Schmidt kernel and has a unique solution after the truncation in the angular momentum of relative motion of the fragments.[2] We describe in the following the procedure of truncation and discretization used in the actual calculations in later chapters of the present review.

Suppose cluster c of channel γ breaks up into two fragments 1 and 2, each in a definite bound state. The model internal wave function of such a state has the form

$$\bar{\phi}_{cl}(k, \xi_c)=[\bar{\phi}_{cl}(k, \boldsymbol{r}_{12}), [\bar{\phi}_1(\xi_1), \bar{\phi}_2(\xi_2)]_s]_{I_cM_c}, \tag{2·6}$$

where the $\bar{\phi}$ are model internal wave functions of 1 and 2, and $\bar{\phi}_{clm}(k, \boldsymbol{r}_{12})$ is the wave function of relative motion between the fragments with wave number k and angular momentum l and its z-component m where $\boldsymbol{r}_{12}$ is the relative coordinate. The spin, I_c, and its z-component, M_c, of cluster c is composed from l and the spins of the fragments as shown in (2·6). The internal energy of cluster c is given by

$$\bar{\varepsilon}_c(k)=\frac{\hbar^2k^2}{2\mu_{12}}, \tag{2·7}$$

where μ_{12} is the reduced mass between 1 and 2. Now, the truncation is made by restricting l and k or ε_c as

$$l\leq l_{c,m} \quad \text{and} \quad k\leq k_{c,m} \quad \text{or} \quad \bar{\varepsilon}_c\leq \varepsilon_{c,m}, \tag{2·8}$$

where the limits $k_{c,m}$ or $\varepsilon_{c,m}$ and $l_{c,m}$ are taken to be such that they satisfy requirements stated in § 2.3. Thus, the space of the eigen-states of $\bar{h}_c$ with the bound states, $\bar{\phi}_{cn}(\xi_c)$, $n=1\sim N_c$, and the continuous states, $\bar{\phi}_{cl}(k, \xi_c)$, is truncated into a space spanned by

$$\{\bar{\phi}_{cn}(\xi_c), \quad n=1\sim N_c; \quad \bar{\phi}_{cl}(k, \xi_c), \quad k\leq k_{c,m}, \quad l\leq l_{c,m}\}. \tag{2·9}$$

Now, this set of infinite number of functions is replaced by a *finite* set of model "state"

wave functions

$$\{\hat{\phi}_{cl,i}(\xi_c),\quad i=1, 2\cdots, N_{cl},\quad l\leq l_{c,m}\}. \tag{2·10}$$

The first N_c functions of the set simulate the bound states, and the rest represents the continuous states of the original set, (2·9). The wave functions of the latter have the form

$$\hat{\phi}_{cl,i}(\xi_c)=[\bar{\phi}_{cl,i}(\boldsymbol{r}_{12}), [\bar{\phi}_1(\xi_1), \bar{\phi}_2(\xi_2)]_s]_{I_cM_c}. \tag{2·11}$$

We assume that the $\hat{\phi}$ are normalized as

$$\langle\phi_{cn}|\phi_{cm}\rangle=\delta_{nm},\quad \langle\phi_{cn}|\phi_{cl,i}\rangle=0\quad\text{and}\quad \langle\hat{\phi}_{cl,i}|\hat{\phi}_{cl,j}\rangle=\delta_{ll'},\ \delta_{ij}. \tag{2·12}$$

One can construct such a discretized set of functions in various ways. We discuss below two methods which are used in the subsequent chapters of the present review : (A) the method of pseudo-states, and (B) the method of momentum bins. A merit of these methods is that the set $\{\phi_{cl,i}\}$ diagonalizes the internal Hamiltonian, $\bar{h}_c$, which greatly facilitates the subsequent calculation. The use of an orthogonal set, however, is not essential ; for example, a set of Strumian functions used by Johnson and Tandy[3] in their pioneering work on the deuteron breakup process in (d, p) reactions.

(A) Method of pseudo-states[4]

In this method, the Hamiltonian $\bar{h}_c$ is diagonalized on a basis of a finite number of normalizable functions

$$\{\varphi_{clm,i}(\boldsymbol{r}),\quad i=1\sim N_{cl},\quad l\leq l_{cm}\}.$$

Thus, $\hat{\phi}_{clm,i}$ is taken to be

$$\hat{\phi}_{clm,i}=\sum_j a_{cl,ij}\varphi_{lm,i}, \tag{2·13}$$

and the $a_{cl,ij}$ are determined so that the $\hat{\phi}_{cl,i}$ given by (2·11) with (2·13) satisfy

$$\langle\hat{\phi}_{cl,i}|\bar{h}_c|\hat{\phi}_{cl,j}\rangle=\hat{\varepsilon}_{cl,i}\delta_{ij} \tag{2·14}$$

and

$$\langle\hat{\phi}_{cl,i}|\hat{\phi}_{cl',j}\rangle=\delta_{ll'}\delta_{ij}. \tag{2·15}$$

Then, $\hat{\phi}_{cl,i}$ and $\hat{\varepsilon}_{cl,i}$ are taken to be the wave function and the energy, respectively, of the i-th discretized "state" of channel cl which is actually a superposition of eigen-states of $\bar{h}_c$. The basis set of diagonalization is chosen in such a way that the set

$$\{\hat{\phi}_{cl,i}(\xi_c),\quad i=1\sim N_{cl},\quad l\leq l_{cm}\}$$

represents the original truncated space of (2·9) well, simulates the bound states well in energy and wave function, and represents the continuum states well, with the $\hat{\varepsilon}_{cl,i}$ for them properly distributed within the range $[0,\ \varepsilon_{c,m}]$.

A set of Gaussian functions

$$\varphi_{c\ell m,i}(\boldsymbol{r})=e^{-\kappa_{ci}r^2}i^{\ell}Y_{\ell m}(\hat{r}), \tag{2·16}$$

is a convenient choice for such a basis and is used in the calculation described in Chapter V.[4d] Other types of functions such as Strumian functions[4a),c)] and Laguerre polynomials times an exponential[4b)] have also been used.

(B) Method of momentum bins[5)]

This method is based on the assumption that the eigen-functions $\bar{\phi}_{c\ell}(k, \xi_\gamma)$ of $\bar{h}_c$ are known for all k in $[0, k_{c,m}]$, an assumption strictly valid for a deuteron, and approximately so for c for which two-cluster model is good. The interval $[0, k_{c,m}]$ is divided into a finite number of sub-intervals $[0, k_1]$, $[k_1, k_2]$, $\cdots$, $[k_{n-1}, k_n=k_{c,m}]$ where $n=N_{c\ell}$. Then, the continuous states within the sub-interval $[k_{i-1}, k_i]$ are represented by a single function $\hat{\phi}_{c\ell,i}(\xi_c)$ with a $\hat{\phi}_{c\ell m,i}(\boldsymbol{r})$ derived from the $\bar{\phi}_{c\ell m}(k, \boldsymbol{r})$ of the continuous states. A definition, which is often used in actual calculations, is

$$\hat{\phi}_{c\ell m,i}(\boldsymbol{r})=\int_{k_{i-1}}^{k_i} w_{ci}(k)\bar{\phi}_{c\ell m}(k, \boldsymbol{r})\mathrm{d}k, \tag{2·17}$$

where $w_{ci}(k)$ is a weight function normalized by

$$\int_{k_{i-1}}^{k_i} w_{ci}^2(k)\mathrm{d}k=1. \tag{2·18}$$

If $w_{ci}(k)$ is taken to be a constant within the interval $[k_{i-1}, k_i]$, (2·18) gives

$$w_{ci}(k)=\frac{1}{\sqrt{\Delta_{ci}}}. \tag{2·19}$$

In either case the $\hat{\phi}_{c\ell,i}$ are normalized as

$$\langle\hat{\phi}_{c\ell,i}|\hat{\phi}_{c\ell',j}\rangle=\delta_{\ell\ell'}\delta_{ij}. \tag{2·20}$$

It should be noted that the set $\{\hat{\phi}_{c\ell,i}\}$ diagonalizes $\bar{h}_c$ in the sense that

$$\langle\hat{\phi}_{c\ell,i}|\bar{h}_c|\hat{\phi}_{c\ell',j}\rangle=\hat{\varepsilon}_{c\ell,i}\delta_{\ell\ell'}\delta_{ij}, \tag{2·21}$$

where $\hat{\varepsilon}_{c\ell,i}$ is the energy of the discretized state $\hat{\phi}_{c\ell,i}$, which is given by

$$\hat{\varepsilon}_{c\ell,i}=(\hbar^2/2\mu_{12})\{(k_i+k_{i-1})^2/4+(\Delta k_i)^2/12\}, \tag{2·22}$$

for (2·17) with (2·19). Hence, this method can also be regarded as a kind of pseudo-state method with the pseudo-states defined by (2·17).

Sometimes, one uses the $\hat{\phi}_{c\ell m,i}$ defined by

$$\hat{\phi}_{c\ell m,i}(\boldsymbol{r})=\bar{\phi}_{c\ell m}(k(i), \boldsymbol{r})/\sqrt{\Delta_{ci}}, \tag{2·23}$$

where $k(i)$ is a certain representative point in the interval $[k_{i-1}, k_i]$. In this case, the energy eigen-value for $\hat{\phi}_{c\ell m,i}$ is

$$\hat{\varepsilon}_{c\ell,i}=\hbar^2k(i)^2/2\mu_{12} \tag{2·24}$$

and the normalization is

$$\langle \phi_{c l m,i} | \phi_{c l' m',j} \rangle = \delta_{ll'} \delta_{mm'} \delta(k(i)-k(j)). \tag{2·25}$$

In addition to the discretized continuum wave functions, the bound state eigenfunctions of $\bar{h}_c$ themselves are taken for the model wave functions, $\hat{\phi}_{cn} = \bar{\phi}_{cn}$ for $n=1 \sim N_c$, to form a set of discretized model wave functions

$$\{\hat{\phi}_{cl,i}(\xi_c), \quad i=1 \sim N_{cl}, \quad l \leq l_{cm}\},$$

which replaces the continuous set, (2·9).

The truncation and discretization of the breakup states of cluster c described above leads to a corresponding replacement of the continuous-channel internal wave functions by those of discretized channels

$$\{\phi_\gamma(\xi_\gamma)\} \longrightarrow \{\hat{\phi}_{\gamma i}(\xi_\gamma), \quad i=1 \sim N_\gamma\}, \tag{2·26}$$

where

$$\hat{\phi}_{\gamma i}(\xi_\gamma) = [\hat{\phi}_{cl,i}(\xi_c), \quad \bar{\phi}_C(\xi_C)]_{\Lambda_\gamma \mu_\gamma} \tag{2·27}$$

is the internal wave function of the i-th discretized state of channel γ. They diagonalize $\bar{h}_\gamma = \bar{h}_c + \bar{h}_C$

$$\langle \hat{\phi}_{\gamma i} | \bar{h}_c + \bar{h}_C | \hat{\phi}_{\gamma j} \rangle = \bar{\varepsilon}_{\gamma i} \delta_{ij}, \tag{2·28}$$

where

$$\bar{\varepsilon}_{\gamma i} = \hat{\varepsilon}_{cl,i} + \bar{\varepsilon}_C \tag{2·29}$$

and

$$\langle \hat{\phi}_{\gamma i} | \hat{\phi}_{\gamma j} \rangle = \delta_{ij}. \tag{2·30}$$

The model internal wave functions thus introduced span a functional space, M, which is the model space of the CDCC calculation. All the subsequent calculations are done in this space. A model wave function Ψ_M is a projection of Ψ onto M, $\Psi_M = P\Psi$, which has a form

$$\Psi_M \equiv P\Psi = \sum_\gamma \sum_i \hat{\Phi}_{\gamma i}(\xi_\gamma, \hat{R}_\gamma) \hat{\chi}_{\gamma i}(R_\gamma), \tag{2·31}$$

which replaces (2·4), where

$$\hat{\Phi}_{\gamma i}(\xi_\gamma, \hat{R}_\gamma) = [\hat{\phi}_{\gamma i}(\xi_\gamma), \ i^{L_\gamma} Y_{L_\gamma}(\hat{R}_\gamma)]_{J\mu} \tag{2·32}$$

and the $\hat{\chi}$ are the corresponding radial functions.

2.3. *"Convergence" of truncation and discretization*

A test of adequacy of the model space M as a substitute for the original space F is to see whether the calculation is a convergent one in the sense that the quantities $\{Q\}$

calculated with M with a specific model Hamiltonian, H_M, and by a specific procedure of calculation does not change when the limits of the truncation, the $l_{c,m}$, $k_{c,m}$ and $\varepsilon_{c,m}$, or the density of the discretization is increased.[6] If the convergence is achieved, M is deemed adequate. It should be noted that the "convergence" is only in the limited sense as stated above and does not necessarily mean a convergence in the wave function, for example. It is, however, enough for the purpose of the CDCC calculation as stated in § 1.

§ 3. Model Hamiltonian

The effective Hamiltonian, H_{eff}, for the original functional space of the model, F, given by (1·10) is an extremely complicated many-body operator because of the projection operator p and the effective interaction potential V_{eff} with the complicated second term on the r.h.s. of (1·11). In CDCC, it is replaced by a proper phenomenological model Hamiltonian, H_M, which is physically reasonable and yet simple enough for numerical works. In the present section, a general prescription for the replacement is described and its application to some special examples are discussed.

3.1. *General prescription for constructing model Hamiltonians*

The prescription is basically to replace the p and V_{eff} in H_{eff} by some reasonable, simple, phenomenological operators, while keeping the total kinetic energy operator K unchanged. It has already been discussed how the projector p for the original functional space of the model, F, spanned by exact internal wave functions, $\{\phi_\gamma\}$, is replaced by $\bar{p}$ for the space $\bar{F}$ spanned by the phenomenological model internal wave functions, $\{\bar{\phi}_\gamma\}$, and eventually by P for the truncated and discretized model space, M, spanned by the discretized internal wave functions, $\{\hat{\phi}_{\gamma i}\}$.

Correspondingly, we first replace H_{eff} by a phenomenological effective Hamiltonian $\bar{H}_{\text{eff}}$ given by

$$\bar{H}_{\text{eff}}=\bar{p}(K+\bar{V}_{\text{eff}})\bar{p}, \tag{3·1}$$

where $\bar{V}_{\text{eff}}$ is a phenomenological effective potential which replaces V_{eff}. We then define the model Hamiltonian H_M by

$$H_M=P(K+\bar{V}_{\text{eff}})P, \tag{3·2}$$

simply replacing $\bar{p}$ in $\bar{H}_{\text{eff}}$ by P. This is reasonable because the same model internal Hamiltonians are used in $\bar{F}$ and M as discussed in § 2.

The replacement of V_{eff} must satisfy two obvious conditions. One condition is that $\bar{V}_{\text{eff}}$ be phenomenologically reasonable and at the same time simple enough to be used in actual CDCC calculations. The other condition is that the replacement be consistent with that of the projection operator described above since the latter involves the replacement of internal Hamiltonians which include some parts of the interaction potential.

Bearing these conditions in mind, we take $\bar{V}_{\text{eff}}$ to be such an operator that it takes a form

$$\bar{V}_{\text{eff}}=\bar{V}_{\text{eff}}^{(\gamma)}\equiv\bar{V}_{\text{c}}+\bar{V}_{\text{C}}+\bar{V}_{\gamma}, \tag{3·3}$$

in every two-cluster channel γ in the model, where $\bar{V}_c$ and $\bar{V}_C$ are phenomenological potentials of interaction *within* clusters c and C, respectively, and $\bar{V}_\gamma$ is that *between* c and C. Note that the original interaction potential, V, has this property, i.e., it takes a form

$$V=V^{(\gamma)}\equiv V_c+V_C+V_\gamma, \tag{3·4}$$

in every two-cluster channel γ. However, V_{eff} does not have this property.

As is well known, the total kinetic energy K can also be written in the form

$$K=K_c+K_C+K_\gamma \tag{3·5}$$

in channel γ where K_c and K_C are the kinetic energy of internal motion of c and C, respectively, and K_γ is that of relative motion between c and C. The center-of-mass kinetic energy of the total system, K_G, is set to zero in (3·5). Equations (3·3) and (3·5) lead to the form of the total Hamiltonian, $H=K+V$, in channel γ

$$H=H^{(\gamma)}\equiv K+V^{(\gamma)}=K_c+V_c+K_C+V_C+K_\gamma+V_\gamma, \tag{3·6}$$

which can also be written as

$$H^{(\gamma)}=h_c+h_C+K_\gamma+V_\gamma, \tag{3·7}$$

where

$$h_c=K_c+V_c \quad \text{and} \quad h_C=K_C+V_C \tag{3·8}$$

are the internal Hamiltonians of c and C, respectively.

Upon inserting (3·3) and (3·5) into (3·1), one gets a form, $\bar{H}_{\text{eff}}^{(\gamma)}$, which $\bar{H}_{\text{eff}}$ takes in channel γ which is completely parallel to (3·7)

$$\bar{H}_{\text{eff}}=\bar{H}_{\text{eff}}^{(\gamma)}\equiv\bar{p}(\bar{h}_c+\bar{h}_C+K_\gamma+\bar{V}_\gamma)\bar{p}, \tag{3·9}$$

where

$$\bar{h}_c=K_c+\bar{V}_c \quad \text{and} \quad \bar{h}_C=K_C+\bar{V}_C \tag{3·10}$$

are the phenomenological internal Hamiltonians for c and C, respectively.

Now, one can satisfy the two conditions for the replacement of V_{eff} by $\bar{V}_{\text{eff}}$ stated earlier. We take $\bar{V}_c$, $\bar{V}_C$ and $\bar{V}_\gamma$ to be reasonable phenomenological substitutes of the corresponding parts of the original potential, V_c, V_C and V_γ, respectively, which include the effect of the excluded channels, and yet simple enough for numerical works in the CDCC calculation. The consistency of $\bar{V}_{\text{eff}}$ with the projection operator $\bar{p}$ can be satisfied by taking $\bar{V}_c$ and $\bar{V}_C$ such that the model internal Hamiltonians $\bar{h}$ are the same as those which define $\bar{F}$, and hence $\bar{p}$. The model Hamiltonian, H_M, is given by $\bar{H}_{\text{eff}}$ with $\bar{p}$ replaced by P, (3·2). Its form in channel γ is given, from (3·9), by

$$H_M=H_M^{(\gamma)}\equiv P(\bar{h}_c+\bar{h}_C+K_\gamma+\bar{V}_\gamma)P. \tag{3·11}$$

3.2. *Application to special cases*

Actual choice of $\bar{V}_{\text{eff}}$, and consequently of $\bar{H}_{\text{eff}}$ and H_M, is done basically case by case,

depending much on the reaction mechanism assumed, i.e., F. We give some examples of practical interest in the following.

(A) One channel model

If one calculates elastic scattering in a channel α with particles a and A, and assumes that no direct process through other channels is important, F includes only channel α. Then, it is clear that $V_{\rm eff}$ given by (1·11) is just the Feshbach generalized optical potential for channel α. Then, it is reasonable to replace it by a phenomenological optical potential, $U_\alpha^{\rm OPT}$ at the energy $E_\alpha=E-\varepsilon_\alpha$. Hence,

$$\bar{V}_{\rm eff}=U_\alpha^{\rm OPT}. \tag{3·12}$$

Then,

$$\bar{H}_{\rm eff}=\bar{p}(\bar{h}_{\rm a}+\bar{h}_{\rm A}+K_\alpha+U_\alpha^{\rm OPT})\bar{p}. \tag{3·13}$$

Since $\bar{p}=P$ in this case, because there is only one channel,

$$H_M=P(\bar{h}_{\rm a}+\bar{h}_{\rm A}+K_\alpha+U_\alpha^{\rm OPT})P=\bar{H}_{\rm eff}. \tag{3·14}$$

(B) Three-body model Hamiltonian

Let us consider a reaction induced by a loosely bound projectile a impinging upon a nucleus A. We consider the case in which (a) no rearrangement process is important, (b) A remains in the ground state, and (c) a can break up into two fragments, 1 and 2, each remaining in the ground state. Then, only elastic scattering and elastic breakup of a are the important processes. Generalization to include excited bound states of A is straightforward.

An obviously appropriate model of reaction mechanism in this case would be multi-step processes within the channels of three bound particles, 1, 2 and A, interacting with each other. This is called a three-body model. The internal wave functions of the channels define the functional space of the model F.

Following the general prescription, we take the phenomenological effective Hamiltonian to be of a form

$$\bar{H}_{\rm eff}=\bar{p}(\bar{h}_{\rm a}+\bar{h}_{\rm A}+K_\alpha+\bar{V}_\alpha)\bar{p}, \tag{3·15}$$

where $\bar{p}$ is the projector onto the space $\bar{F}$ spanned by the eigen-functions of $\bar{h}_{\rm a}$ and $\bar{h}_{\rm A}$, of which $\bar{h}_{\rm a}$ has a form

$$\bar{h}_{\rm a}=K_{12}+\bar{V}_{12}+\bar{h}_1+\bar{h}_2, \tag{3·16}$$

where K_{12} and $\bar{V}_{12}$ are the kinetic and model potential energy operators of relative motion between 1 and 2, respectively, and $\bar{h}_1$ and $\bar{h}_2$ are the model internal Hamiltonians of 1 and 2, respectively.

Now, we choose $\bar{V}_\alpha$. One possible choice[5e] is $\bar{V}_\alpha=\sum_{i\in{\rm a},j\in{\rm A}}\bar{V}_{ij}$ where $\bar{V}_{ij}$ is an effective two-nucleon potential given by, say, the G-matrix theory. Another reasonable choice is

$$\bar{V}_\alpha=\bar{V}_{1{\rm A}}+\bar{V}_{2{\rm A}}, \tag{3·17}$$

where $\bar{V}_{1A}$ and $\bar{V}_{2A}$ are potentials of interaction of 1 and 2 with A, respectively. It is not altogether clear in our approach what to take for $\bar{V}_{1A}$ and $\bar{V}_{2A}$. A reasonable choice would be the optical potentials for the pairs (1, A) and (2, A). Optical potentials, however, depend on energy, and the energies of 1 and 2 relative to A are not well defined because the two fragments exchange energies through mutual interaction, $\bar{V}_{12}$. Furthermore, if the $\bar{V}$, and hence $\bar{H}_{\text{eff}}$, depended on the energy of the individual fragments, one would have to deal with a very difficult problem of solving a Schroedinger equation with a Hamiltonian which depends on the energy of subsystems. A theoretical discussion of the nature of the $\bar{V}$ has been given elsewhere,[7] and we do not discuss it any further here.

In the subsequent chapters except Chapter VI, the $\bar{V}$ are taken to be the optical potentials U_{1A}^{OPT} and U_{2A}^{OPT} at the most probable energies of relative motion between 1 and A, and 2 and A, E_{1A} and E_{2A}, respectively. Thus,

$$\bar{H}_{\text{eff}}=\bar{p}(\bar{h}_{\text{a}}+\bar{h}_{\text{A}}+K_{\alpha}+U_{1A}^{\text{OPT}}(E_{1A})+U_{2A}^{\text{OPT}}(E_{2A}))\bar{p}. \tag{3·18}$$

This is the phenomenological effective Hamiltonian of the three-body model which is used in actual calculations. If all the breakup states are included in $\bar{F}$, $\bar{p}$ commutes with the operators inside the parentheses, and so may be omitted with the understanding that $\bar{H}_{\text{eff}}$ operates onto wave functions within $\bar{F}$.

The three-body character of $\bar{H}_{\text{eff}}$ becomes even more apparent if one writes it in the form

$$\bar{H}_{\text{eff}}=\bar{p}(\bar{h}_{\text{A}}+\bar{h}_{1}+\bar{h}_{2}+K_{12}+K_{\alpha}+U_{1A}^{\text{OPT}}+U_{2A}^{\text{OPT}}+\bar{V}_{12})\bar{p}. \tag{3·19}$$

If A is much heavier than 1 and 2,

$$K_{12}+K_{\alpha}\approx K_{1A}+K_{2A}, \tag{3·20}$$

where K_{1A} and K_{2A} are the kinetic energies of 1 and 2 relative to A, one can approximate $\bar{H}_{\text{eff}}$ as

$$\bar{H}_{\text{eff}}\approx\bar{p}(\bar{h}_{\text{A}}+\bar{h}_{1}+\bar{h}_{2}+K_{1A}+K_{2A}+U_{1A}^{\text{OPT}}+U_{2A}^{\text{OPT}}+\bar{V}_{12})\bar{p}. \tag{3·21}$$

This form of $\bar{H}_{\text{eff}}$ is sometimes convenient for theoretical discussions.[7]

Finally, the model Hamiltonian H_M is obtained from $\bar{H}_{\text{eff}}$ by the replacement of the $\bar{p}$ by the P,

$$H_M=P(\bar{h}_{\text{a}}+\bar{h}_{\text{A}}+K_{\alpha}+U_{1A}^{\text{OPT}}(E_{1A})+U_{2A}^{\text{OPT}}(E_{2A}))P \tag{3·22}$$

or

$$H_M=P(\bar{h}_{\text{A}}+\bar{h}_{1}+\bar{h}_{2}+K_{12}+K_{\alpha}+U_{1A}^{\text{OPT}}+U_{2A}^{\text{OPT}}+\bar{V}_{12})P. \tag{3·23}$$

An important example of three-body Hamiltonian is that for deuteron induced reactions in which only elastic scattering and elastic breakup process are important. In that case, the phenomenological effective Hamiltonian discussed above is given by

$$\bar{H}_{\text{eff}}=\bar{p}(\bar{h}_{\text{d}}+\bar{h}_{\text{A}}+K_{\text{dA}}+U_{\text{pA}}^{\text{OPT}}+U_{\text{nA}}^{\text{OPT}})\bar{p}, \tag{3·24}$$

where

$$\bar{h}_{\mathrm{d}}=K_{\mathrm{pn}}+\bar{V}_{\mathrm{pn}}, \tag{3·25}$$

and the nucleon optical potentials, $U_{\mathrm{pA}}^{\mathrm{OPT}}$ and $U_{\mathrm{nA}}^{\mathrm{OPT}}$, are those at half the incident deuteron energy, E_{d}, $E_{\mathrm{pA}}=E_{\mathrm{nA}}=E_{\mathrm{d}}/2$. Again, (3·24) can be rewritten as

$$\bar{H}_{\mathrm{eff}}=\bar{p}(\bar{h}_{\mathrm{A}}+K_{\mathrm{pn}}+K_{\mathrm{dA}}+U_{\mathrm{pA}}^{\mathrm{OPT}}+U_{\mathrm{nA}}^{\mathrm{OPT}}+\bar{V}_{\mathrm{pn}})\bar{p}, \tag{3·26}$$

which may be approximated for A much heavier than the nucleons as

$$\bar{H}_{\mathrm{eff}}\approx\bar{p}(\bar{h}_{\mathrm{A}}+K_{\mathrm{pA}}+K_{\mathrm{nA}}+U_{\mathrm{pA}}^{\mathrm{OPT}}+U_{\mathrm{nA}}^{\mathrm{OPT}}+\bar{V}_{\mathrm{pn}})\bar{p}. \tag{3·27}$$

Finally, the model Hamiltonian is given by $\bar{H}_{\mathrm{eff}}$ with $\bar{p}$ replaced by P,

$$H_M=P(\bar{h}_{\mathrm{d}}+\bar{h}_{\mathrm{A}}+K_{\mathrm{dA}}+U_{\mathrm{pA}}^{\mathrm{OPT}}+U_{\mathrm{nA}}^{\mathrm{OPT}})P \tag{3·28}$$

or

$$H_M=P(\bar{h}_{\mathrm{A}}+K_{\mathrm{pn}}+K_{\mathrm{dA}}+U_{\mathrm{pA}}^{\mathrm{OPT}}+U_{\mathrm{nA}}^{\mathrm{OPT}}+\bar{V}_{\mathrm{pn}})P, \tag{3·29}$$

which for A much heavier than the nucleons can be approximated as

$$H_M\approx P(\bar{h}_{\mathrm{A}}+K_{\mathrm{pA}}+K_{\mathrm{nA}}+U_{\mathrm{pA}}^{\mathrm{OPT}}+U_{\mathrm{nA}}^{\mathrm{OPT}}+\bar{V}_{\mathrm{pn}})P. \tag{3·30}$$

The optical potentials are those at $E_{\mathrm{pA}}=E_{\mathrm{nA}}=E_{\mathrm{d}}/2$.

The $\bar{H}_{\mathrm{eff}}$ given by (3·18) and (3·24) and the corresponding H_M are used in the calculations described in Chapters III[5c] and IV.[5d]

(C) Rearrangement process

If rearrangement processes are important in a reaction, due to strong coupling of the rearranged channels with the incident channel, F must include such channels. One, therefore, has to deal with more than one partitions of the system. Let us take an example of just two partitions (a, A) and (b, B) with various internal states. We denote the channels with (a, A) by α and those with (b, B) by β. We assume that F includes breakup states of cluster a, while all the other clusters are in bound states.

According to our general prescription, the phenomenological effective Hamiltonian, $\bar{H}_{\mathrm{eff}}$, in this case takes two different forms, $\bar{H}_{\mathrm{eff}}^{(\alpha)}$ and $\bar{H}_{\mathrm{eff}}^{(\beta)}$ in channels α and β, respectively. For channels α with breakup states of a, it is appropriate to take a three-body model Hamiltonian $\bar{H}_{\mathrm{eff}}{}^{(\alpha)}$ of the form (3·18) or (3·19). For channels β with only bound states,

$$\bar{H}_{\mathrm{eff}}^{(\beta)}=\bar{p}(\bar{h}_{\mathrm{B}}+K_{\mathrm{pB}}+\bar{V}_{\mathrm{pB}})\bar{p}, \tag{3·31}$$

is appropriate. The set $\{\bar{H}_{\mathrm{eff}}^{(\alpha)}, \bar{H}_{\mathrm{eff}}^{(\beta)}\}$ defines $\bar{H}_{\mathrm{eff}}$, and hence H_M.

An example of this situation is a (d, p) reaction,

$$\mathrm{A}+\mathrm{d}(\mathrm{p}+\mathrm{n})\rightarrow\mathrm{B}(\mathrm{A}+\mathrm{n})+\mathrm{p}$$

with a strong coupling of the proton channel with the deuteron channels including breakup states. We take $\bar{H}_{\mathrm{eff}}$ in this case to be the three-body model Hamiltonian of (3·24) in the

deuteron channels

$$H_{\rm eff}^{\rm (d)}=\bar{p}(\bar{h}_{\rm d}+\bar{h}_{\rm A}+K_{\rm dA}+U_{\rm pA}^{\rm OPT}(E_{\rm pA}=E_{\rm d}/2)+U_{\rm nA}^{\rm OPT}(E_{\rm nA}=E_{\rm d}/2))\bar{p} \tag{3·32}$$

with

$$\bar{h}_{\rm d}=K_{\rm pn}+\bar{V}_{\rm pn}, \tag{3·33}$$

and in the proton channel

$$\bar{H}_{\rm eff}^{\rm (p)}=\bar{p}(\bar{h}_{\rm B}+K_{\rm pB}+\bar{V}_{\rm pB})\bar{p}. \tag{3·34}$$

Since B consists of A and n, the model internal Hamiltonian $\bar{h}_{\rm B}$ can be written in the form

$$\bar{h}_{\rm B}=\bar{h}_{\rm A}+K_{\rm nA}+\bar{V}_{\rm nA}, \tag{3·35}$$

where $\bar{V}_{\rm nA}$ is a model interaction potential between n and A. Likewise it is reasonable to assume that $\bar{V}_{\rm pB}$ is of the form

$$\bar{V}_{\rm pB}=\bar{V}_{\rm pA}+\bar{V}_{\rm pn}, \tag{3·36}$$

and take $\bar{V}_{\rm pn}$ to be the same as the one in $\bar{h}_{\rm d}$ of (3·33). Putting (3·35) and (3·36) into (3·34) one has

$$\bar{H}_{\rm eff}^{\rm (p)}=\bar{p}(\bar{h}_{\rm A}+K_{\rm pB}+K_{\rm nA}+\bar{V}_{\rm pA}+\bar{V}_{\rm nA}+\bar{V}_{\rm pn})\bar{p}. \tag{3·37}$$

In the extreme single particle model, $\bar{V}_{\rm nA}$ is a single particle potential,

$$\bar{V}_{\rm nA}=U_{\rm nA}(\boldsymbol{r}_{\rm nA}). \tag{3·38}$$

One could also take $\bar{V}_{\rm pA}$ to be an optical potential

$$\bar{V}_{\rm pA}=U_{\rm pA}^{\rm OPT}, \tag{3·39}$$

at the outgoing proton energy. Then, (3·37) becomes

$$\bar{H}_{\rm eff}^{\rm (p)}=\bar{p}(\bar{h}_{\rm A}+K_{\rm pB}+K_{\rm nA}+U_{\rm pA}^{\rm OPT}+U_{\rm nA}+\bar{V}_{\rm pn})\bar{p}. \tag{3·40}$$

Again, the model Hamiltonian, H_M, is given by $\bar{H}_{\rm eff}$ of (3·32) and (3·37) or (3·40) with the $\bar{p}$ replaced by the P.

Now, it is noticed that the forms of $\bar{H}_{\rm eff}^{\rm (p)}$ given by (3·37) and (3·40) are quite similar to that of $\bar{H}_{\rm eff}^{\rm (d)}$ in the approximation (3·27)

$$\bar{H}_{\rm eff}^{\rm (d)}\approx\bar{p}(\bar{h}_{\rm A}+K_{\rm nA}+K_{\rm pA}+U_{\rm pA}^{\rm OPT}+U_{\rm nA}^{\rm OPT}+\bar{V}_{\rm pn})\bar{p}. \tag{3·41}$$

In fact, the right-hand side of (3·40) is the same as that of (3·41) for a heavy A for which $K_{\rm pB}\approx K_{\rm nA}$ if $U_{\rm nA}$ is changed to $U_{\rm nA}^{\rm OPT}$. This is the reason why sometimes $\bar{H}_{\rm eff}^{\rm (d)}$ and $\bar{H}_{\rm eff}^{\rm (p)}$ are regarded as a same three-body Hamiltonian with a neutron-nucleus potential which depends on the neutron energy, an optical potential for a neutron in the continuum and a real binding potential for a neutron in a bound state.

The form of (3·41), however, is only an approximate one, correct only for heavy A.

Furthermore, a three-body Hamiltonian which depends on the energy of a subsystem, the neutron, seems likely to lead to the same kind of difficulty as mentioned in the case of the nucleon optical potentials in the deuteron breakup channels. There is no such difficulty with the general prescription of the present paper for constructing $\bar{H}_{\text{eff}}$.

The $\bar{H}_{\text{eff}}$ given by (3·32) and (3·34) is the one used in the calculations described in Chapter V.[4d)]

§ 4. Model Schroedinger equation and boundary condition

We are now in the position to determine the model wave function given by

$$\Psi_M \equiv P\Psi = \sum_{\gamma}\sum_{i} \hat{\Phi}_{\gamma i}(\xi_\gamma, \hat{R}_\gamma)\hat{\chi}_{\gamma i}(R_\gamma), \tag{4·1}$$

by solving the model Schroedinger equation

$$H_M \Psi_M = E\Psi_M, \tag{4·2}$$

which is equivalent to

$$(\hat{\Phi}_{\gamma i}(\xi_\gamma, \hat{R}_\gamma)|H_M - E|\sum_{\mu j}\hat{\Phi}_{\mu j}(\xi_\mu, \hat{R}_\mu)\hat{\chi}_{\mu i}(R_\gamma)\rangle = 0, \tag{4·3}$$

for all the γi in M, where the left parenthesis signifies the integration over the coordinates in $\hat{\Phi}_{\gamma i}$ only. If one uses (3·11), (2·27) and (2·30), one can rewrite (4·3) as

$$(K_\gamma + U_{\gamma i} - E_{\gamma i})\hat{\chi}_{\gamma i} = -\sum_{\mu j \neq \gamma i}(\hat{\Phi}_{\gamma i}|H - E|\hat{\Phi}_{\mu j}\hat{\chi}_{\mu j}\rangle, \tag{4·4}$$

where

$$U_{\gamma i} = \langle \hat{\Phi}_{\gamma i}|\bar{V}_\gamma|\hat{\Phi}_{\gamma i}\rangle \tag{4·5}$$

and

$$E_{\gamma i} = E - \bar{\varepsilon}_{\gamma i}, \tag{4·6}$$

where $\bar{\varepsilon}_{\gamma i}$ is the internal energy associated with $\hat{\Phi}_{\gamma i}$, given by (2·29). Equations (4·3) and (4·4) are general forms of the coupled equations of CDCC for the unknown radial functions of relative motion, $\hat{\chi}_{\gamma i}(R_\gamma)$. The quantity

$$F(\gamma i, \mu j) \equiv (\hat{\Phi}_{\gamma i}|H - E|\hat{\Phi}_{\mu j}) \tag{4·7}$$

is called the form factor of coupling between channels γi and μj. The finiteness of the dimension of M guarantees a unique solution of (4·2) through (4·4).

In the case of the three-body model with H_M given by (3·22) discussed in § 3, (4·4) takes the form

$$(K_\alpha + U_{\alpha i} - E_{\alpha i})\hat{\chi}_{\alpha i} = -\sum_{j \neq i}(\hat{\Phi}_{\alpha i}|U_{1\text{A}}^{\text{OPT}}(E_{1\text{A}}) + U_{2\text{A}}^{\text{OPT}}(E_{2\text{A}})|\hat{\Phi}_{\alpha j}), \tag{4·8}$$

because of (2·28) and (2·30).

In the case of coupled rearranged channels, discussed in § 3, situation is somewhat complicated because of the non-orthogonality of rearranged channels. The form factor of coupling between rearranged channels, α and β

$$F(\alpha, \beta)=(\hat{\Phi}_\alpha|H_M-E|\hat{\Phi}_\beta), \tag{4·9}$$

is now an integral operator acting on $\bar{\chi}_\alpha$ because R_α is a function of ξ_β. There is an ambiguity as to which of the forms of H_M to take, $H_M^{(\alpha)}$ or $H_M^{(\beta)}$. In principle, H_M ought to be so chosen that either form gives the same result. In practice, however, this may not necessarily be the case. If we take $H_M^{(\beta)}$ of the form (3·29), then,

$$F(\alpha, \beta)=(\Phi_\alpha|K_\beta+\bar{V}_\beta-E_\beta|\Phi_\beta), \tag{4·10}$$

$$=F_{\alpha\beta}+N_{\alpha\beta}, \tag{4·11}$$

where

$$F_{\alpha\beta}=(\Phi_\alpha|\bar{V}_\beta-U_\beta|\Phi_\beta) \tag{4·12}$$

and

$$N_{\alpha\beta}=(\Phi_\alpha|K_\beta+U_\beta-E_\beta|\Phi_\beta), \tag{4·13}$$

where U_β is an auxiliary potential which is a function of $\boldsymbol{R}_\beta$, introduced to reduce $\bar{V}_\beta$ to the "residual interaction", $\bar{V}_\beta-U_\beta$. $F_{\alpha\beta}$ is called the interaction term, and $N_{\alpha\beta}$ the non-orthogonality term of the coupling form factor. $N_{\alpha\beta}$ would be zero if channels α and β were orthogonal to each other. As the operator in (4·12) shows, it has a long range which makes the calculation rather complicated. We do not go into any further discussion of the subject, and refer the reader to the papers of Ref. 8).

The boundary condition for the model wave function is assumed to be that $\hat{\chi}_{\gamma i}(R_\gamma)$ have the same asymptotic form as that of $\bar{\chi}_\gamma(R_\gamma)$ in $\bar{p}\Psi$ which corresponds to the energy of relative motion $E_{\gamma i}$. For a reaction initiated in channel α, the asymptotic form of the $\bar{\chi}_\gamma$ is given by

$$R\bar{\chi}_\gamma(R)\sim u_{\gamma L_\gamma}^{(-)}(P_{\gamma i}, R)\delta_{\alpha\gamma}-\bar{S}_{\gamma\alpha}(P_{\gamma i})u_{\gamma L_\gamma}^{(+)}(P_{\gamma i}, R), \quad (R\to\infty) \tag{4·14}$$

if channel γ is open at $E_{\gamma i}$, and

$$R\bar{\chi}_\gamma(R)\sim W_{L_\gamma}(\varkappa_{\gamma i}, R), \quad (R\to\infty) \tag{4·15}$$

if channel γ is closed at $E_{\gamma i}$, where $P_{\gamma i}=(2\mu_\gamma E_{\gamma i}/\hbar^2)^{1/2}$ for $E_{\gamma i}\geq 0$ and $\varkappa_{\gamma i}=(-2\mu_\gamma E_{\gamma i}/\hbar^2)^{1/2}$ for $E_{\gamma i}\leq 0$ where μ_γ is the reduced mass in channel γ. $\bar{S}_{\gamma\alpha}(P_{\gamma i})$ is the model S-matrix element of process $\alpha\to\gamma$ at wave number $P_{\gamma i}$, and the $u^{(\pm)}$ are the usual outgoing and incoming Coulomb wave functions with the asymptotic forms

$$u_{\gamma L_\gamma}^{(\pm)}(P_{\gamma i}, R)\sim\exp[\pm i(P_{\gamma i}R-\eta_{\gamma i}\ln 2P_{\gamma i}R-L_\gamma\pi/2)]/\sqrt{v_{\gamma i}}, \tag{4·16}$$

where $v_{\gamma i}=\hbar P_{\gamma i}/\mu_\gamma$, and $\eta_{\gamma i}=Z_c Z_c e^2/\hbar v_{\gamma i}$ is the Sommerfeld parameter.

Correspondingly, the asymptotic form of $\hat{\chi}_{\gamma i}(R)$ is set to

$$R\hat{\chi}_{\gamma i}(R)\sim u^{(-)}_{\gamma L_\gamma}(P_{\gamma i}, R)\delta_{\alpha\gamma}-\hat{S}_{\gamma i,\alpha}u^{(+)}_{\gamma L_\gamma}(P_{\gamma i}, R), \quad (R\to\infty) \tag{4·17}$$

for $E_{\gamma i}\geq 0$, and

$$R\hat{\chi}_{\gamma i}(R)\sim W_{L_{\gamma i}}(\chi_i, R), \quad (R\to\infty) \tag{4·18}$$

for $E_{\gamma i}\leq 0$.

The relation between $\hat{S}_{\gamma i,\alpha}$ and $\bar{S}_{\gamma\alpha}$ is rather involved. It is not always reasonable to associate $\hat{S}_{\gamma i,\alpha}$ directly to $\bar{S}_{\gamma\alpha}(P_{\gamma i})$ because $\hat{\phi}_{\gamma j}$ with $j\neq i$ may contain a component of $\bar{\phi}_\gamma(k, \xi_\gamma)$ with k in $[k_{i-1}, k_i]$, in general. In the case of discretization by the momentum-bin method with constant weight functions, (2·19), however, the relation is direct

$$\bar{S}_{\gamma\alpha}(P_{\gamma i})=\hat{S}_{\gamma i,\alpha}/\sqrt{\Delta_{\gamma i}}. \tag{4·19}$$

In actual numerical calculations, the boundary condition (4·16) or (4·17) is set at a large but finite R_γ, say $R_{\gamma,\mathrm{m}}$. In order for a $\hat{\chi}_{\gamma i}(R_\gamma)$ be close to the $\bar{\chi}_\gamma(R_\gamma)$ which it is supposed to represent, it is necessary that $R_{\gamma,\mathrm{m}}$ be so large that the asymptotic form of (4·14) and (4·15) are at least approximately valid for the $\bar{\chi}_\gamma(R_\gamma)$. However, it must not be so large as to jeopardize the l truncation, because the coupling between breakup channels of high l become increasingly important as R_γ becomes large. It is an assumption of CDCC that a set of the $R_{\gamma,\mathrm{m}}$ can be found in such a way as to satisfy the both requirements.

The boundary condition described above seems to be the most reasonable one under this assumption. It should be borne in mind, however, that the model wave function, Ψ_M, thus obtained has three-body breakup parts with wrong asymptotic forms. In fact, it has been shown[9] that in the asymptotic region of three-body breakup channels γ, Ψ_M decreases as R^{-3} rather than $R^{-5/2}$, as in the correct asymptotic form, where R is the hyperradius, $R=(R_\gamma^2+r_{12}^2)^{1/2}$. Hence, Ψ_M *cannot* be equal to $p\Psi$ or $\bar{p}\Psi$ in the entire configuration space. This would be catastrophic from the point of view of approximating the wave function. This is, however, not the case for CDCC because its aim is to calculate some specific physical quantities rather than wave function: The asymptotic form of the wave function is often irrelevant, depending on the quantities to be calculated. This point is discussed in the next section.

§ 5. Calculation of physical quantities

The model wave function, Ψ_M, found in the way described in the preceding sections is used for the calculation of the desired physical quantities $\{Q\}$, with the aid of model operators $\{\bar{Q}\}$ corresponding to $\{Q\}$ in general. However, the procedure of calculation is by no means unique. We explain this below for the case of calculation of transition matrix elements.

Suppose, for example, we wish to calculate $T_{\beta\alpha}(P_\beta)$ of a reaction with the initial and final channels α and β, respectively for the final momentum of relative motion P_β. One can calculate it from the $\hat{S}$-matrix elements defined in the previous section, through calculation of $\bar{S}_{\beta\alpha}(P_\beta)$. The procedure of calculating $\bar{S}_{\beta\alpha}(P_\beta)$ from the $\hat{S}$, however, depends on the method of discretization of the continuum. For example, if it is done by the momentum-bin method with constant weight functions, (2·19), $\bar{S}_{\beta\alpha}(P_\beta)$ may be obtained by an inter-

polation of the $\hat{S}_{\beta i,\alpha}/\sqrt{\Delta_{\beta i}}$, which can be identified with $\bar{S}_{\beta\alpha}(P_{\beta i})$ as (4·19) shows, for a P_β between the $P_{\beta i}$. This is actually the procedure that is used in Chapters III,[5c] IV[5d] and VI.[5e]

One can, however, calculate $T_{\beta\alpha}$ also from the well-known integral formula in the post form

$$T_{\beta\alpha}=\langle e^{iP_\beta\cdot R_\beta}\cdot\phi_\beta|\, V_\beta|\,\Psi_\alpha^{(+)}\rangle, \tag{5·1}$$

substituting the wave functions and the potential with corresponding model ones

$$\bar{T}_{\beta\alpha}=\langle e^{iP_\beta\cdot R_\beta}\cdot\bar{\phi}_\beta|\,\bar{V}_\beta|\,\Psi_{M\alpha}^{(+)}\rangle \tag{5·2}$$

or from the formula corresponding to the prior form of $T_{\beta\alpha}$

$$\bar{T}_{\beta\alpha}=\langle\Psi_{M\beta}^{(-)}|\,\bar{V}_\alpha|e^{iP_\alpha\cdot R_\alpha}\cdot\bar{\phi}_\alpha\rangle, \tag{5·3}$$

where $\Psi_{M\alpha}^{(+)}$ has the same scattering state boundary condition as $\Psi_\alpha^{(+)}$, and $\Psi_{M\beta}^{(-)}$ as $\Psi_\beta^{(-)}$. Note that the model operators, i.e., the barred potentials are used in (5·2) and (5·3), hence the bar in $\bar{T}_{\beta\alpha}$.

Still another procedure is to calculate $\bar{S}_{\beta\alpha}$ by a variational method such as the Coupled-Channel Variational Method (CCVM) discussed in Chapter V,[4d] using $\Psi_{M\alpha}^{(+)}$ and $\Psi_{M\beta}^{(-)}$ as trial functions. These and other possible procedures give $T_{\beta\alpha}$ which differ from each other in general, in the value and in the expected accuracy. It is important that the procedure matches well with the model space and the model Hamiltonian to give optimal results. In fact, the model space, the model Hamiltonian, and the calculational procedure should be taken as a set, as is done in the previous sections.

Let us compare in more detail the two calculational procedures given above, one from the $\hat{S}$, and the other from the integral formulae. In order to fix the ideas, let us consider the T-matrix elements of deuteron induced reactions, (d,d), (d,p) and (d,pn). The nucleons are assumed to be spinless.

The calculation from the $\hat{S}$ relies on the model wave function at the boundary of the region in which actual CDCC calculations are made. Errors in the calculated T-matrix elements are directly proportional to the error in Ψ_M there. In order to obtain $T_{\mathrm{pn,d}}$ for continuous momenta of the outgoing p and n, one calculates the $\bar{S}_{\mathrm{d}^*\mathrm{d}}(P_{\mathrm{d}^*})$ for the continuous P_{d^*} from the discrete $\hat{S}$, although this procedure is not unique as already mentioned.

The model T-matrix elements in the integral forms are, for example,

$$\bar{T}_{\mathrm{dd}}=\langle e^{i\boldsymbol{k}_\mathrm{d}\cdot\boldsymbol{R}_\mathrm{d}}\bar{\phi}_\mathrm{d}(\boldsymbol{r}_\mathrm{pn})\Phi_\mathrm{A}(\xi_\mathrm{A})|\,U_\mathrm{pA}^{\mathrm{OPT}}(R_\mathrm{pA})+U_\mathrm{nA}^{\mathrm{OPT}}(R_\mathrm{nA})|\,\Psi_{M\mathrm{d}}^{(+)}\rangle, \tag{5·4}$$

$$\bar{T}_{\mathrm{pd}}=\langle\bar{\chi}_\mathrm{p}^{(-)}(\boldsymbol{R}_\mathrm{pB})\bar{\Phi}_\mathrm{B}(\boldsymbol{r}_\mathrm{nA},\,\xi_\mathrm{A})|\,\bar{V}_\mathrm{pn}(\boldsymbol{r}_\mathrm{pn})+(\bar{V}_\mathrm{pA}-U_\mathrm{pB}^{\mathrm{OPT}}(R_\mathrm{pB}))|\,\Psi_{M\mathrm{d}}^{(+)}\rangle, \tag{5·5}$$

$$\bar{T}_{\mathrm{pn,d}}=\langle e^{i\boldsymbol{k}_\mathrm{p}\cdot\boldsymbol{r}_\mathrm{p}}e^{i\boldsymbol{k}_\mathrm{n}\cdot\boldsymbol{r}_\mathrm{n}}\bar{\Phi}_\mathrm{A}(\xi_\mathrm{A})|\,U_\mathrm{pA}^{\mathrm{OPT}}+U_\mathrm{nA}^{\mathrm{OPT}}+\bar{V}_\mathrm{pn}|\,\Psi_{M\mathrm{d}}^{(+)}\rangle, \tag{5·6}$$

where ϕ_d, Φ_A, and Φ_B are the bound state wave functions of deuteron, nucleus A, and nucleus B, respectively, $\bar{\chi}_\mathrm{p}^{(-)}$ is the distorted wave in the auxiliary potential $U_\mathrm{pB}^{\mathrm{OPT}}$ which is taken to be the proton-B optical potential at the outgoing proton energy. The term $(\bar{V}_\mathrm{pA}-U_\mathrm{pB}^{\mathrm{OPT}})$ on the r.h.s. of (5·5) is eventually neglected, as in usual DWBA calculations.

It is noted that the integrands of (5·4) and (5·5) are significant only within a limited

region of the configuration space, say $r_{pn} \leq r_m$ and $R_d \leq R_m$, because of the finite range of the potentials and the bound state wave functions. Hence, $\bar{T}_{dd}$ and $\bar{T}_{pd}$ are affected only by the value of $\Psi^{(+)}_{Md}$ within this region. This has a great advantage because it allows a truncation of l with a relatively small l_m since in the limited region, $R_d \leq R_m$, coupling of d* states with high l turns out to be small, so that multi-step processes through them are negligible in the reaction starting from the deuteron ground state channel.

Now, it is easy to see that T_{dd} and T_{pd} calculated by the two procedures are actually the same if the same model wave function is used. There is, however, an advantage of great practical importance of the integral formula for T_{pd} over the calculation from the $\hat{S}$ when the coupling of the proton channel with the deuteron channels is weak. In that case, one can neglect the p channel in the CDCC calculation of $\Psi^{(+)}_{Md}$, and use that $\Psi^{(+)}_{Md}$ in (5·5) to calculate $\bar{T}_{pd}$. In the $\hat{S}$ procedure, the same model space would obviously give a null T_{pd} since the model wave function is zero in the proton channel.

The calculation of $T_{pn,d}$ is subtle, because there is no bound state wave function which limits the range of the final state interaction. As mentioned in § 4, Ψ_M has a wrong asymptotic form in the space of breakup channels. This implies that a CDCC calculation in a finite region bounded by $R_d \leq R_{d,m}$ contains an error in the calculated $T_{pn,d}$ which depends on $R_{d,m}$. This is true both in the calculation from the $\hat{S}$ and that from the integral formula. As long as the l truncation is valid, the error is a decreasing function of $R_{d,m}$. One, therefore, takes as large $R_{d,m}$ as possible to minimize the error. However, one cannot make the error arbitrarily small by taking $R_{d,m}$ arbitrarily large, because that would make the l truncation inconsistent since the coupling of channels with high l becomes increasingly important as R_d becomes large. One, therefore, would have to contrive other methods, in order to correct for the error.

There are advantages in the integral formula over the $\hat{S}$ procedure. The interpolation for continuous momenta, k and P_{d*}, is automatically done through the momenta in the final state wave functions in the integral. Also, it contains components of $\bar{T}_{pn,d}$ with the l not included in the model space, i.e., $l \geq l_{d,m}$, because the integral yields such components even if $\Psi^{(+)}_{Md}$ does not contain them. A great disadvantage of the integral formula, however, is the extra integral that has to be carried out after getting $\Psi^{(+)}_{Md}$ which is, of course, unnecessary in the $\hat{S}$ procedure. For this reason, the $\hat{S}$ procedure has been used in practice as reviewed in Chapter III.[5c)]

Finally, the calculated results are compared with experimental data. The quality of agreement between them is interpreted as the measure of how real the model of reaction mechanism, etc., are. If it is insufficient, improvement of the model has to be looked for. If the agreement is satisfactory, the model is deemed realistic and the model wave function Ψ_M is assumed to contain all the main important information on the wave function Ψ relevant to the calculated quantities $\{Q\}$, especially detailed information on the reaction mechanism relevant to $\{Q\}$. The best hope is that Ψ_M is a good approximation to $p\Psi$, at least within the limited region of the configuration space relevant to the calculation of $\{Q\}$, although this cannot be true for the entire configuration space as already mentioned. This is, however, probably too optimistic a hope in general because of the phenomenological steps involved in the calculation.

§ 6. Summary

Basic ideas and assumptions of CDCC are reviewed. The method is characterized as a phenomenological method of calculating some specific physical quantities in a reaction, rather than a method of approximately solving a Schroedinger equation with a given (model) Hamiltonian. The steps of actual CDCC calculations are described which are summarized as follows.

There are some specific physical quantities $\{Q\}$ in a specific reaction to be calculated. A model reaction mechanism of some multi-step direct processes is assumed with a procedure of the calculation of $\{Q\}$ fixed. The model is specified by a set of channels, including some continuous channels of broken up particles, among which the multi-step processes take place. The channel wave functions define a functional space of the model, F. For the sake of feasibility of actual calculations, the internal wave functions of the channels in F are substituted by phenomenological model wave functions, which define a phenomenological substitute, $\bar{F}$, for F. Then, the continuum channels in $\bar{F}$ are truncated and discretized into a finite number of "channels", which define the model space of the CDCC calculation, M. Two methods of discretization are described: the method of pseudo-states and the method of momentum-bins. Adequacy of the truncation and discretization is tested by the "convergence" of the calculated quantities.

A general prescription for constructing the model Hamiltonian of a CDCC calculation is given. One starts from the Feshbach effective Hamiltonian H_{eff} for the space F. One replaces the effective interaction potential, V_{eff}, in H_{eff} by a phenomenological one, $\bar{V}_{\text{eff}}$, to define a phenomenological effective Hamiltonian $\bar{H}_{\text{eff}}$ which is consistent with the space $\bar{F}$. One then defines the model Hamiltonian H_M by simply replacing $\bar{p}$, the projection operator onto $\bar{F}$, in $\bar{H}_{\text{eff}}$ by P, that onto M. Application to a one-channel model for elastic scattering, a three-body model for processes involving breakup of a projectile into two fragments, and that with a coupling of rearrangement channels are discussed, with examples of (d, d), (d, pn) and (d, p) as special cases.

The model Schroedinger equation with H_M is solved for a model wave function Ψ_M. A set of boundary conditions is set at the boundary of a finite region of the configuration space which is discussed in some detail.

Finally, the desired quantities $\{Q\}$ are calculated with the model wave function by some specific procedures associated with the model. The reality of the model is judged by the quality of agreement of the calculated results with experimental data. If it is good, the model is deemed realistic, and then the model wave function Ψ_M is assumed to contain all the main important information on the wave function Ψ relevant to the quantities $\{Q\}$, in particular the reaction mechanism involved.

Justification of CDCC has so far been empirical, relying almost entirely on the intuitive plausibility and agreement with experimental data. Theoretical investigation of the validity of CDCC is complicated by the fact that CDCC is not simply a mathematical method of approximately solving a Schroedinger equation with a given Hamiltonian, as clarified by the summary given above. It must eventually include justification of various phenomenological steps as well. However, even an examination of the effect of the truncation and discretization of the continuum channels on the wave function of a three-body model effective Hamiltonian, $\bar{H}_{\text{eff}}$, would be very instructive as a first step of such

investigation. In view of the remarkable success of CDCC as a phenomenological theory, clarification of its theoretical foundation is highly desirable in any case.

Acknowledgements

The author wishes to thank Drs. M. Kamimura, M. Yahiro and Prof. R.C. Johnson for very helpful discussions. He also wishes to thank Professors N. Austern and T. Sawada for their illuminating correspondences on the subject of the theoretical basis of CDCC.

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