General Formalism for the Transition Matrix of Nuclear Reaction Theory and Its Application to the Study of Potential Scattering

R. B. Perez
Neutron Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830
(Received 2 May 1972)

One develops a general integrodifferential equation for the transition matrix of nuclear reaction theory in terms of the physical parameters of the nuclear reaction. One derives, as a corollary of the main result, a system of equations which describes the motion of the poles and residues of the collision matrix as a function of the parameters entering in the reaction formalism. Some applications to the study of the potential-scattering problem are also shown.

I. INTRODUCTION

In the last ten years there has been an increased activity in the development of new methods to compute resonant cross sections based on various nuclear reaction theories. The problem at hand is that of calculating resonance parameters and cross sections from the Hamiltonian pertinent to the nucleus and its interaction with the incoming projectile.

The present work arises from the concern about the role and choice of the several parameters which enter in the various nuclear reaction formalisms. Examples on the effect of the channel radii and boundary condition numbers are given in the work of Lejeune and Mahaux.[1] Tobocman and collaborators,[2,3] and also Takeuchi and Moldauer[4] have pointed out and discussed the relationship between the convergence of R-matrix expansions and the value of the channel radius. These are by no means the only parameters of interest. One is also concerned with the strength, deformation, and diffusiveness of the channel potentials, and last but not least with the analytical properties of the collision matrix as a function of energy and angular momentum. Within the framework of R-matrix theory, some of these problems have been studied by Wigner,[5] Teichmann and Wigner,[6] Altman,[7] and Mockel and Perez.[8] The results of these investigations is a general differential equation, frequently a Ricatti-matrix-type equation which, starting from a given initial configuration, defines, the R matrix at any "later" value of the parameter of interest. There is at least one technical and one philosophical reason to repeat this kind of treatment for the transition T matrix.[9] The technical point has to do with the numerical problems arising from the singularities of the R matrix on the real energy axis. Despite the fact that there are several devices to go around these singular points, the problem can be avoided altogether by the use of the T matrix. From the philosophical viewpoint, the transition matrix has the attractive feature of being a function directly related to observable quantities such as phase shifts and cross sections.

Historically, the usual approach to this general problem goes in two steps. First, one performs a nuclear structure calculation from which one obtains the channel eigenfunctions, φ_c, which depend on the internal and angular coordinates of the system. Expansion of the total wave function in terms of the channel functions leads to a set of coupled radial Schrödinger equations, the so-called coupled channel of Breit,[10] Newton,[9] Tamura,[11] Buck,[12] and Feshbach,[13] among others. The second step has to do with the use and interpretation of the channel equations in the light of the various nuclear reaction formalisms.

There are two main avenues of approach to this latter problem. The first approach consists of the direct use of some nuclear formalism. The second utilizes shell-model eigenfunctions in the framework of an appropriate nuclear reaction theory.

In the first category the use of the Wigner-Eisenbud R-matrix theory[14] was proposed by Haglund and Robson[15] and investigated with great detail by Buttle[16] and by Lejeune and Mahaux.[1] The general idea is to develop the radial solutions in terms of R-matrix states obtained via the solution of the uncoupled-channel equations which satisfy rigorous R-matrix boundary conditions. This procedure yields the contribution of the nearby levels. The contribution of the slowly varying background, due to the levels unaccounted for in the calculation, is estimated by the introduction of a background R matrix obtained in a prescribed manner.

The second category employs as a basic tool the shell model applied to the calculation of nuclear continuum states (Mahaux and Weidenmuller[17]). There are, in principle, well-known problems involved in this approach. Firstly, one has to generalize the shell model so that the continuum part of the total wave function can be properly generated. Second, the shell-model functions have the wrong asymptotic behavior. There are various methods to avoid these pitfalls. In this connection, two subcategories of methods can be distinguished. First, one can consider those theories which do not use an interaction region. To this class belong the Bloch-Gillet[18] theory, the projection-operator formalism of Feshbach,[13] and the reaction theory derived by MacDonald.[19]

The second subclass contains the techniques which separate configuration space into an "inner" or interaction region and an asymptotic region. These theories are essentially R-matrix theories. Takeuchi and Moldauer[14] compute the shell-model functions for a Woods-Saxon potential with the requirement that the logarithmic radial derivatives of the single-particle states should have a certain fixed real value at the boundary radius. On this basis one obtains the R-matrix states from which the collision matrix can be computed.

The use of shell-model eigenfunctions in R-matrix theory has been also made possible by means of other devices. Tobocman and Nagarajan[2] force the shell-model functions to satisfy appropriate boundary conditions by introducing the latter as constraints in a variational principle, or through the use of the Green's function to relate the wave function inside the interaction region to its logarithmic derivative at the boundary. A generalization of this approach is the extended R-matrix theory of Garside and Tobocman.[3] In this method one introduces three channel radii for each channel, each of them performing one specific function. The extra parameters that appear in this case are treated either as free parameters of the theory or optimized by means of a variational principle.

Fortunately for the scientific historian, Lane and Robson in a series of papers[20-23] have developed a comprehensive formalism in which utilizing the very clever Bloch's $\mathcal{L}$ operator[24] they were able to unify the various nuclear theory formalisms as well as their application to cross-section calculations. The usefulness of this approach has been illustrated by Purcell.[25] The purpose of this work is twofold: First, to convert the multichannel coupled equations into a set of equations in terms of the Green's function; secondly, on the basis of the relation between the Green's function and the T-matrix operator, to generate a formalism allowing the evaluation of the variation of the transition matrix versus changes in the parameters entering in the theory.

In Sec. II one derives the relation between the collision and transition matrices with the multichannel Green's function. Section III is devoted to obtaining the variation of the T matrix by the use of invariant-imbedding techniques similar to the method employed by Mockel and Perez.[8] The "equation of motion" of the poles and residues of the T matrix are derived in Sec. IV. In Sec. V we discuss the generation of the Kapur-Peierls theory parameters[26] from the R-matrix parameters, utilizing the equations of motion previously derived. This problem is of interest in order to find the statistical properties of the U-matrix poles and residues. Finally in Secs. VI and VII one derives and generalizes various expressions related to the scattering of spinless particles by a central potential.

The present work makes extensive use of Bloch's $\mathcal{L}$ operator and from this viewpoint it can be incorporated into the comprehensive formalism of Lane and Robson. It is then hoped that its appearance will not increase the entropy of the field of nuclear reaction theory.

II. COUPLED-CHANNEL FORMALISM AND THE COLLISION MATRIX

Our starting point is the set of radial coupled-channel equations (see, for example, Tamura,[11] and Newton[9])

$$(D_c{}^2+E_c)\phi_c(r_c)-\sum_{c''}V_{cc''}(r_c)\phi_{c''}(r_c)=0\,, \tag{1}$$

where

$$D_c{}^2=\frac{\hbar^2}{2M_c}\,\frac{d^2}{dr_c{}^2}\,, \tag{2}$$

M_c is the reduced mass in channel c, $E_c=E-Q_c$ (Q_c is the threshold energy for channel c),

$$V_{cc'}(r_c)=(\varphi_c\,|\,V(\vec{r})+\frac{\hbar^2}{2M_c}\,\frac{l(l+1)}{r_c{}^2}\,|\varphi_{c'})\,. \tag{3}$$

In Eq. (3) l_c is the channel angular momentum, and the round brackets indicate that the integrations are performed over the angular and internal coordinates, keeping the radial coordinates constant. The channel eigenfunctions, φ_c, are those defined in the Lane and Thomas article.[27]

We now introduce the adjoint-channel Green's functions $G^{+}_{cc'}(r_c|r_{c'})$, satisfying the radial equations

$$(D_c{}^2+E_c)G^{+}_{cc'}(r_c|r_{c'})-\sum_{c''} V^{+}_{cc''}(r_c)G^{+}_{c''c'}(r_c|r_{c'})=-\delta(r_c-r_{c'})\delta_{cc'} \tag{4}$$

and the boundary conditions

$$\frac{\hbar^2}{2M_c}\frac{d}{dr_c}G^{+}_{cc'}(r_c|r_{c'})|_{r_c=a_c}=-B_c G^{+}_{cc'}(a_c|r_{c'}), \tag{5}$$

where the boundary-condition functions B_c are those used in the Kapur-Peierls formalism[26]:

$$B_c=-\frac{\hbar^2}{2M_c}\frac{L_c}{a_c} \tag{6}$$

with

$$L_c=S_c+iP_c, \tag{7}$$

where S_c and P_c are the usual shift and penetration factors, respectively. Following Bloch,[24] Eqs. (4) and (5) can be combined in the form:

$$(D_c{}^2+E_c)G^{+}_{cc'}(r_c|r_{c'})-\sum_{c''} V^{+}_{cc''}(r_c)G^{+}_{c''c'}(r_c|r_{c'})+\sum_{c''}\mathcal{L}_{cc''}(r_c|r_{c'})=-\delta(r_c-r_{c'})\delta_{cc'} \tag{8}$$

with Bloch's $\mathcal{L}$ operator defined as

$$\mathcal{L}_{cc'}=-\delta(r_c-a_{c'})(\delta_{c'}+B_{c'}), \tag{9}$$

$$\delta_c=\frac{\hbar^2}{2M_c}\frac{d}{dr_c}. \tag{10}$$

Utilization of an obvious matrix notation leads to our writing Eqs. (1) and (8) in the compact form:

$$\underline{H}\,\underline{\phi}=0, \tag{11}$$

$$\underline{H}=\underline{D}^2-\underline{V}+\underline{E} \qquad (E_{cc'}=E_c\,\delta_{cc'}), \tag{12}$$

$$(\underline{H}^{+}+\underline{\mathcal{L}})\underline{G}^{+}=-\underline{M} \tag{13}$$

with

$$\underline{H}^{+}=(\underline{H}^{*})^T; \qquad V^{+}_{cc'}=(V^{*}_{cc'})^T=V_{c'c}. \tag{14}$$

In Eq. (13) $\underline{\mathcal{L}}$ is a matrix of elements defined in Eq. (9), $\underline{M}$ is a diagonal matrix of element $\delta(r_c-r_{c'})$, and $\underline{\phi}$ is a column vector of components $\phi_c(r_c)$.

After these preliminary developments we can now proceed with the derivation of the relation between the channel Green's functions and the collision matrix $U_{cc'}$. To this end we apply Green's theorem between Eqs. (11) and (13). One obtains on account of (12) and (14), the result

$$\begin{aligned}\phi_c(r_{c''})\delta(r_c-r_{c''})=\sum_{c''}&\big[G^{+}_{c''c}(r_{c''}|r_c)D_{c''}{}^2\phi_{c''}(r_{c''})-\phi_{c''}(r_{c''})D_{c''}{}^2G^{+}_{c''c}(r_{c''}|r_c)\\&-\sum_{c'''}\phi_{c''}(r_{c''})\mathcal{L}_{c''c'''}G^{+}_{c'''c}(r_{c'''}|r_c)\big].\end{aligned} \tag{15}$$

Operating on Eq. (15) with $\int_0^{a_{c''}} dr_{c''}$, followed by an integration by parts yields

$$\begin{aligned}\phi(r_c)=\sum_{c''}\{&G^{+}_{c''c}(a_{c''}|r_c)[\delta_{c''}\phi_{c''}(a_{c''})+B_{c''}\phi_{c''}(a_{c''})]\\&-\phi_{c''}(a_{c''})\sum_{c'''\neq c''}\int_0^{a_{c''}} dr_{c''}\,\delta(r_{c''}-a_{c'''})(\delta_{c'''}+B_{c'''})G_{c'''c}(r_{c'''}|r_c)\}.\end{aligned} \tag{16}$$

In view of the boundary conditions (5) the last term in the curly bracket above vanishes, leading to the relation

$$\phi_c(r_c)=\sum_{c''} G^{+}_{c''c}(a_{c''}|r_c)[\delta_{c''}\phi_{c''}(a_{c''})+B_{c''}\phi_{c''}(a_{c''})] \tag{17}$$

which gives the radial channel wave function in terms of the channel Green's functions and the associated boundary conditions. We now split in the usual manner the channel wave functions into incoming and outgoing components, i.e.,

$$\phi_c(r_c) = y_c \left(\frac{M_c}{\hbar k_c}\right)^{1/2} u_c^{(-)}(r_c) - x_c \left(\frac{M_c}{\hbar k_c}\right)^{1/2} u_c^{(+)}(r_c), \tag{18}$$

where the incident- and outgoing-wave coefficients y_c and x_c, respectively, are related via the collision matrix

$$x_c = \sum_{c'} U_{cc'} y_{c'} \tag{19}$$

with

$$u_c^{(-)} = \left(\frac{k_c r_c}{P_c}\right)^{1/2} e^{i\xi_c}; \quad u_c^{(+)} = u_c^{(-)*}, \tag{20}$$

$$k_c = \left(\frac{2M_c}{\hbar^2} E_c\right)^{1/2},$$

$$\xi_c = k_c r_c - \tfrac{1}{2} l_c \pi, \tag{21}$$

$$\frac{d}{dr_c} u_c^{(+)}(r_c) = \frac{L_c}{r_c} u_c^{(+)}(r_c). \tag{22}$$

Upon insertion of Eq. (18) into (17) and use of the relations (20, (22), and (6) one obtains

$$x_c = \sum_{c'} e^{i\xi_c(r_c)}[e^{i\xi_c(r_c)} \delta_{cc'} + i\eta_c(r_c)\eta_{c'}(a_c) \times G^+_{cc'}(a_{c'}|r_{c'}) e^{i\xi_{c'}(a_{c'})}] y_{c'} \tag{23}$$

and by direct comparison of the above result with the relation (19), one comes up with the following expression for the collision matrix

$$U_{cc'}(a_{c'}|r_c) = e^{i[\xi_c(r_c) + \xi_{c'}(r_c)]} \delta_{cc'} + i\eta_c(r_c)\eta_{c'}(a_c) \times G^+(a_{c'}|r_{c'}) e^{i[\xi_{c'}(a_{c'}) + \xi_c(r_c)]}, \tag{24}$$

where

$$\eta_c(r_c) = \left(\frac{\hbar^2 P_c(r_c)}{M_c r_c}\right)^{1/2}. \tag{25}$$

Alternatively, from the relation below, between the transition matrix, $T_{cc'}$, and the collision matrix, $U_{cc'}$,

$$T_{cc'}(a_{c'}|r_c) = e^{-i\xi_c(r_c)} U_{cc'}(a_{c'}|r_c) e^{-\xi_{c'}(a_c)} - \delta_{cc'} \tag{26}$$

one obtains

$$T_{cc'}(a_{c'}|r_c) = i\eta_c(r_c)\eta_{c'}(a_{c'}) G^+_{cc'}(a_{c'}|r_c). \tag{27}$$

Clearly the general T matrix $T_{cc'}(r|r')$ is closely related to the Green's function in that it connects a "disturbance" occurring at r', with the "response" at the radial location, r. For $r = r' = a_c$ it becomes the usual transition matrix. In view of the relation, Eq. (26), and the unitarity of the collision U matrix, the T matrix is constrained to satisfy the general optical theorem $[\underline{T}\,\underline{T}^* + 2\mathrm{Re}(\underline{T}) = 0]$. This constraint insures the independence of the cross section from the channel radii introduced in the formal computational scheme. The usefulness of the Bloch $\mathcal{L}$ operator is now illustrated in two examples. First we expand the Green's function in Eq.(27) in terms of the eigenfunctions $\chi_{\lambda c}(r_c)$ satisfying the wave equation[28]

$$(D_c^2 + \epsilon_\lambda)\chi_{\lambda c}(r_c) - \sum_{c''} V_{cc''}(r_c)\chi_{\lambda c''}(r_c) = 0 \tag{28}$$

and the boundary conditions (5), with the complex eigenvalues

$$\epsilon_\lambda = \mu_\lambda - i\nu_\lambda. \tag{29}$$

Upon introduction of the expression

$$G^+_{cc'}(r_c|r_{c'}) = \sum_\lambda g_\lambda^{cc'} \chi^+_{\lambda c}(r_c)\chi_{\lambda c'}(r_{c'}) \tag{30}$$

into Eq. (27) one obtains the well-known expression for the T matrix in the Kapur-Peierls formalism

$$T_{cc'} = i\sum_\lambda \frac{g_{\lambda c} g_{\lambda c'}}{\epsilon_\lambda - E}, \tag{31}$$

where the complex partial widths $g_{\lambda c}$ are given by

$$g_{\lambda c} = \eta_c \chi_{\lambda c}(r_c) = (2P_c)^{1/2}\tilde{\gamma}_{\lambda c} \tag{32}$$

with the reduced complex widths defined as

$$\tilde{\gamma}_{\lambda c} = \left(\frac{\hbar^2}{2M_c r_c}\right)^{1/2} \chi_{\lambda c}(a_c). \tag{33}$$

In a second example we utilize a set of eigenfunctions which do not satisfy the boundary condition (5). We choose the internal eigenfunctions of R-matrix theory, satisfying the equation

$$(D_c{}^2 + E_\lambda) f^+_{\lambda c}(r_c) - \sum_{c''} V^+_{c''c}(r_c) f^+_{\lambda c''}(r_c) = 0, \tag{34}$$

$$\delta_c f^+_{\lambda c}(r_c)|_{a_c} = \frac{\hbar^2}{2M_c}\frac{b_c}{a_c} f^+_{\lambda c} \qquad (f^+_{\lambda c} = f_{\lambda c}), \tag{35}$$

where both the eigenvalues E_λ and the boundary-condition number, b_c, are real. Then use of the expansion

$$G_{cc'}(r_c|r_{c'}) = \sum_{\lambda,\lambda} g^{cc'}_{\lambda\lambda'} f^+_{\lambda c}(r_c) f_{\lambda' c'}(r_{c'}) \tag{36}$$

leads to

$$(E_\lambda - E_c) g^{cc'}_{\lambda\lambda'} - \sum_{c''}\sum_{\lambda''} [iP_{c''} + (S_{c''} - b_{c''})] \frac{\hbar^2}{2M_{c''}a_{c''}} \times f_{\lambda c''}(a_{c''}) f_{\lambda'' c''}(a_{c''}) g^{c''c'}_{\lambda''\lambda'} = \delta_{\lambda\lambda'}\delta_{cc'} \tag{37}$$

which with the definitions

$$\gamma_{\lambda c} = \left(\frac{\hbar^2}{2M_c a_c}\right)^{1/2} f_{\lambda c}(a_c), \tag{38}$$

$$\Gamma_{\lambda\lambda' c} = 2P_c \gamma_{\lambda c}\gamma_{\lambda' c}, \tag{39}$$

$$\Delta_{\lambda\lambda' c} = -(S_c - b_c)\gamma_{\lambda c}\gamma_{\lambda' c}, \tag{40}$$

$$\Gamma_{\lambda\lambda'} = \sum_c \Gamma_{\lambda\lambda' c}; \quad \Delta_{\lambda\lambda'} = \sum_c \Delta_{\lambda\lambda' c}, \tag{41}$$

and Eqs. (36) and (37) provides us with the following expression for the T matrix

$$T_{cc'} = i\sum_{\lambda,\lambda'} (\Gamma_{\lambda c}\Gamma_{\lambda' c'})^{1/2} A_{\lambda\lambda'}, \tag{42}$$

where $A_{\lambda\lambda'}$ is the Wigner level matrix

$$(A_{\lambda\lambda'})^{-1} = (E_\lambda - E)\delta_{\lambda\lambda'} + (\Delta_{\lambda\lambda'} - \tfrac{1}{2} i \Gamma_{\lambda\lambda'}). \tag{43}$$

III. DERIVATION OF A GENERAL INTEGRODIFFERENTIAL EQUATION FOR THE TRANSITION MATRIX

The goal of this section is to find the variation of the transition matrix upon changes of the parameters entering in the formalism. To this end we follow a technique previously utilized by Mockel and Perez[8] and form the matrix functional $N(\tau)$ in the form:

$$\underline{N}(\tau) = \Big\{ -\int_0^{a_{c''}(\tau_0)} dr_{c''}\, \underline{G}^+(r_{c''}|r_\beta(\tau),\tau)[\underline{H}(\tau_0) + \mathcal{L}(\tau_0)]\, \underline{G}(r_{c''}|r_\alpha(\tau),\tau_0)$$
$$+ \int_0^{a_{c''}(\tau)} dr_{c''}\, \underline{G}(r_{c''}|r_\alpha(\tau_0),\tau_0) \times [\underline{H}^+(\tau) + \mathcal{L}(\tau)]\, \underline{G}^+(r_{c''}|r_\beta(\tau_0),\tau) \Big\} \tag{44}$$

or

$$\underline{N}(\tau) = \underline{G}^+(r_\alpha(\tau)|r_\beta(\tau),\tau) - \underline{G}(r_\beta(\tau_0)|r_\alpha(\tau_0),\tau_0), \tag{45}$$

where τ represents any of the parameters pertinent to the theory, such as energy, angular momentum, coupling constants, and so forth, and we introduced the Green's function $\underline{G}(r_{c''}|r_\alpha,\tau)$, which satisfies the equation

$$(\underline{H} + \underline{\mathcal{L}})\underline{G} = -\underline{M}, \tag{46}$$

where all the operators and symbols have been previously defined. Notice at this point that the radial coordinates r_α and r_β are taken to be functions of the parameter τ. The same applies to the limits of integration in the second integral of the two introduced in the right-hand side of Eq. (44). Next, integration by parts in Eq. (44) yields, in explicit form after use is made of the boundary conditions, the result

$$
\begin{aligned}
&G^+_{cc'}(r_\alpha(\tau)\,|\,r_\beta(\tau),\tau) - G_{cc'}(r_\alpha(\tau_0)\,|\,r_\beta(\tau_0),\tau_0)\\
&= \sum_{c''}\Big\{ G^+_{c''c}(a_{c''}(\tau_0)\,|\,r_\beta(\tau),\tau)B_{c''}(\tau_0)G_{c''c'}(a_{c''}(\tau_0)\,|\,r_\alpha(\tau),\tau_0)\\
&\quad - G_{c''c}(a_{c''}(\tau)\,|\,r_\alpha(\tau_0),\tau_0)B_{c''}(\tau)G^+_{c''c'}(a_{c''}(\tau)\,|\,r_\beta(\tau_0),\tau)\\
&\quad + \frac{\hbar^2}{2M_{c''}}\Big[\int_0^{a_{c''}(\tau_0)} dr_{c''}\Big(\frac{d}{dr_{c''}}G^+_{c''c}(r_{c''}\,|\,r_\beta(\tau),\tau)\Big)\Big(\frac{d}{dr_{c''}}G_{c''c'}(r_{c''}\,|\,r_\alpha(\tau),\tau_0)\Big)\\
&\qquad - \int_0^{a_{c''}(\tau)} dr_{c''}\Big(\frac{d}{dr_{c''}}G_{c''c}(r_{c''}\,|\,r_\alpha(\tau_0),\tau_0)\Big)\Big(\frac{d}{dr_{c''}}G^+_{c''c'}(r_{c''}\,|\,r_\beta(\tau_0),\tau)\Big)\Big]\Big\}\\
&+\sum_{c'',c'''}\Big\{\int_0^{a_{c''}(\tau)} dr_{c''}G_{c''c}(r_{c''}\,|\,r_\alpha(\tau),\tau_0)[E_{c'''}(\tau)\delta_{c''c'''} - V^+_{c''c'''}(r_{c''}\,|\,\tau)]\,G^+_{c'''c'}(r_{c''}\,|\,r_\beta(\tau_0),\tau)\\
&\qquad - \int_0^{a_{c''}(\tau_0)} dr_{c''}G^+_{c''c}(r_{c''}\,|\,r_\beta(\tau),\tau)[E_{c'''}(\tau_0)\delta_{c''c'''} - V^+_{c''c'''}(r_{c''}\,|\,\tau_0)]\,G_{c'''c'}(r_{c''}\,|\,r_\alpha(\tau),\tau_0)\Big\}\,.
\end{aligned}
\tag{47}
$$

The above equation evaluated at $\tau=\tau_0$ yields, in view of the relation (14), the result

$$G^+_{c'c}(r_{c'}\,|\,r_c,\tau_0) = G_{cc'}(r_c\,|\,r_{c'},\tau_0) \tag{48}$$

which is the expression of the reciprocity principle satisfied by the Green's function.

We now proceed on with our task of computing the derivative of the Green's function with respect to the parameter τ. To this end we apply the operator $d/d\tau$ on both sides of Eq. (47) and use the well-know differentiation formula

$$\frac{d}{d\tau}\int_0^{a(\tau)} dx f(x,\tau) = \int_0^{a(\tau_0)} dx\Big(\frac{d}{d\tau}f(x,\tau)\Big)_{\tau_0} + f(x,\tau_0)\Big(\frac{da(\tau)}{d\tau}\Big)_{\tau_0}\,. \tag{49}$$

One obtains after some algebra, involving simple integrations by parts and repeated use of the boundary conditions (5) the result:

$$
\begin{aligned}
\frac{d}{d\tau}G^+_{cc'}(r_\alpha\,|\,r_\beta,\tau) &= \sum_{c''}\Big[G_{c''c}(a_{c''}\,|\,r_\alpha,\tau)\Big(\frac{2M_{c''}}{\hbar^2}B_{c''}{}^2\frac{da_{c''}}{d\tau} - \frac{d}{d\tau}B_{c''}(\tau)\Big)G^+_{c''c'}(a_{c''}\,|\,r_\beta,\tau)\\
&\quad + \Big(\frac{d}{dr'}G^+_{c''c}(r_\alpha\,|\,r',\tau)\Big)_{r'=r_\beta}\frac{dr_\beta}{d\tau} + \Big(\frac{d}{dr'}G_{c''c'}(r_\beta\,|\,r',\tau)\Big)_{r'=r_\alpha}\frac{dr_\alpha}{d\tau}\Big]\\
&\quad + \sum_{c''}\sum_{c'''}\Big[G_{c''c}(a_{c''}\,|\,r_\alpha,\tau)[E_{c'''}(\tau)\delta_{c''c'''} - V^+_{c''c'''}(a_{c''},\tau)]\,G^+_{c'''c'}(a_{c''}\,|\,r_\beta,\tau)\frac{da_{c''}(\tau)}{d\tau}\\
&\qquad + \int_0^{a_{c''}} dr_{c''}G_{c''c}(r_{c''}\,|\,r_\alpha,\tau)\Big(\frac{d}{d\tau}[E_{c'''}(\tau)\delta_{c''c'''} - V^+_{c''c'''}(r_{c''},\tau]\Big)G^+_{c'''c'}(r_{c''}\,|\,r_\beta,\tau)\Big]\,.
\end{aligned}
\tag{50}
$$

To evaluate the last two terms we multiply Eq. (13) by $\int_{r_\alpha}^{a_{c''}} dr_{c''}$ and Eq. (46) by $\int_{r_\beta}^{a_{c''}} dr_{c''}$. Assuming $r_\alpha < r_\beta$ one obtains:

$$
\begin{aligned}
\Big(\frac{d}{dr'}G^+_{c''c}(r'\,|\,r_\beta,\tau)\Big)_{r'=r_\alpha} &= \frac{2M_{c''}}{\hbar^2}\Big\{\delta_{c''c} - B_{c''}(\tau)G^+_{c''c}(a_{c''}\,|\,r_\beta,\tau)\\
&\quad + \sum_{c'''}\int_{r_\alpha}^{a_{c''}} dr_{c''}[E_{c'''}(\tau)\delta_{c''c'''} - V^+_{c''c'''}(r_{c''},\tau)]\,G^+_{c'''c}(r_{c''}\,|\,r_\beta,\tau)\Big\}
\end{aligned}
\tag{51}
$$

and

$$\left[\frac{d}{dr'}G_{c''c'}(r'|r_\alpha,\tau)\right]_{r_\beta}=\frac{2M_{c''}}{\hbar^2}\left[-B_{c''}(\tau)G_{c''c'}(a_{c''}|r_\alpha,\tau)\right.$$

$$\left.+\sum_{c'''}\int_{r_\beta}^{a_{c''}}dr_{c''}[E_{c'''}(\tau)\delta_{c''c'''}-V_{c''c'''}(r_{c''},\tau)]\,G_{c'''c'}(r_{c''}|r_\alpha,\tau)\right]. \tag{52}$$

Introduction of Eqs. (51) and (52) into Eq. (50) yields the final expression for the derivative of the channel Green's function

$$\frac{d}{d\tau}G^+_{cc'}(r_\alpha|r_\beta,\tau)=\sum_{c''}\frac{2M_{c''}}{\hbar^2}\begin{Bmatrix}\frac{dr_\alpha}{d\tau}\,\delta_{c''c}; & r_\alpha>r_\beta\\ \frac{dr_\beta}{d\tau}\,\delta_{c''c'}; & r_\beta>r_\alpha\end{Bmatrix}$$

$$-\sum_{c''}\frac{2M_{c''}}{\hbar^2}B_{c''}(\tau)\left(G^+_{c''c}(a_{c''}|r_\beta,\tau)\,\frac{dr_\beta}{d\tau}+G^+_{c'c''}(r_\alpha|a_{c''},\tau)\,\frac{dr_\alpha}{d\tau}\right)$$

$$+\sum_{c'',c'''}G^+_{cc''}(r_\alpha|a_{c''},\tau)\left\{\left[\left(\frac{2M_{c''}}{\hbar^2}B_{c'''}{}^2+E_{c'''}\right)\delta_{c''c'''}-V^+_{c''c'''}(a_{c''},\tau)\right]\frac{da_{c''}}{d\tau}\right.$$

$$\left.-\frac{dB_{c'''}}{d\tau}\,\delta_{c''c'''}\right\}G^+_{c'''c'}(a_{c''}|r_\beta,\tau)$$

$$+\sum_{c''}\sum_{c'''}\frac{2M_{c''}}{\hbar^2}\left[\frac{dr_\beta}{d\tau}\left(\int_{r_\beta}^{a_{c''}}dr_{c''}[E_{c''}(\tau)\delta_{c''c'''}-V^+_{c''c'''}(r_{c''},\tau)]\,G^+_{c'''c}(r_{c''}|r_\beta,\tau)\right)\right.$$

$$\left.+\frac{dr_\alpha}{d\tau}\left(\int_{r_\beta}^{a_{c''}}dr_{c''}[E_{c'''}(\tau)\delta_{c''c'''}-V^+_{c''c'''}(r_{c''},\tau)]\,G^+_{c'''c'}(r_{c''}|r_\alpha,\tau)\right)\right]$$

$$+\sum_{c''}\sum_{c'''}\int_0^{a_{c''}}dr_{c''}\,G^+_{cc''}(r_\alpha|r_{c''},\tau)\left(\frac{d}{d\tau}[E_{c'''}(\tau)\delta_{c''c'''}-V^+_{c''c'''}(r_{c''},\tau)]\right)G^+_{c''c'}(r_{c''}|r_\beta,\tau), \tag{53}$$

where use was made of the reciprocity relation (48) and the expression (6) for the boundary-condition function B_c.

The result (53) shows that the variation of the Green's function is made up of the following contributions: (a) variations due to changes in the radial coordinates r_α and r_β, measured by their derivatives $dr_\alpha/d\tau$ and $dr_\beta/d\tau$; (b) spherically symmetric changes of the channel radii, a_c; (c) the variations produced by changes in the boundary conditions; and (d) variations which arise from changes in the channel potentials $V^+_{cc'}$, as well as those variations which may arise from the potentials chosen within a particular channel due to variations of Q_c and hence E_c.

The relation between parameter changes and the ensuing variation of the transition matrix is immediately obtained from Eqs. (53) and (27). The result is:

$$\frac{d}{d\tau}T_{cc'}(r_\alpha|r_\beta,\tau)=\sum_{c''}\left[i\,\eta_c(r_\alpha)\eta_{c'}(r_\beta)\,\frac{2M_{c''}}{\hbar^2}\,\frac{dr_>}{d\tau}\begin{Bmatrix}\delta_{c''c}\\ \delta_{c''c'}\end{Bmatrix}+\left(\frac{d}{d\tau}\ln[\eta_{c''}(r_\alpha)\eta_{c'}(r_\beta)]\right)T_{c''c'}(r_\alpha|r_\beta,\tau)\delta_{c''c}\right.$$

$$\left.-\frac{2M_{c''}}{\hbar^2}B_{c''}\left(\frac{\eta_{c'}(r_\beta)}{\eta_{c''}(a_{c''})}\,T_{c''c}(a_{c''}|r_\beta,\tau)\,\frac{d}{d\tau}r_\beta+\frac{\eta_c(r_\alpha)}{\eta_{c''}(a_{c''})}\,T_{c'c''}(r_\alpha|a_{c''},\tau)\,\frac{dr_\alpha}{d\tau}\right)\right]$$

$$-i\sum_{c''}\sum_{c'''}\left([\eta_{c''}(a_{c''})\eta_{c'''}(a_{c''})]^{-1}T_{cc''}(r_\alpha|a_{c''},\tau)\right.$$

$$\times\left\{\left[\left(\frac{2M_{c''}}{\hbar^2}B_{c'''}{}^2(\tau)+E_{c'''}(\tau)\right)\delta_{c''c'''}-V^+_{c''c'''}(a_{c''},\tau)\right]\frac{da_{c''}}{d\tau}\right.$$

$$\left.\left.-\frac{d}{d\tau}B_{c''}(\tau)\delta_{c''c'''}\right\}T_{c'''c'}(a_{c''}|r_\beta,\tau)\right)$$

$$+\sum_{c''}\sum_{c'''}\left[\frac{2M_{c''}}{\hbar^2}\left(\eta_{c'}(r_\beta)\frac{dr_\beta}{d\tau}\int_{r_\alpha}^{a_{c''}}dr_{c''}\,\eta_{c'''}{}^{-1}(r_{c''})[E_{c'''}(\tau)\delta_{c''c'''}-V^{+}_{c''c'''}(r_{c''},\tau)]\,T_{c'''c}(r_{c''}|r_\beta,\tau)\right.\right.$$
$$+\eta_c(r_\alpha)\frac{dr_\alpha}{d\tau}\int_{r_\beta}^{a_{c''}}dr_{c''}\,\eta_{c'''}{}^{-1}(r_{c''})[E_{c'''}(\tau)\delta_{c''c'''}$$
$$\left.\left.-V^{+}_{c''c'''}(r_{c''},\tau)]\,T_{c''c'''}(r_\alpha|r_{c''},\tau)\right)\right]$$
$$-i\sum_{c''}\sum_{c'''}\int_0^{a_{c''}}dr_{c''}[\eta_{c''}(r_{c''})\eta_{c'''}(r_{c''})]^{-1}T_{cc''}(r_\alpha|r_{c''},\tau)$$
$$\times\left(\frac{d}{d\tau}[E_{c'''}(\tau)\delta_{c''c'''}-V^{+}_{c''c'''}(r_{c''},\tau)]\right)T_{c'''c'}(r_{c''}|r_\beta,\tau)\,, \tag{54}$$

where $r_>$ is the largest of the two radial coordinates r_α, r_β.

For what follows it turns out to be convenient to work with two versions of Eq. (54). First, we assume the parameter, τ, to be the channel radius, a_{co}; we also make $r_\alpha=a_c$, $r_\beta=a_{c'}$, and assume that all the channel radii are of the same length. This leads to the equation:

$$\frac{d}{da_{co}}T_{cc'}(a_{co})=\sum_{c''}\left[i\,\eta_c(a_{co})\eta_{c'}(a_{co})\frac{2M_{c''}}{\hbar^2}\delta_{c''co}\delta_{c'co}\begin{Bmatrix}\delta_{c''c}\\ \delta_{c''c'}\end{Bmatrix}+\left(\frac{d}{da_{co}}\ln[\eta_c(a_{co})]\right)T_{c''c'}(a_{co})\delta_{cco}\delta_{c'co}\delta_{c''c}\right.$$
$$\left.-\frac{2M_{c''}}{\hbar^2}B_{c''}\left(\frac{\eta_{c'}(a_{co})}{\eta_{c''}(a_{c''})}\delta_{c'co}T_{c''c}(a_{co})+\frac{\eta_c(a_{co})}{\eta_{c''}(a_{co})}\delta_{cco}T_{c'c''}(a_{co})\right)\right]$$
$$-i\sum_{c''}\sum_{c'''}\left\{[(\eta_{c''}(a_{co})\eta_{c'''}(a_{co})]^{-1}T_{cc''}(a_{co})\left[\left(\frac{2M_{c''}}{\hbar^2}B_{c'''}{}^2+E_{c'''}\delta_{c''c'''}-V^{+}_{c''c'''}(a_{co})\right)\delta_{c''co}\right.\right.$$
$$\left.\left.-\frac{d}{da_{co}}B_{c''}\delta_{c''c'''}\right]T_{c'''c'}(a_{co})\right\}, \tag{55}$$

where $T_{cc'}(a_{co})=T_{cc'}(a_{co}|a_{co})$. The second form of Eq. (54) is obtained by keeping constant the set of channel radii (i.e., $\tau\neq a_c$)

$$\frac{d}{d\tau}T_{cc'}(r_\alpha|r_\beta,\tau)=\sum_{c''}\sum_{c'''}\left[\left(\frac{d}{d\tau}\ln[\eta_{c''}(r_\alpha)\eta_{c'''}(r_\beta)]\right)T_{c''c'''}(r_\alpha|r_\beta,\tau)\delta_{c''c}\delta_{c'''c'}\right.$$
$$+i[\eta_{c''}(a_{c''})\eta_{c'''}(a_{c''})]^{-1}T_{cc''}(r_\alpha|a_{c''},\tau)\frac{d}{d\tau}B_{c'''}\delta_{c''c'''}T_{c'''c'}(a_{c''}|r_\beta,\tau)$$
$$-\int_0^{a_{c''}}dr_{c''}[\eta_{c''}(r_{c''})\eta_{c'''}(r_{c''})]^{-1}T_{cc''}(r_\alpha|r_{c''},\tau)$$
$$\left.\times\left(\frac{d}{d\tau}[E_{c'''}(\tau)\delta_{c''c'''}-V^{+}_{c''c'''}(r_{c''},\tau)]\right)T_{c'''c'}(r_{c''}|r_\beta,\tau)\right]. \tag{56}$$

The relation (55) and (56) cover most of the cases needed in the applications to nuclear reaction theory.

IV. EQUATIONS OF MOTION OF THE RESIDUES AND POLES OF THE TRANSITION MATRIX

The residues and complex poles of the transition matrix are, in principle, observable quantities, whence the convenience of deriving equations for the variation of these entities as a function of the parameters entering the theory. This problem was first studied for the R-matrix parameter by Wigner,[5] Teichmann,[6] and generalized by Altman[7] and Mockel and Perez.[8] We follow here the technique used in the latter reference. The starting point is Eq. (56) and the following expansion of the T matrix, based on Eq. (31):

$$T_{cc'}(r_\alpha|r_\beta,\tau)=i\sum_\lambda\frac{g_{\lambda c}(r_\alpha,\tau)g_{\lambda c'}(r_\beta,\tau)}{\epsilon_\lambda(\tau)-E}, \tag{57}$$

where the residues $g_{\lambda c}(r_\alpha,\tau)$ are related to the radial eigenfunctions, $\chi_{\lambda c}(r_\alpha)$, satisfying Eq. (28), by [see also Eq. (32)]

$$g_{\lambda c}(r_\alpha,\tau)=\eta_c(r_\alpha,\tau)\chi_{\lambda c}(r_\alpha,\tau) \tag{58}$$

and the complex poles are defined in Eq. (29). Introduction of the expansion (57) into Eq. (56) yields

$$\sum_{\lambda}\frac{d}{d\tau}\left(\frac{g_{\lambda c}(r_\alpha,\tau)g_{\lambda c'}(r_\beta,\tau)}{\epsilon_\lambda(\tau)-E}\right)=\sum_{\lambda}\left(\frac{d}{d\tau}[\ln\eta_c(r_\alpha)\eta_{c'}(r_\beta)]\,\frac{g_{\lambda c}(r_\alpha,\tau)g_{\lambda c'}(r_\beta,\tau)}{[\epsilon_\lambda(\tau)-E]}\right)$$

$$+\sum_{\lambda}\sum_{\lambda'}\left(\frac{g_{\lambda c}(r_\alpha,\tau)\Omega_{\lambda\lambda'}(\tau)g_{\lambda' c'}(r_\beta,\tau)}{[\epsilon_\lambda(\tau)-E]}\right), \tag{59}$$

where

$$\Omega_{\lambda\lambda'}(\tau)=\sum_{c''c'''}\left\{\int_0^{a_{c''}}dr_{c''}\left[\frac{g_{\lambda c''}(r_{c''},\tau)}{\eta_{c''}(r_{c''})}\left(\frac{d}{d\tau}[E_{c'''}(\tau)\delta_{c''c'''}-V^{+}_{c''c'''}(r_{c''},\tau)]\right)\frac{g_{\lambda' c'''}(r_{c''},\tau)}{\eta_{c'''}(r_{c''})}\right]\right.$$

$$\left.-\eta_{c''}^{-1}(a_{c''})g_{\lambda c''}(a_{c''},\tau)\frac{d}{d\tau}B_{c'''}(\tau)\delta_{c''c'''}\eta_{c'''}^{-1}(a_{c''})g_{\lambda c'''}(a_{c''},\tau)\right\}. \tag{60}$$

Next we introduce the identity

$$\sum_{\lambda}\sum_{\lambda'}\frac{g_{\lambda c}(r_\alpha,\tau)\Omega_{\lambda\lambda'}(\tau)g_{\lambda' c'}(r_\beta,\tau)}{\epsilon_\lambda(\tau)-E}\equiv\sum_{\lambda}\frac{g_{\lambda c}(r_\alpha,\tau)\Omega_{\lambda\lambda}(\tau)g_{\lambda c'}(r_\beta,\tau)}{[\epsilon_\lambda(\tau)-E]^2}$$

$$+\sum_{\lambda}\sum_{\lambda'\neq\lambda}\{[\epsilon_{\lambda'}(\tau)-\epsilon_\lambda(\tau)][\epsilon_\lambda(\tau)-E]\}^{-1}$$

$$\times[g_{\lambda c}(r_\alpha,\tau)\Omega_{\lambda\lambda'}(\tau)g_{\lambda' c'}(r_\beta,\tau)+g_{\lambda' c}(r_\alpha,\tau)\Omega_{\lambda'\lambda}g_{\lambda c'}(r_\beta,\tau)] \tag{61}$$

into Eq. (59), take the indicated derivative in the left-hand side of (59) and finally proceed to equate terms of equal powers in $(\epsilon_\lambda - E)^{-1}$. The result after putting $c=c'$, $r_\alpha = r_\beta$, is:

$$\frac{d}{d\tau}g_{\lambda c}(r_\alpha,\tau)=\left(\frac{d}{d\tau}\ln[\eta_c(r_\alpha)]\right)g_{\lambda c}(r_\alpha,\tau)+\frac{1}{2}\sum_{\lambda'\neq\lambda}[\epsilon_{\lambda'}(\tau)-\epsilon_\lambda(\tau)]^{-1}[\Omega_{\lambda\lambda'}(\tau)+\Omega_{\lambda'\lambda}(\tau)]g_{\lambda' c}, \tag{62}$$

$$\frac{d}{d\tau}[\epsilon_\lambda(\tau)-E(\tau)]=-\Omega_{\lambda\lambda}(\tau). \tag{63}$$

The set of Eqs. (62) and (63) associated with the appropriate initial conditions at $\tau=\tau_0$ defines an initial value problem. One can consider these equations as the ones describing the motion of the generalized dynamical variables $\epsilon_{\lambda c}$ and ϵ_λ, subject to the "forces" $\Omega_{\lambda\lambda''}$. In principle they allow a start from a solvable R-matrix problem and henceforth generate the transition matrix for a given set of channel-coupling potentials. An illustrative example of the use of the equations of motion will be given in the next section.

V. APPLICATION OF THE EQUATIONS OF MOTION TO THE GENERATION OF THE KAPUR-PEIERLS PARAMETERS FROM A GIVEN SET OF R-MATRIX PARAMETERS

The Kapur-Peierls[26] dispersion theory leads to a very convenient parametrization of the cross section. This is especially true for the fissile nuclei, where level interference and channel effects are of importance (Adler and Adler[29]). The only drawback of these types of cross-section parametrization is that very little is known about the statistical properties of the Kapur-Peierls-type parameters. However, from the existing relationships between these parameters and the R-matrix parameters, whose statistical properties are known, one can infer the statistical distribution of the former set by various techniques (Adler and Adler,[30] Moldauer,[31] Garrison,[32] Hwang,[33] Harris,[34] and deSaussure and Perez[35]).

We should like to show how a simple application of the equation of motion of the residues and poles of the collision matrix affords a method to perform the conversion of the R-matrix parameters into the Kapur-Peierls-type parameters. The residues and poles in the R-matrix formalism arise from an eigenvalue problem associated with real, momentum-independent values of the logarithmic derivatives at the nuclear surface. In the case of the collision matrix formalism the boundary-condition functions B_c, Eq. (6), are complex and momentum-dependent. Whence the transition between both formalisms is performed by letting $\tau=B_c$ vary between $\tau_0=-(\hbar^2/2M_c a_c)b_c\equiv B_{c,0}$, and $\tau=B_c$. With the latter identification the matrix elements $\Omega_{\lambda\lambda'}$ become, from Eq. (60)

$$\Omega_{\lambda\lambda'}(B_c)=\sum_{c''c'''}\eta_{c''}^{-1}(a_{c''})g_{\lambda c''}(a_{c''},B_c)\frac{dB_{c'''}}{dB_c}\delta_{c''c'''}\eta_{c'''}(a_{c''})g_{\lambda' c'''}(a_{c''},B_c). \tag{64}$$

The various B_c functions are interrelated via the channel momenta, k_c, with the energy of the incoming particle. Hence

$$\frac{dB_{c'''}}{dB_c}=\frac{dB_{c'''}}{dE}\frac{dE}{dB_{c''}}\ . \tag{65}$$

From the definition (6) of the boundary-condition function, B_c, as well as from $k_c=[(2M/h^2)(E-Q_c)]^{1/2}$, Eq. (65) becomes

$$\frac{dB_{c'''}}{dB_c}=\frac{k_c}{k_{c'''}}F(\rho_c|\rho_{c'''}) \tag{66}$$

with

$$F(\rho_c,\rho_{c'''})=(dL_{c'''}/d\rho_{c'''})/(dL_c/d\rho_c)\ , \tag{67}$$

$$\rho_c=k_c a_c\ . \tag{68}$$

Introduction of Eqs. (64) and (65) into the equations of motion (62) and (63) yields, after making $r_\alpha=a_c=a_{c''}$,

$$\frac{d}{dB_c}g_{\lambda c}(B_c)=-\sum_{c''}\sum_{\lambda'\neq\lambda}\left([\epsilon_{\lambda'}(B_c)-\epsilon_\lambda(B_c)]^{-1}\eta_{c''}^{-2}(a_c)\frac{k_c}{k_{c''}}F(\rho_c|\rho_{c''})g_{\lambda'c}(B_c)g_{\lambda c''}(B_c)g_{\lambda'c''}(B_c)\right)\ , \tag{69}$$

$$\frac{d}{dB_c}\epsilon_\lambda(B_c)=\sum_{c''}\eta_{c''}^{-2}(a_c)\frac{k_c}{k_{c''}}F(\rho_c|\rho_{c''})g_{\lambda c''}^{2}(B_c)\ . \tag{70}$$

For $B_c=B_{c0}$, the complex partial widths $g_{\lambda c}$ and poles ϵ_λ become the corresponding quantities in the R-matrix theory framework. Hence the initial conditions associated with the equations of motion (69) and (70) are

$$g_{\lambda c}(B_{c,0})=\Gamma_c^{1/2}(k_c)\ , \tag{71}$$

$$\epsilon_\lambda(B_{c,0})=E_\lambda\ . \tag{72}$$

The above initial value problem can be solved numerically by means of various techniques. The solution of this Cauchy problem will in fact "march" the solution from its R-matrix initial configuration to the residues and poles of the collision matrix.

Analytical approximations can be obtained by the use of perturbation techniques. To illustrate this point, consider the generation of the Kapur-Peierls[26] parameters from a given set of R-matrix parameters for s-wave neutrons. In this instance

$$L_c(\rho_c)=iP_c=ik_c a_c\ , \tag{73}$$

$$B_{c,0}=0\ , \tag{74}$$

whence from Eq. (67)

$$F(\rho_c|\rho_{c''})=k_{c''}/k_c\ . \tag{75}$$

Also from Eqs. (25) and (73)

$$\eta_{c''}^{-2}(a_c)=\frac{M_{c''}}{\hbar^2 k_{c''}}\ . \tag{76}$$

In view of Eqs. (75) and (76) the equations of motion (69) and (70) become for s-wave neutrons:

$$\frac{d}{dB_c}g_{\lambda c}(B_c)=-\sum_{c''}\sum_{\lambda'\neq\lambda}[\epsilon_{\lambda'}(B_c)-\epsilon_\lambda(B_c)]^{-1}\frac{\hbar^2 k_{c''}}{M_{c''}}g_{\lambda'c}(B_c)g_{\lambda c''}(B_c)g_{\lambda'c''}(B_c)\ , \tag{77}$$

$$\frac{d}{dB_c}\epsilon_\lambda(B_c)=\sum_{c''}\left(\frac{\hbar^2 k_{c''}}{M_{c''}}\right)^{-1}g_{\lambda c''}^{2}(B_c)\ . \tag{78}$$

Our perturbation method consists of expanding the complex partial widths and complex poles in powers of

B_c, i.e.,

$$g_{\lambda c} = g_{\lambda c}(0) + B_c\left(\frac{dg_{\lambda c}}{dB_c}\right)_0 + \frac{1}{2!}B_c^{\,2}\frac{d^2 g_{\lambda c}}{dB_c}, \tag{79}$$

$$\epsilon_\lambda = \epsilon_\lambda(0) + B_c\left(\frac{d\epsilon_\lambda}{dB_c}\right)_0 + \frac{1}{2!}B_c^{\,2}\frac{d^2\epsilon_\lambda}{dB_c^{\,2}} + \frac{1}{3!}B_c^{\,3}\frac{d^3\epsilon_\lambda}{dB_c^{\,2}}, \tag{80}$$

where the pertinent derivatives can be computed from the equations of motion. The results, after putting $M_c = M_{c''}$; $k_c = k_{c''} = k$, are:

$$\left(\frac{d\epsilon_\lambda}{dB_c}\right)_0 = \frac{M_c}{\hbar^2 k}\Gamma_{\lambda\lambda}, \tag{81}$$

$$\left(\frac{dg_{\lambda c}}{dB_c}\right)_0 = -\frac{M_c}{\hbar^2 k}\sum_{\lambda'\neq\lambda}\frac{\Gamma_{\lambda' c}^{\,1/2}\Gamma_{\lambda\lambda'}}{E_{\lambda'} - E_\lambda}, \tag{82}$$

$$\left(\frac{d^2\epsilon_\lambda}{dB_c^{\,2}}\right)_0 = -2\left(\frac{M_c}{\hbar^2 k}\right)^2\sum_{\lambda'\neq\lambda}\frac{\Gamma_{\lambda\lambda'}^{\,2}}{(E_{\lambda'} - E_\lambda)}, \tag{83}$$

$$\left(\frac{d^2 g_{\lambda c}}{dB_c^{\,2}}\right)_0 = \left(\frac{M_c}{\hbar^2 k}\right)^2\sum_{\lambda'\neq\lambda}(E_{\lambda'} - E_\lambda)^{-1}\left[\frac{(\Gamma_{\lambda'\lambda''} - \Gamma_{\lambda\lambda})}{(E_{\lambda''} - E_\lambda)}\Gamma_{\lambda\lambda'}\Gamma_{\lambda' c}^{\,1/2} + \sum_{\lambda''\neq\lambda}\frac{\Gamma_{\lambda''\lambda'}\Gamma_{\lambda''\lambda}}{(E_{\lambda''} - E_\lambda)}\Gamma_{\lambda' c}^{\,1/2} + \sum_{\lambda''\neq\lambda'}\frac{\Gamma_{\lambda\lambda''}\Gamma_{\lambda'\lambda''}}{(E_{\lambda''} - E_{\lambda'})}\Gamma_{\lambda' c}^{\,1/2} + \sum_{\lambda''\neq\lambda'}\frac{\Gamma_{\lambda'\lambda''}\Gamma_{\lambda\lambda'}}{(E_{\lambda''} - E_{\lambda'})}\Gamma_{\lambda'' c}^{\,1/2}\right], \tag{84}$$

and

$$\left(\frac{d^3\epsilon_\lambda}{dB_c^{\,3}}\right)_0 = 3!\left(\frac{M_c}{\hbar^2 k}\right)^3\left[\sum_{\lambda'\neq\lambda}\frac{(\Gamma_{\lambda'\lambda'} - \Gamma_{\lambda\lambda})\Gamma_{\lambda\lambda'}^{\,2}}{(E_{\lambda'} - E_\lambda)^2} + \sum_{\lambda'\neq\lambda}\sum_{\substack{\lambda''\neq\lambda \\ \lambda\neq\lambda'}}\frac{\Gamma_{\lambda\lambda'}\Gamma_{\lambda'\lambda''}\Gamma_{\lambda''\lambda}}{(E_{\lambda'} - E_\lambda)(E_{\lambda''} - E_{\lambda'})}\right]. \tag{85}$$

Introduction of Eqs. (81) up to (85) in the expansions (79) and (80), followed by separation of real and imaginary parts, yields, taking into account the Eq. (6) for B_c, specialized to s-wave neutrons:

$$\mathrm{Re}(g_{\lambda c}) = \Gamma_{\lambda c}^{\,1/2} - \frac{1}{8}\sum_{\lambda'\neq\lambda}(E_{\lambda'} - E_\lambda)^{-1}\left[\frac{(\Gamma_{\lambda'\lambda'} - \Gamma_{\lambda\lambda})}{(E_{\lambda'} - E_\lambda)}\Gamma_{\lambda\lambda'}\Gamma_{\lambda' c}^{\,1/2} + \sum_{\lambda''\neq\lambda}\frac{\Gamma_{\lambda\lambda''}\Gamma_{\lambda''\lambda'}}{(E_{\lambda''} - E_\lambda)}\Gamma_{\lambda' c}^{\,1/2} + \sum_{\lambda''\neq\lambda'}\frac{\Gamma_{\lambda'\lambda''}}{(E_{\lambda''} - E_{\lambda'})}(\Gamma_{\lambda\lambda''}\Gamma_{\lambda' c}^{\,1/2} + \Gamma_{\lambda\lambda'}\Gamma_{\lambda'' c}^{\,1/2})\right], \tag{86}$$

$$\mathrm{Im}(g_{\lambda c}) = \frac{1}{2}\sum_{\lambda'\neq\lambda}\frac{\Gamma_{\lambda\lambda'}}{E_{\lambda'} - E_\lambda}\Gamma_{\lambda' c}^{\,1/2}, \tag{87}$$

$$\mu_\lambda = E_\lambda + \frac{1}{4}\sum_{\lambda'\neq\lambda}\frac{\Gamma_{\lambda\lambda'}^{\,2}}{E_{\lambda'} - E_\lambda}, \tag{88}$$

$$\nu_\lambda = \frac{1}{2}\Gamma_{\lambda\lambda} + \frac{1}{8}\sum_{\lambda'\neq\lambda}\frac{(\Gamma_{\lambda\lambda} - \Gamma_{\lambda'\lambda'})\Gamma_{\lambda\lambda'}^{\,2}}{(E_{\lambda'} - E_\lambda)^2} - \frac{1}{8}\sum_{\lambda'\neq\lambda}\sum_{\substack{\lambda''\neq\lambda \\ \lambda\neq\lambda'}}\frac{\Gamma_{\lambda\lambda'}\Gamma_{\lambda'\lambda''}\Gamma_{\lambda''\lambda}}{(E_{\lambda'} - E_\lambda)(E_{\lambda''} - E_{\lambda'})}. \tag{89}$$

The results contained in Eqs. (86) up to (89) were first obtained by Adler and Adler.[30] Notice that the expansions (79) and (80) in powers of B_c correspond in fact to the expansion of the U-matrix residues and poles in terms of the ratio $\Gamma_{\lambda\lambda'}/(E_{\lambda'} - E_\lambda)$, $(\lambda'\neq\lambda)$ which measures the degree of level interference.

The present formalism has the advantage that one can handle with the same ease the higher angular momenta. This is of interest for the extrapolation to the unresolved resonance region in fissile nuclei.

VI. SCATTERING OF SPINLESS PARTICLES BY A CENTRAL POTENTIAL

Nonrelativistic potential theory has been a valuable source of information in the study of the analytical properties of the scattering amplitude.[36] The variation of the scattering phase shifts, δ_l, as a function of energy, angular momentum, and range of the central potential has been studied by several techniques and authors (Robinson and Hirschfelder,[37] Calogero,[38] Devooght,[39] and Newton,[9] among others). Here we show how all these treatments and results are particular cases of the general equations (55) and (56), particularized to the single-channel case.

We first consider Eq. (55), which for the one-channel case ($a_c = a$), becomes

$$\frac{d}{da} T_l(a) = 2i \frac{P_l(ka)}{a} + [2(L_l/a) + \frac{\hbar^2}{M}\frac{d}{da}(P_l/a)]\, T_l(a) - i \frac{Ma}{\hbar^2 P_l(a)} \times [E - V_l(a) + \frac{\hbar^2}{2M}(L_l/a)^2 - \frac{\hbar^2}{2M}\frac{d}{da}(L_l/a)]\, T_l^2(a), \tag{90}$$

where we used the expressions (6) and (25) and defined the T function $T_l(a) = T_{c=c'=l}(a|a)$.

From Eq. (58), where the parameter τ is now any parameter of the theory with the condition that the channel radius is constant, one obtains

$$\frac{d}{d\tau} T_c(a,\tau) = \left(\frac{d}{d\tau}\ln[P_c(ka)]\right) T_c(a,\tau) - i\,\frac{a}{2P_c(ka)}\frac{d}{d\tau}\frac{L_c(ka)}{a}\, T_c^2(a,\tau) - i\,\frac{M_c}{\hbar^2}\int_0^a dr \left[\frac{T(a|r,\tau)}{P_c(kr)/r}\left(\frac{d}{d\tau}[E - V_c(r,\tau)]\right)\frac{T(r|a,\tau)}{P_c(kr)/r}\right]. \tag{91}$$

The above results are conveniently expressed in terms of the observable phase shifts. Upon use of the Green's function

$$G_c(a|r) = \frac{2M}{\hbar^2}\, e^{i[\delta_c(ka)+\xi_c(ka)]}\,\psi_c(r), \tag{92}$$

where $\psi_c(r)$ is the solution of the radial Schrödinger equation pertinent to this problem, and has the asymptotic behavior

$$\psi_c(r) \underset{r\to\infty}{=} k^{-1}\sin[\delta_c + \xi_c(r)] \tag{93}$$

and from the definition (27) of the transition matrix and the relations (92) and (93), one obtains

$$T_l(a) = e^{2i[\delta_c(ka)+\xi(ka)]} - 1, \tag{94}$$

where $T_l(a)$ is the transition matrix for $r = r' = a$. Also

$$T_c(a|r) = 2i\,\frac{P_c(kr)P_c(ka)}{ar}\, e^{i[\delta_c(ka)+\xi_c(ka)]}\psi_c(r). \tag{95}$$

Introduction of the result (94) into Eq. (90) yields

$$\frac{d}{da}\delta_l(ka) = -\left(\frac{P_l(ka)}{a} - k\right) - \frac{1}{2i}\left[\frac{\hbar^2}{Ma}\left(\frac{d}{da}P_l(ka) - \frac{1}{a}P_l(ka)\right) - \frac{2}{a}L_l(ka)\right](1 + e^{-2i[\delta_c(ka)+\xi_c(ka)]}) + \frac{a}{P_l(ka)}\left[k^2 - \frac{2M}{\hbar^2}V_l(a) + \left(\frac{L_l(ka)}{a}\right)^2\right] + \frac{1}{a}\left[\frac{1}{a}L_l(ka) - \frac{d}{da}L_l(ka)\right]\sin^2[\delta_l(ka) + \xi_l(ka)]. \tag{96}$$

This result is equivalent to the expression obtained by Calogero[38] for the derivative $d[\delta_l(ka)]/da$. Calogero's result[38] is given in terms of the phases of the Ricatti-Bessel functions, instead of the appearance of the more physically meaningful shift and penetration functions in our result.

Introduction of Eq. (95) into Eq. (91) yields

$$\frac{d}{d\tau}[\delta_c(ka,\tau) + \xi_c(ka,\tau)] = \frac{1}{2}\left(\frac{d}{d\tau}\ln P_c(ka,\tau)\right)\sin\{2[\delta_c(ka,\tau) + \xi_c(ka,\tau)]\} - \left(\frac{1}{P_c(ka,\tau)}\right)\left(\frac{d}{d\tau}S_c(ka,\tau)\right)\sin^2[\delta_c(ka,\tau) + \xi_c(ka,\tau)] + 2\,\frac{M}{\hbar^2}\,\frac{P_c(ka,\tau)}{a}\int_0^a dr\,\psi_c(r)\left(\frac{d}{d\tau}[E(\tau) - V_c(r,\tau)]\right)\psi_c(r). \tag{97}$$

There are three cases of interest which can be obtained from the general result (97): For $\tau = l$,

$$\frac{d}{dl}(\delta_l) = \frac{1}{2}\pi + \frac{1}{2}\left(\frac{d}{dl}\ln(P_l)\right)\sin^2(\delta_l+\xi_l) - \left(\frac{1}{P_l}\frac{d}{dl}S_l\right)\sin^2(\delta_l+\xi_l) - \frac{P_l}{a}\int_0^a dr\,\psi_l(r)\frac{2l+1}{r^2}\psi_l(r); \tag{98}$$

for $\tau = k$,

$$\frac{d}{dk}\delta_l = -a + \frac{1}{2}\frac{d}{dk}\ln(P_l)\sin[2(\delta_l+\xi)] - \left(\frac{1}{P_l}\frac{d}{dk}S_l\right)\sin^2(\delta_l+\xi_l) + 2\frac{P_l}{a}k\int_0^a dr\,\psi_l^2(r). \tag{99}$$

For $\tau=\epsilon$, where ϵ is the strength coupling constant of the potential; i.e., $V(r,\tau)=\epsilon V_0(r)$, one obtains

$$\frac{d}{d\epsilon}\delta_l = -\frac{2M}{\hbar^2}\frac{P_l}{a}\int_0^a dr\,\psi_l(r)V_0(r)\psi_l(r). \tag{100}$$

For s-wave neutrons, $P_0 = ka$, $S_0 = 0$, and one obtains from Eqs. (96) and (99), respectively,

$$\frac{d}{da}\delta_0 = -\frac{2M}{\hbar^2 k}V_0(a)\sin^2(\delta_0+\xi_0), \tag{101}$$

$$2i\frac{d}{dk}\delta_0 = i\,k^{-1}\sin[2(\delta_0+\xi_0)] + 4i\,k^2\int_0^a dr\,\psi_0^2(r) - 2ia. \tag{102}$$

The results (101) and (102) for s-wave neutrons have been given by Devooght[39] and Newton,[9] respectively.

VII. SCATTERING LENGTH FOR s-WAVE NEUTRONS

To illustrate the use of the equations derived previously, let us consider the derivation of an expression for the scattering length for s-wave neutrons. The scattering length[40] $\alpha(a)$ is defined as the limit

$$\alpha(a) = -\lim_{k\to 0}\frac{\tan\delta_0}{k}. \tag{103}$$

From Eq. (101) for the phase shifts, δ_0, one obtains, for a definite negative potential,

$$\frac{d}{da}\delta_0 = \frac{1}{k}W(a)(\sin\delta_0\cos\xi_0 + \cos\delta_0\sin\xi_0)^2 \tag{104}$$

with

$$\xi_0 = ka, \tag{105}$$

$$W(a) = \frac{2M}{\hbar^2}|V_0(a)|. \tag{106}$$

Now we expand the phase shift, δ_0, in powers of the momentum, k, i.e.,

$$\tan\delta_0 = \alpha k + \tfrac{1}{3}\beta k^3. \tag{107}$$

Introduce Eq. (107) into Eq. (104) and equate equal powers in the momentum variable. This procedure yields

$$-\frac{d\alpha}{da} = W(a)[a^2 - 2a\alpha(a) + \alpha^2(a)] \tag{108}$$

which is a Ricatti differential equation for the scattering length with the initial condition $\alpha(0)=0$. Equation (108) can then be solved with the only restriction that the potential $V_0(a)$ must decrease not faster than a^{-2}. Besides the numerical integration by the Runge-Kutta technique, for example, one can obtain several analytical approximations through the use of various techniques. We shall use here a linearization procedure subject to a large degree of generalization. To this end we start splitting the solution into the zeroth-order solution $\alpha^{(0)}(a)$ and a small deviation $Y(a)$, i.e.,

$$\alpha(a) = \alpha^{(0)}(a) + Y(a), \tag{109}$$

where from Eq. (108)

$$\alpha^{(0)}(a) = -\int_0^a da'\,W(a')a'^2. \tag{110}$$

Introduction of Eq. (109) into the Ricatti equation (108) yields

$$-\frac{d}{da}Y(a) = H_0(a) + H_1(a)Y(a) \tag{111}$$

with

$$H_0(a) = W(a)[\alpha^{(0)2}(a) - 2a\alpha^{(0)}(a)], \tag{112}$$

$$H_1(a) = 2W(a)[-a + \alpha^{(0)}(a)]. \tag{113}$$

Integration of the differential Eq. (111) and use of the relation (109) yields the following approximation

$$-\alpha^{(1)}(a) = -\alpha^{(0)}(a) + \exp\left[-\int_0^a H_1(a')da'\right] \times \left\{ \int_0^a da' H_0(a') \exp\left[+\int_0^{a'} da'' H_1(a'')\right] \right\} . \tag{114}$$

This operation can be repeated by replacing $\alpha^{(0)}(a)$ by $\alpha^{(1)}(a)$ in Eq. (109) and repeating the previous procedure. In order to illustrate the degree of accuracy involved in the first iteration $\alpha^{(1)}(a)$, consider the case of a square well potential, $V_0(a) = V_0$. In this instance the exact solution is, Messiah[41, 42]

$$-\alpha(a) = \left(\frac{\tan b}{b} - 1\right) a \tag{115}$$

with

$$b = W^{1/2} a = \left(\frac{2M}{\hbar^2} V_0 a^2\right)^{1/2} . \tag{116}$$

With the change of variables (116) various integrals in Eq. (114) can be performed after expansion of the exponential functions in the integrand, one obtains:

$$-\alpha^{(1)}(a) = \tfrac{1}{3} b^2 a + a b^4 \left(\tfrac{2}{15} - \tfrac{5}{63} b^2 + \tfrac{1}{81} b^4\right) e^{b^2[1+(1/6)b^2]} . \tag{117}$$

Expansion of the exponential terms in Eq. (117)

$$e^{b^2[1+(1/6)b^2]} \approx 1 + b^2 + \tfrac{4}{6} b^4 \tag{118}$$

and keeping only terms up to b^8 yields

$$-\alpha^{(1)}(a) = \tfrac{1}{3} b^2 a + \tfrac{2}{15} b^4 a + \tfrac{17}{315} b^6 a + \tfrac{62}{2835} b^8 a . \tag{119}$$

The first term in Eq. (119) is the first Born approximation, while the whole expression coincides with the first four terms of the exact solution (115) upon expansion of $\tan b$ in powers of the parameter b.

VIII. DISCUSSION AND CONCLUSIONS

The main result of this work is embodied in Eq. (54), which gives an integrodifferential equation for the T matrix in terms of the physical parameters of the system. Together with the initial conditions, the problem of computing the transition matrix, and hence cross sections, has been converted into a generalized Cauchy problem. This technique affords, in principle, a new alternate method of solution of the coupled-channel equations.

The direct solution of Eq. (54) offers the advantage of conserving unitarity within the limits of the numerical approximations utilized.

Starting from Eq. (54) one has derived a set of equations, the so-called equations of motion (62) and (63) from which one can compute energy levels and widths, starting from the corresponding quantities in the R-matrix uncoupled case. An application has been shown to the generation of the complex residues and poles of the collision matrix in Sec. VI. The procedure shown there can be easily extended to higher angular momenta, which is of interest in order to study the extrapolation from the resolved into the unresolved resonance region.

To further illustrate the power of the method, we have derived general differential-integral equations for the phase shifts which describe the scattering of spinless particles by a central potential. In this manner various results previously derived by other methods for s-wave scattering have been generalized and unified. As a result of this treatment, an equation for the scattering length, $\alpha(a)$, as a function of the range of the potential, a_0, has been obtained. By linearization of this equation, one arrives at a first-order approximation to the scattering length, which is equivalent to the first four terms of the expansion of the true solution in terms of the parameter, b, given by Eq. (115).

In conclusion, the T-matrix treatment of the coupled-channel equations affords several advantages:

(a) It offers a large degree of flexibility in the choice of boundary conditions.

(b) The formalism gives explicitly the dependence of the T matrix on the pertinent physical parameter.

(c) Unitarity is conserved.

ACKNOWLEDGMENT

The author is indebted to Dr. A. J. Mockel and Dr. G. de Saussure for their advice and many illuminating discussions.

---

[1]A. Lejeune and C. Mahaux, Nucl. Phys. A145, 613 (1970).

[2]W. Tobocman and M. A. Nagarajan, Phys. Rev. 138, B1351 (1965).

[3]L. Garside and W. Tobocman, Phys. Rev. 173, 1047 (1968).

[4]K. Takeuchi and P. A. Moldauer, Phys. Rev. C 2, 925 (1970); Phys. Rev. C 2, 920 (1970).

[5]E. P. Wigner, in E. Vogt, Rev. Mod. Phys. 34, 723 (1962). A generalization to the multichannel case is also presented in Professor Wigner's contribution to the Breit Celebration Volume.

[6]T. Teichmann and E. P. Wigner, Phys. Rev. 77, 506 (1950); Phys. Rev. 87, 123 (1952).

[7]A. Altman, Phys. Rev. 138, B78 (1965).

[8]A. J. Mockel and R. B. Perez, Phys. Rev. C 2, (1970).

[9]R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw Hill, New York, 1966).

[10]G. Breit, Phys. Rev. 69, 472 (1946).

[11]T. Tamura, Rev. Mod. Phys. 37, 679 (1965).

[12]B. Buck, Phys. Rev. 130, 712 (1963).

[13]H. Feshbach, Ann. Phys. (N.Y.) 5, 357 (1958); Ann. Phys. (N.Y.) 19, 287 (1962).

[14]E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947).

[15]M. E. Haglund and D. Robson, Phys. Rev. Letters 14, 225 (1965).

[16]P. J. A. Buttle, Phys. Rev. 160, 719 (1967).

[17]C. Mahaux and H. W. Weidenmuller, *Shell-Model Approach to Nuclear Reactions* (North-Holland, Amsterdam, 1969).

[18]C. Bloch and V. Gillet, Phys. Letters 16, 62 (1965).

[19]W. M. MacDonald, Nucl. Phys. 54, 343 (1964); Nucl. Phys. 56, 636 (1964); Nucl. Phys. 56, 647 (1964).

[20]A. M. Lane and D. Robson, Phys. Rev. 151, 774 (1966).

[21]D. Robson and A. M. Lane, Phys. Rev. 161, 982 (1967).

[22]A. M. Lane and D. Robson, Phys. Rev. 185, 1403 (1969).

[23]A. M. Lane and D. Robson, Phys. Rev. 178, 1715 (1969).

[24]C. Bloch, Nucl. Phys. 4, 503 (1957).

[25]J. E. Purcell, Phys. Rev. 185, 1279 (1969).

[26]P. L. Kapur and R. E. Peierls, Proc. Roy. Soc. (London), 166, 277 (1928).

[27]A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30, 257 (1958).

[28]The general properties of the functions $\chi_{\lambda c}$ and their adjoints are studied with great detail by Bloch (Ref. 24).

[29]D. B. Adler and F. T. Adler, ANL Report No. ANL-6792, 1963 (unpublished), p. 695.

[30]D. B. Adler and F. T. Adler, ANL Report No. COO-1546-4, 1967 (unpublished).

[31]P. A. Moldauer, Phys. Rev. 135, B642 (1966); also, P. H. Moldauer, R. N. Thomas, and B. S. Garbow in ANL Report No. ANL-7590, 1969 (unpublished).

[32]J. D. Garrison, Ann. Phys. (N.Y.) 30, 269 (1964).

[33]R. N. Hwang, Nucl. Sci. Eng. 36, 67 (1969).

[34]D. R. Harris, LASL Report No. LA-4327, 1969 (unpublished).

[35]G. de Saussure and R. B. Perez, ORNL Report No. ORNL-TM-2599, 1969 (unpublished).

[36]R. Blankenbecker, M. L. Goldberger, N. N. Khuri, and S. B. Treiman, Ann. Phys. (N.Y.) 10, 62 (1960).

[37]P. Robinson and J. Hirschfelder, Phys. Rev. 129, 1391 (1963).

[38]F. Calogero, *Variable Phase Approach to Potential Scattering* (Academic, New York, 1967).

[39]J. Devooght, J. Math. Phys. 7, 1764 (1966).

[40]For simplicity we have chosen the range of the potential $V_0(a)$ to be the channel radius.

[41]A. Messiah, *Mechanique Quantique* (Dunod, Paris, 1960), Vol. II.

[42]Of course, for this constant potential case the exact solution (115) is also obtained from the Ricatti equation (109). To this end make the substitution $X = a - \alpha(a)$ to obtain

$$\int_0^X \frac{dX}{1+WX^2} = a$$

or $\tan(W^{1/2}a) = \tan b = W^{1/2}[a - \alpha(a)]$, from which the result (115) follows.