Treatment of large perturbations of the Hamiltonian and the boundary conditions in scattering and reaction calculations*

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On the basis of an integrodifferential equation which was derived in a previous work for the T matrix of nuclear reaction theory, we have developed a general formalism to treat large perturbations in both the Hamiltonian and the boundary conditions of a quantum mechanical system. As a result of this formalism, a set of first order differential equations, in terms of any of the physical parameters of the system, is given for the widths and poles of the collision U matrix. The technique is illustrated by the conversion of a set of R-matrix resonance parameters into its equivalent set of U-matrix widths and poles, which corresponds to the passage from the R-matrix boundary conditions to the complex, momentum-dependent boundary conditions associated with the Kapur-Peierls reaction formalism. The case of large perturbations of the Hamiltonian is illustrated by the calculation of the elastic and inelastic scattering cross sections in a strongly coupled two-channel system which was proposed by Tobocman and has been widely used as testing grounds for reaction theories.

I. INTRODUCTION

The physical problem most usually encountered in quantum mechanics is that one related to perturbations of the interaction term in the Hamiltonian. However, in dealing with finite systems, such as those found in nuclear reaction theory, one can also face a situation in which the boundary conditions satisfied by the interior eigenfunctions on the nuclear surface may be markedly altered. An example of this is afforded by the R-matrix theory of nuclear reactions of Wigner and Eisenbud,[1] and its relationship with the Kapur-Peierls theory.[2] The former utilizes real, energy-independent boundary conditions. The corresponding level widths and poles are then real and momentum-independent. In contrast the Kapur-Peierls formalism introduces complex energy-dependent boundary conditions to construct directly the collision U matrix. The two techniques are of course equivalent and can be related on the basis of a change in the boundary conditions.

Situations in which both the boundary conditions and the Hamiltonian of the system are perturbed arise in the calculation of resonant cross sections based on various nuclear reaction theories, as discussed by Tobocman and Nagarajan,[3] Garside and Tobocman,[4] Purcell,[5] and Lejeune and Mahaux[6] among others. These formalisms have in common the feature that the basic set of eigenfunctions does not usually satisfy boundary conditions consistent with the U-matrix formalism. The perturbation of the Hamiltonian of the system is introduced when the channel residual potentials and channel coupling potential are "turned on." The various techniques available to solve these problems have been unified and thoroughly discussed by Lane and Robson.[7-9]

In a previous work, Perez[10] has developed an integrodifferential equation satisfied by the transition T matrix in terms of any of the physical parameters of the system. This equation together with the initial conditions on the T matrix establishes an initial value problem, defining this transition matrix at any "later" value of the physical parameter chosen to describe the system. The advantage of this formalism is that the perturbations of the boundary conditions can be incorporated in the Hamiltonian by means of Bloch's L operator.[11] The purpose of the present work is to develop a novel technique for the calculation of the collision U matrix for highly perturbed systems.

As an illustration of the present technique we show two applications. One is concerned with a problem involving the change of boundary conditions between the R-matrix and collision-matrix formalisms. The second application is related to perturbations of the Hamiltonian , such as the ones taking place in coupled channels potential scattering problems.

First we discuss the classical eigenfunction expansion method, utilizing as the basic set the R-matrix states corresponding to the unperturbed Hamiltonian. This method leads to a set of first order differential equations for the widths and poles of the collision matrix, which is then used to perform the transformation of a set of R-matrix resonance parameters into equivalent U-matrix parameters.

An objectionable feature of the usual eigenfunction expansion method is the fact that level truncation effects destroy the unitarity of the collision matrix. The main practical effect is a poor description of the background introduced by the "far-away" levels. Although there are several prescriptions to estimate these effects, via the introduction of a background R matrix,[12] it appears useful to explore the direct integration of the initial value problem. This is done in Sec. V where some applications to a two-channel problem are presented.

II. GENERAL THEORY

In Ref. 10 we introduced the radial channel $G^+_{ij}(r|r',\tau)$, where τ represents any of the physical parameters of the nuclear system except the channel radii a_i. There it was shown that this function satisfied the following integrodifferential equation:

$$\frac{d}{d\tau}G^+_{ij}(r|r') = \sum_{kl}\left\{-G^+_{ik}(r|a_i)\left(\frac{d}{d\tau}B_l\right)\delta_{kl}G^+_{lj}(a_j|r') + \int_0^{a_i} dr''G^+_{ik}(r|r'')\left[\left(\frac{d}{d\tau}E_l\right)\delta_{lk} - \frac{d}{d\tau}V_{kl}\right]G^+_{lj}(r''|r')\right\}, \tag{1}$$

where B_i, the logarithmic boundary condition functions are given by

$$B_i = -\frac{C_i^2 L_i}{a_i} \tag{2}$$

with

$$C_i = \left(\frac{\hbar^2}{2M_i}\right)^{1/2}, \tag{3}$$

$$L_i = S_i + iP_i, \tag{4}$$

S_i = level shift factor, P_i = penetration factor, M_i = channel reduced mass,

$$E_l = E - Q_l, \tag{5}$$

Q_l = energy threshold, and V_{ij} = channel potentials.

The Green's function was also seen to be related to the transition matrix T_{ij} by

$$T_{ij}(r|r') = i\eta_i(r)\eta_j(r')G^+_{ij}(r|r') \tag{6}$$

while the following relation holds between the T matrix and the collision matrix U_{ij}:

$$T_{ij}(r|r') = e^{-i\phi_i(r)}U_{ij}(r|r')e^{-i\phi(r')} - \delta_{ij}, \tag{7}$$

where $\phi_i(r)$ is the hard sphere scattering factor and

$$\eta_i(r) = C_i[2P_i(r)/r]^{1/2}. \tag{8}$$

Introduction of the relation (6) into Eq. (1) yields the following integrodifferential equation for the transition matrix

$$\frac{d}{d\tau}T_{ij}(r|r') = \sum_{kl}\left\{\left[\frac{d}{d\tau}\ln(\eta_k(r)\eta_l(r'))\right]T_{kl}(r|r')\delta_{ki}\delta_{lj} + i[\eta_k(a_k)\eta_l(a_l)]^{-1}T_{ik}(r|a_k)\left(\frac{d}{d\tau}B_l\right)\delta_{kl}T_{lj}(a_l|r')\right.$$
$$\left. - i\int_0^i dr''[\eta_k(r'')\eta_l(r'')]^{-1}T_{ik}(r|r'')\left[\left(\frac{dE}{d\tau}l\right)\delta_{kl} - \frac{d}{d\tau}V_{kl}(r'')\right]T_{lj}(r''|r')\right\}. \tag{9}$$

We shall use either the result Eq. (1) or Eq. (9) as is convenient.

We also recapitulate various relations from Ref. 10 and R-matrix theory.[13] To this end, call $\phi_{\lambda i}(r)$ the orthogonal set of radial channel eigenfunctions of an R-matrix problem, satisfying real, energy independent logarithmic boundary conditions:

$$\left(\frac{d}{dr}\phi_{\lambda i}(r)\right)_{a_i} = \left(\frac{b_i}{a_i}\right)\phi_{\lambda i}(a_i), \tag{10}$$

where b_i is the boundary condition number of R-matrix theory.[13] Then one defines the widths and

level shifts

$$\gamma_{\lambda i} = (C_i/a_i^{1/2})\phi_{\lambda i}(a_i) , \tag{11}$$

$$\Gamma_{\lambda\nu i} = 2P_i\gamma_{\lambda i}\gamma_{\nu i} = (\Gamma_{\lambda i}\,\Gamma_{\nu i})^{1/2} , \tag{12}$$

$$\Delta_{\lambda\nu i} = -(S_i - b_i)\gamma_{\lambda i}\gamma_{\nu i} , \tag{13}$$

$$\Gamma_{\lambda\nu} = \sum_i \Gamma_{\lambda\nu i} , \tag{14}$$

$$\Delta_{\lambda\nu} = \sum_i \Delta_{\lambda\nu i} . \tag{15}$$

Furthermore, we shall write the transition matrix in the form

$$T_{ij}(r \mid r') = i \sum_\lambda (\epsilon_\lambda - E)^{-1} g_{\lambda i}(r) g_{\lambda j}(r') , \tag{16}$$

where $g_{\lambda i}(r)$ are complex width functions, and ϵ_λ the complex collision matrix poles are written in the form

$$\epsilon_\lambda = \mu_\lambda - i\nu_\lambda . \tag{17}$$

III. EXPANSION IN TERMS OF R-MATRIX RADIAL EIGENFUNCTIONS

In this section the Green's function of the system will be expanded in terms of R-matrix theory states. The starting point is the R-matrix self-adjoint eigenfunction set, $\phi_{\lambda c}(r)$, solution of an uncoupled channel Schrödinger equation, which satisfies the boundary conditions, Eq. (10). The Green's function in Eq. (1) can then be expanded in the form

$$G^+_{ij}(r \mid r', \tau) = \sum_{\lambda\nu} f_{\lambda\nu}(\tau)\phi_{\lambda i}(r)\phi_{\nu j}(r') , \tag{18}$$

where the parameter, τ, is left arbitrary and the amplitudes $f_{\lambda\nu}(\tau)$ satisfy the initial condition, at $\tau = \tau_0$

$$f_{\lambda\nu}(\tau 0) = \delta_{\lambda\nu}/(E_\lambda - E) , \tag{19}$$

where E_λ is an R-matrix pole. We now insert the expansion (18) into Eq. (1) for the Green's function to obtain

$$\frac{d}{d\tau}\underline{F} = \underline{F}\,\underline{\Omega}\,\underline{F} \tag{20}$$

which is the degenerated case of the Ricatti-matrix equation for the matrix $(\underline{F})_{\lambda\nu} = f_{\lambda\nu}$. The matrix $\underline{\Omega}$ is given by

$$\Omega_{\lambda\nu} = \sum_{ij}\left[-\phi_{\lambda i}(a_i)\left(\frac{d}{d\tau}B_i\right)\delta_{ij}\phi_{\nu j}(a_j) + \left(\frac{d}{d\tau}E_j\right)\delta_{ij}\delta_{\lambda\nu} - \frac{d}{d\tau}V_{ij\lambda\nu}\right] , \tag{21}$$

where we introduced the matrix elements $V_{ij\lambda\nu}$ of the radial channel potentials, i.e.,

$$V_{ij\lambda\nu} = \langle \phi_{\lambda i} \mid V_{ij} \mid \phi_{\nu j} \rangle . \tag{22}$$

The result, Eq. (20), together with the knowledge of the initial matrix $F(\tau_0)$, defines an initial value problem for the calculation of the Green's function appropriate to the coupled channel case with the rigorous boundary coniditions, because the Ω matrix contains the coupling potentials and the boundary condition changes. Utilization of the relation, Eq. (6), between the Green's function and the transition T matrix allows the calculation of cross sections. The formal solution of Eq. (20) is easily obtained:

$$\underline{F}(\tau) = \left[\underline{I} - \underline{F}(\tau_0)\int_{\tau_0}^{\tau} d\tau'\,\underline{\Omega}(\tau')\right]^{-1}\underline{F}(\tau_0) , \tag{23}$$

$$(I)_{\lambda\nu} = \delta_{\lambda\nu} . \tag{24}$$

Whenever the parameter, τ, enters in the Hamiltonian only as a multiplicative constant, the matrix elements, $\Omega_{\lambda\nu}$, become τ-independent. One can then set τ equal to its "final" value and obtain the perturbed Green's function by matrix inversion. In other instances, for example, in dealing with deformed nuclei, τ can be considered one of the deformation parameters in which case the matrix $\underline{\Omega}$ is now dependent on the τ parameter. Instead of using the closed result, Eq. (23), which involves an integration over τ, and matrix inversion for each value of the parameter, it is more expedient to solve the Ricatti-matrix Eq. (20) by other techniques such as the Runge-Kutta[14] method or the Lie-series approach.[15]

IV. EQUATIONS FOR THE CALCULATION OF THE WIDTHS AND POLES OF THE COLLISION MATRIX

The results obtained in the previous section will now be utilized to derive a set of equations for the complex widths and poles of the collision matrix. Our starting point is Eq. (20), into which we introduce the expansion

$$f_{\lambda\nu} = \sum_\alpha \frac{\beta_{\lambda\alpha}\beta_{\nu\alpha}}{\epsilon_\alpha - E} \tag{25}$$

in terms of the complex poles ϵ_α, and the complex modal amplitudes $\beta_{\lambda\alpha}$. One obtains

$$\sum_\alpha \frac{d}{d\tau}\left(\frac{\beta_{\lambda\alpha}\beta_{\nu\alpha}}{\epsilon_\alpha - E}\right) = \sum_\alpha\left(\frac{H^{\lambda\nu}_{\alpha\alpha}}{(\epsilon_\alpha - E)^2} + \sum_{\beta\neq\alpha}\frac{H^{\lambda\nu}_{\alpha\beta} + H^{\nu\lambda}_{\beta\alpha}}{(\epsilon_\beta - \epsilon_\alpha)(\epsilon_\alpha - E)}\right) \tag{26}$$

with

$$H^{\lambda\nu}_{\alpha\beta} = \sum_{\gamma\delta}\beta_{\lambda\alpha}\beta_{\gamma\lambda}\Omega_{\gamma\delta}\beta_{\delta\beta}\beta_{\nu\beta} , \tag{27}$$

$$H^{\lambda\nu}_{\alpha\beta} = H^{\nu\lambda}_{\beta\alpha} . \tag{28}$$

Next we perform the derivative indicated in (26) and equate equal powers in $(\epsilon_\alpha - E)^{-1}$. The result is

$$\frac{d}{d\tau}\beta_{\lambda\alpha} = \sum_{\beta\neq\alpha}(\epsilon_\beta - \epsilon_\alpha)^{-1}P_{\alpha\beta}\beta_{\lambda\beta}\,, \tag{29}$$

$$\frac{d}{d\tau}(\epsilon_\alpha - E) = -P_{\alpha\alpha}\,, \tag{30}$$

where we introduced the matrix functional

$$P_{\alpha\beta} = \sum_{\gamma\delta}\beta_{\gamma\alpha}\Omega_{\gamma\delta}\beta_{\delta\beta}\,. \tag{31}$$

The set of Eqs. (29) and (30) together with the initial conditions

$$\epsilon_\alpha(\tau_0) = E\,, \tag{32}$$

$$\beta_{\lambda\alpha}(\tau_0) = \delta_{\lambda\alpha} \tag{33}$$

defines an initial value problem for the computation of the model amplitudes $\beta_{\lambda\alpha}$ and the U-matrix poles, ϵ_α. The complex widths, $g_{\alpha i}(a_i)$, are given in terms of the modal amplitudes by

$$g_{\alpha i} = \sum_\gamma \beta_{\gamma\alpha}[\eta_i(a_i)\phi_{\gamma i}(a_i)] \tag{34}$$

which is obtained by combination of Eqs. (6), (16), (18), and (25).

Frequently the matrix elements $\Omega_{\gamma\delta}$ are independent of the parameter, τ, with the important exception when τ describes a degree of freedom associated with nuclear deformation. In this case a useful alternate set of equations to the system formed by Eqs. (29) and (30) can be easily found. To this end take derivatives in both sides of Eq. (31) to obtain

$$\frac{d}{d\tau}P_{\alpha\beta} = \sum_{\gamma\delta}\left(\frac{d}{d\tau}\beta_{\gamma\alpha}\Omega_{\gamma\delta}\beta_{\delta\beta} + \beta_{\gamma\alpha}\Omega_{\gamma\delta}\frac{d}{d\tau}\beta_{\delta\beta}\right); \tag{35}$$

next introduce Eq. (29) and the definition (31) of the matrix elements $P_{\alpha\beta}$ to find

$$\frac{d}{d\tau}P_{\alpha\beta} = \sum_{\gamma\neq\alpha}\frac{P_{\alpha\gamma}P_{\gamma\beta}}{\epsilon_\gamma - \epsilon_\alpha} + \sum_{\gamma\neq\beta}\frac{P_{\alpha\gamma}P_{\gamma\beta}}{\epsilon_\gamma - \epsilon_\beta} \tag{36}$$

which is a set of differential equations for the matrix functional P. In many instances, as we shall illustrate with an example, it is more convenient to use Eqs. (36) and (30) followed by substitution in Eq. (29) rather than Eq. (29) in conjunction with Eq. (30).

V. GENERATION OF THE COLLISION MATRIX WIDTHS AND POLES FROM A GIVEN SET OF R-MATRIX PARAMETERS FOR FISSILE NUCLEI

The correct parametrization of the neutron cross sections in fissile nuclei demands the use of analytical representations of cross sections which account for both level interference and multichannel effects. Such an appropriate formulation is afforded by various versions of the collision matrix theory like the Kapur-Peierls dispersion theory[2] and the Adler-Adler formalism,[16] among others. In the latter formalism, the expressions for the resonance lines are given in a form which preserves the main features of the single-level Breit-Wigner line shape formula and at the same time includes level interference effects via the introduction of asymmetric terms. As an illustration, the reaction cross section for s-wave neutrons is given in the form

$$\sqrt{E}\,\sigma_{nx} = \sum_\lambda \frac{\nu_\lambda G_\lambda^{(x)} + (\mu_\lambda - E)H_\lambda^{(x)}}{(\mu_\lambda - E)^2 + \nu_\lambda^2}\,, \tag{37}$$

where $G_\lambda^{(x)}$ and $H_\lambda^{(x)}$ define the symmetric and asymmetric parts of the resonance line. Similar relations are shown to apply for the resonance contributions to the scattering and total neutron cross sections where the symmetric coefficients A_λ, $G_\lambda^{(T)}$, $G_\lambda^{(n)}$ and asymmetric coefficients B_λ and $H_\lambda^{(T)}$, $H_\lambda^{(n)}$ are introduced. These coefficients are related to the widths of the poles of the collision matrix by the relations[16]

$$A_\lambda + iB_\lambda = 2cg_J E^{-1/2} g_{\lambda n}{}^2\,, \tag{38}$$

$$H_\lambda^{(T)} - iG_\lambda^{(T)} = 2cg_J E^{-1/2} g_{\lambda n}{}^2 e^{(2i\phi_n)}\,, \tag{39}$$

$$H_\lambda^{(n)} - iG_\lambda^{(n)} = (2cg_J E^{-1}) \times \sum_\nu (\epsilon_\nu^* - \epsilon_\lambda)^{-1}(g_{\lambda n} g_{\nu n}^*)^2\,, \tag{40}$$

$$H_\lambda^{(x)} - iG_\lambda^{(x)} = (2cg_J E^{-1/2}) \times \sum_\nu (\epsilon_\nu^* - \epsilon_\lambda)^{-1}(g_{\lambda x} g_{\lambda n} g_{\nu x}^* g_{\nu n}^*)\,, \tag{41}$$

where $g_{\lambda n}$ are the level widths for the neutron channel, $g_{\lambda x}$ the widths for one of the various reaction channels, and g_J is the statistical spin factor, with $c = 6.15\times 10^5$ (b eV). The asymmetric coefficients satisfy the sum rule

$$\sum_\lambda H_\lambda^{(x,n,T)} = 0 \tag{42}$$

and in view of unitarity one has the relations

$$A_\lambda = G_\lambda^{(n)} + \sum_x G_\lambda^{(x)}\,, \tag{43}$$

$$B_\lambda = H_\lambda^{(n)} + \sum_x H_\lambda^{(x)}\,. \tag{44}$$

The usual way to obtain the complex widths and poles of the U matrix is by the inversion of Wigner's level matrix.[13] Alternatively, Reich and Moore[17] have developed a formalism for

fissile nuclei which eliminates the capture channels through the use of the random-phase approximation and replaces the inversion of Wigner's level matrix by the inversion of a much smaller matrix in channel space, comprising only the neutron channel and a few fission channels. Hence, the collision matrix is computed by inversion of a small matrix at each energy point. The method is very efficient and has been widely used for cross section fitting in the case of various fissile nuclei.[18,19] However, it does not lend itself to an explicit cross section parametrization as in the case of the previously discussed Kapur-Peierls U-matrix formalism. The analytical representation given by the latter allows the calculation of Doppler-broadening, resonance self-shielding factors, and other functionals of the cross sections relevant to nuclear reactor calculations in a very straightforward manner. In particular, average reaction cross sections are easily obtained, as they are proportional to $\sum_\lambda G_\lambda^{(\gamma)}$. Unfortunately very little is known about the statistical properties of the U-matrix widths and poles, a fact preventing the statistical extrapolation of the cross section to the unresolved energy region. The opposite situation appears in the case of the R-matrix formalism, where the statistical features of the R-matrix parameters can be obtained from general considerations of the properties of the nuclear Hamiltonian.[20,21] The usual approach to this problem is to utilize the existing relationships between the U-matrix parameters and the R-matrix parameters in order to infer the statistical properties of the former set of parameters. In view of the previous discussion, there is interest in performing the conversion of a set of R-matrix resonance parameters into a set of equivalent U-matrix parameters. This conversion has been achieved in several ways. Adler and Adler,[22] as well as Moldauer,[23] utilize techniques based on the diagonalization of the level matrix. Harris[24] obtains the U-matrix parameters by perturbation methods (valid for small level width to level spacing ratios); de Saussure and Perez[25] based their work on the direct partial fraction expansion of the Reich-Moore[17] formalism. In most instances the methods have been restricted to s-wave neutrons.

The purpose of this section is to show a general method to perform the conversion between the two formalisms, which applies to any value of the angular momentum. The necessary tools have been developed in Sec. III. Involved in the conversion is a change from the momentum-independent, real boundary conditions of R-matrix theory to the complex, energy-dependent boundary condition functions B_c [Eq. (2)]. The matrix elements $\Omega_{\lambda\nu}$, Eq. (21), are given now by

$$\Omega_{\lambda\nu} = -\sum_i \phi_{\lambda i}(a_i)(B_i - B_{0i})\phi_{\nu i}(a_i) , \tag{45}$$

where we used the expression

$$B_i(\tau) = \tau(B_i - B_{0i}) + B_{0i} \tag{46}$$

to evaluate the change in the boundary conditions for $0 \leq \tau \leq 1$ and defined the initial boundary condition numbers B_{0i} as

$$B_{0i} = -(C_1^2/a_i)b_i . \tag{47}$$

From Eqs. (31), (45), and (34) one obtains the matrix elements $P_{\alpha\beta}$, in terms of the complex widths

$$P_{\alpha\beta} = \sum_i \eta_i^{-2}(B_i - B_{0i})g_{\alpha i}g_{\beta i} . \tag{48}$$

An equation for these complex widths is arrived at by multiplication of Eq. (29) by $\eta_i\phi_{\alpha i}(a_i)$ and summation over the level subindex, α. Use of the relation (34) between widths and modal amplitudes yields the desired result

$$\frac{d}{d\tau} g_{\alpha i} = \sum_{\alpha \neq \beta} (\epsilon_\beta - \epsilon_\alpha)^{-1} P_{\alpha\beta} g_{\beta i} . \tag{49}$$

In connection with the fissile nuclei, one encounters the problem of the many participating capture channels, which will make the set of equations, (49), too large to be tractable. This is a situation in which the introduction of the matrix-functional $\underline{P}$, proves to be extremely useful. One divides the channel space into two subsets: the first with only the neutron and fission channels and the second set containing the capture channels, i_γ. Equations (36) and (30) in which the channel-dependent magnitudes do not enter explicitly are first solved. This leads to the determination of the matrix, $P_{\alpha\beta}$, and the eigenvalues, ϵ_α, from which the widths for the neutron and fission channels can be obtained by means of Eq. (49). The initial conditions associated with Eqs. (36), (30), and (49) are:

$$\epsilon_\alpha(\tau = 0) = E_\alpha , \tag{50}$$

$$g_{\alpha i}(\tau = 0) = \eta_i(a_i)\phi_{\alpha i}(a_i) = \Gamma_{\alpha i}{}^{1/2} , \tag{51}$$

where the E_α are the R-matrix poles and $\Gamma_{\alpha c}$ the R-matrix partial level widths [see Eqs. (8), (11), and (12)]. In order to find the initial value of the matrix functional $\underline{P}$, we utilize the results (2), (8), (12) up to (15), together with (48) and (51) to obtain

$$P_{\alpha\beta}(\tau = 0) = \Delta_{0\alpha\beta} + \tfrac{1}{2} i \Gamma_{0\alpha\beta} + \tfrac{1}{2} i \sum_{i(\gamma)} (\Gamma_{\alpha i}\Gamma_{\beta i})^{1/2} , \tag{52}$$

where $\Delta_{0\alpha\beta}$ and $\Gamma_{0\alpha\beta}$ are the level shift factors and level widths contributed by the fission and neutron channels only, while the sum in Eq. (52) goes over the capture channels. To treat this last term, we make use of the random phase approximation

$$\sum_{i(\gamma)} (\Gamma_{\alpha i}\Gamma_{\beta i})^{1/2} = \Gamma_{\alpha c}\delta_{\alpha\beta}, \tag{53}$$

arriving then to the final expression

$$P_{\alpha\beta}(\tau = 0) = -\Delta_{0\alpha\beta} + (\tfrac{1}{2}i)(\Gamma_{0\alpha\beta} + \Gamma_{\alpha c}\delta_{\alpha\beta}), \tag{54}$$

where $\Gamma_{\alpha c}$ is the capture level width.

After the computation of the complex poles ϵ_α and the complex widths $g_{\alpha i}$ for neutron and fission channels, one obtains the cross-section parameters A_α, B_α, $G_\alpha^{(f)}$, and $H_\alpha^{(f)}$ for the neutron and fission channels via the relations (38) up to (41). The parameters $G_\alpha^{(c)}$ and $H_\alpha^{(c)}$ for the capture cross sections are obtained from the unitarity relations (43) and (44).

The initial value problem, formed by the first order differential Eqs. (36) and (30), with the initial conditions, Eqs. (50), (51), and (54), was solved utilizing a second order Runge-Kutta[14] technique. The size of the marching step, $\Delta\tau$ $(0 \leq \tau \leq 1)$ is chosen on the basis of the following condition

$$\Delta\tau \leq \left\{ W \Big/ \left[\text{Max2} \left| \frac{P_{\alpha\beta}}{(\epsilon_\beta - \epsilon_\alpha)} \right| \right] \right\}, \quad \alpha \neq \beta, \tag{55}$$

where $W(\sim 0.01)$ is an appropriate fixed weight, and the denominator in Eq. (55) is the maximum absolute value of the ratio $2P_{\alpha\beta}/(\epsilon_\beta - \epsilon_\alpha)$, which is the degree of level interference. The step length $\Delta\tau$ is adjusted after each step in the "marching" towards the final U-matrix parameter set. To illustrate the method, we have chosen a simple s-wave neutron two-level problem. The initial R-matrix parameters are given in Table I. The initial degree of interference is [from Eq. (54) and the parameters in Table I]:

$$2\left|\frac{P_{12}}{E_1 - E_2}\right| = \frac{\Gamma_{012}}{D} = \frac{1}{D}\left[(\Gamma_{1n}\Gamma_{2n})^{1/2} + (\Gamma_{1f}\Gamma_{2f})^{1/2}\right] = 4.004, \tag{56}$$

TABLE I. Input R-matrix parameters for the two level problem shown in Fig. 1.

E_0 (eV)	Γ_n (meV)	Γ_γ (eV)	Γ_f (eV)
1.0	4.0	0.4	4.0
2.0	4.0	0.1	4.0

where D is the average level spacing. This case corresponds to a large pertrubation of the boundary conditions. The trajectories described by the two complex poles are shown in Fig. 1. The point, $\tau = 0$, corresponds to $\mu_1 = E_1$, $\mu_2 = E_2$, $\nu_1 = \nu_2 = 0$, that is to the real poles of R-matrix theory. As the value of τ increases from zero to unity, the real part of the two complex poles quickly approach each other, while the widths, ν_1 and ν_2 go together initially and for $\tau \geq 0.25$ start in divergent trajectories. This is characteristic of systems with a high degree of level interference, where some of the levels "pick up" large widths, ν, as in the case shown here. The point $\tau = 0.25$ corresponds to the closest approach of the two pole-trajectories yielding the maximum value for the degree of interference which has been plotted in Fig. 2.

A further illustrative example of the present method is afforded by the U-matrix parametrization of the neutron induced reactions in ^{247}Cm. Moore *et al.*[18] have analyzed the neutron cross sections of ^{247}Cm and published a set of R-matrix

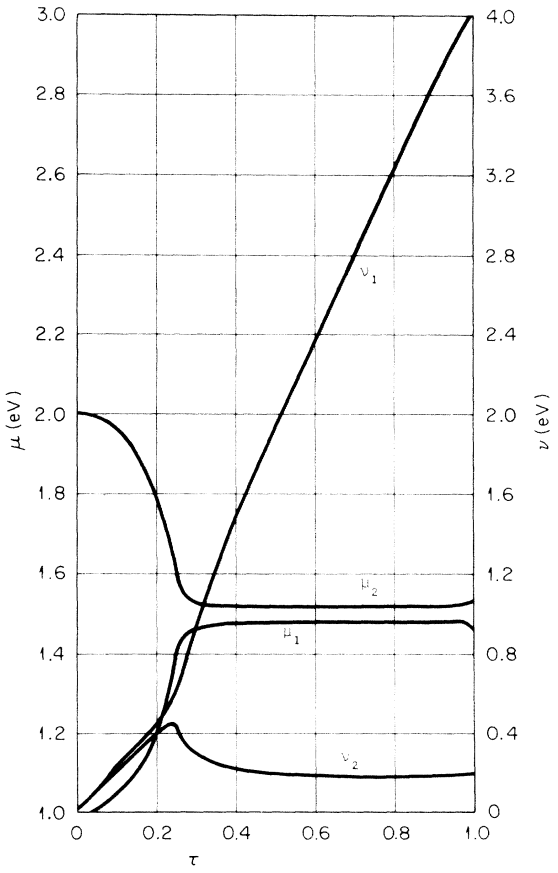

FIG. 1. Trajectories followed by the U-matrix complex poles as a function of changes in the boundary conditions.

parameters with which the cross sections of this isotope can be constructed in the range 20–60 eV. These parameters which include two fission channels per level are given in Table II. The corresponding U-matrix parameters in the Adler-Adler[16] formulation obtained by the method developed in this work are shown in Table III and the fission and capture cross sections for neutron energies between 20 and 60 eV are shown in Figs. 3 and 4, respectively. Inspection of these results shows the consistency between the R-matrix and the U-matrix calculation with the parameters obtained by the present method. The advantage of the latter is, however, the fact that rather than inverting a matrix for each energy point (the level matrix in R-matrix theory, or a reduced channel matrix in the Reich-Moore formalism[17]) one can represent the cross sections in the more attractive and practical form given by Eq. (37).

VI. DIRECT SOLUTION OF THE T-MATRIX INTEGRODIFFERENTIAL EQUATION

In this section we discuss an alternate method to the eigenfunction expansion technique. The new method is based on the direct solution of the integrodifferential Eq. (9) for the transition matrix. We consider for $\tau = 0$ a coupled channel problem

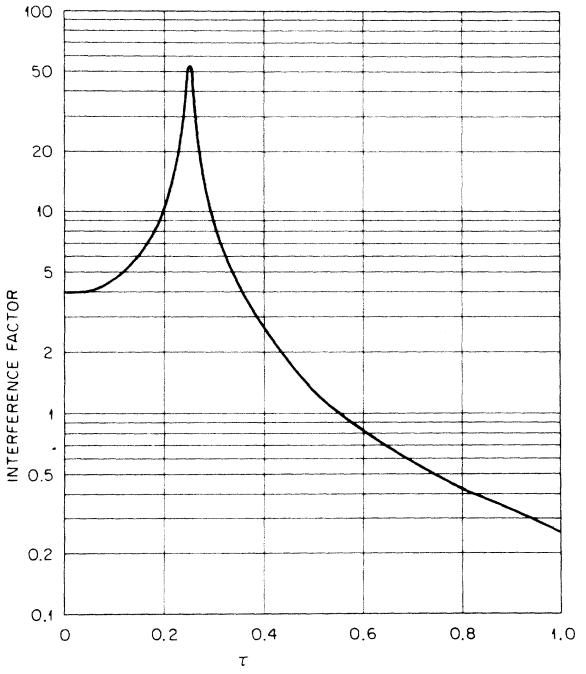

FIG. 2. Level interference as a function of changes in the boundary conditions. [The interference factor is defined in Eq. (56) in the text.]

in which all the coupling potentials, V_{ij} $(i \neq j)$, and channel residual potentials, V_{ii}, are turned off. In this initial configuration the boundary conditions are taken to be the R-matrix boundary conditions, B_{0i} [Eq. (47)] while the channel potentials are assumed to be square well potentials V_{0ti}. This configuration corresponds to an uncoupled R-matrix problem which can be solved exactly (Appendix A). The resulting initial T matrix, (T_{00c}), is diagonal and is given by

$$T_{cc}^{(00)}(r\,|\,r') = \frac{2iP_c}{K_c a_c} D_{cu}^{-1} Q_c(r) j_{1c}(r') \quad (r \geq r') \tag{57}$$

with

$$Q_c(r) = D_{cw} j_{1c}(r) - D_{cu} n_{1c}(r) \tag{58}$$

and

$$T_{ci}^{(00)}(r\,|\,r') = 0, \quad c \neq i\,, \tag{59}$$

where a_c is the channel radius, and K_c has been defined in Appendix A, along with the channel momenta, k_c, and the functions, D_{cu} and D_{cw}. The re-

TABLE II. Multilevel resonance parameters for the reaction (^{247}Cm + n) between 20 and 60 eV (from M. S. Moore *et al.* Ref. 18).

E_0 (eV)	$2g\Gamma_n^0$ (mV)	Γ_γ (mV)	Γ_{f1}^1 (mV)	Γ_{f2} (mV)
21.30	0.027	(40)	−353	196
24.03	0.009	(40)	−61	−119
25.35	0.002	(40)	−25	−6
26.19	0.003	(40)	171	−138
28.04	0.011	(40)	30	43
30.25	0.627	(40)	−4	−0.3
30.62	0.034	(40)	−26	45
32.23	0.089	(40)	−26	−1
36.36	0.270	(40)	−38	48
37.74	0.004	(40)	−252	−494
37.76	0.217	(40)	−0.5	−13
39.52	0.001	(40)	−206	−674
39.95	0.015	(40)	54	158
40.01	0.005	(40)	−35	−33
41.25	0.103	(40)	19	−5
41.76	0.008	(40)	−104	536
43.39	0.029	(40)	4	−2
44.87	0.313	(40)	6	31
45.21	0.086	(40)	−52	−29
47.92	0.169	(40)	−158	42
48.85	0.973	(40)	35	74
50.08	0.334	(40)	−44	−33
50.69	0.447	(40)	19	48
51.78	0.231	(40)	−6	-13
52.19	0.175	(40)	−3	3
53.63	0.062	(40)	278	−167
55.10	0.072	(40)	38	1
56.18	0.088	(40)	61	31
59.66	2.037	(40)	−106	43

TABLE III. Collision matrix parameters for (^{247}Cm + n) between 20 and 60 eV.

μ (eV)	ν (eV)	A (b eV$^{3/2}$)	B (b eV$^{3/2}$)	G_F (b eV$^{3/2}$)	H_F (b eV$^{3/2}$)	G_c (b eV$^{3/2}$)	H_c [a] (b eV$^{3/2}$)
21.31	0.294	17.4	3.27	16.2	3.26	1.2	−0.3
24.04	0.108	5.9	0.23	4.8	0.23	1.1	0.4
25.35	0.035	1.3	0.05	0.6	0.05	0.74	−0.2
26.20	0.175	2.0	−0.72	1.8	−0.72	0.23	−1.8
28.04	0.057	7.1	0.33	4.6	0.33	2.5	1.4
30.25	0.022	408.7	2.97	38.9	2.75	364.1	38.1
30.62	0.055	22.2	−0.03	14.4	0.03	7.8	−36.4
32.23	0.033	58.1	−0.64	23.3	−0.64	34.8	−1.3
36.36	0.062	176.4	−1.02	119.0	−1.07	57.0	−14.4
37.87	0.381	10.2	−2.00	9.5	−2.03	0.6	36.0
37.76	0.021	134.6	0.62	7.5	0.65	126.5	−49.9
39.50	0.568	−4.9	0.61	−4.9	0.64	−0.0	−31.0
39.89	0.060	12.9	0.95	8.3	0.88	4.6	64.0
40.59	0.045	2.9	−0.59	1.5	−0.58	1.4	−13.4
41.25	0.030	69.9	−2.07	22.1	−1.93	47.7	−167.0
41.72	0.335	3.2	4.64	2.8	4.46	0.4	180.9
43.39	0.023	18.8	−0.32	2.1	−0.33	16.6	−2.3
44.87	0.039	204.3	−9.12	95.1	−8.56	108.4	−709.7
45.20	0.060	56.2	12.09	35.0	11.39	21.1	716.2
47.92	0.121	110.8	−5.14	92.1	−5.24	18.6	−51.5
48.85	0.075	634.4	−3.05	458.8	−3.30	171.4	−63.7
50.08	0.059	216.3	−3.27	138.5	−3.03	77.1	−268.0
50.68	0.053	292.3	4.55	178.4	4.39	112.7	325.5
51.78	0.029	151.5	5.68	46.8	5.70	104.1	27.7
52.19	0.023	114.4	−3.05	13.8	−2.91	100.2	−14.6
53.62	0.0243	40.0	3.76	36.6	3.75	3.4	29.9
55.10	0.039	46.6	−2.28	23.0	−2.27	23.6	−8.0
56.17	0.066	56.4	−7.78	39.2	−7.77	17.2	−14.8
59.65	0.095	1328.9	1.36	1033.9	1.85	280.7	16.3

[a] The values in this column are to be multiplied by 10^{-3}.

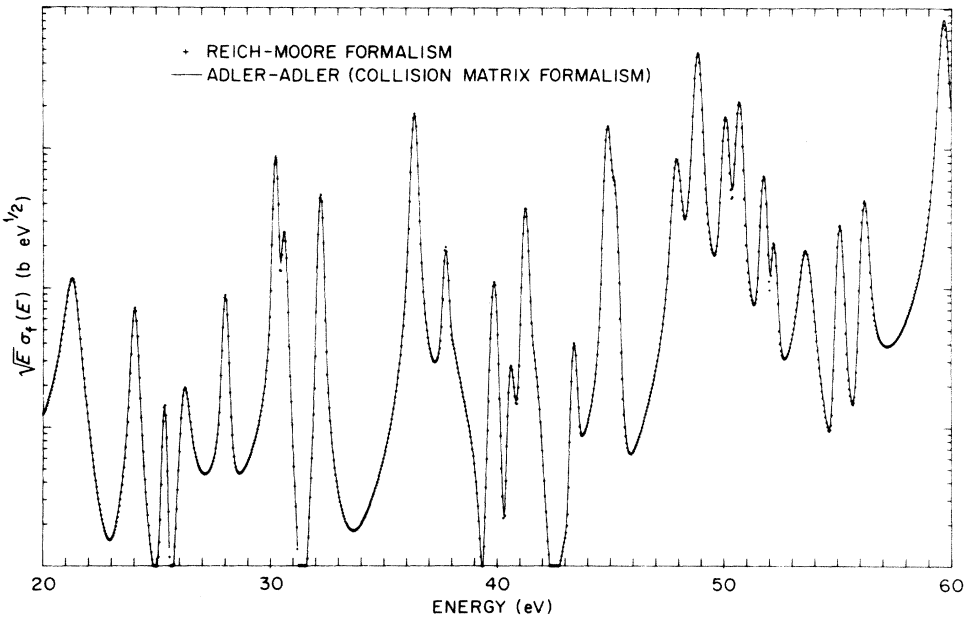

FIG. 3. Comparison of the fission cross sections for ^{247}Cm, between 20 and 60 eV, computed by the Reich-Moore formalism (***R***-matrix parameters) and by the Adler-Adler formalism, with the equivalent set of collision matrix parameters obtained by the method developed in this work.

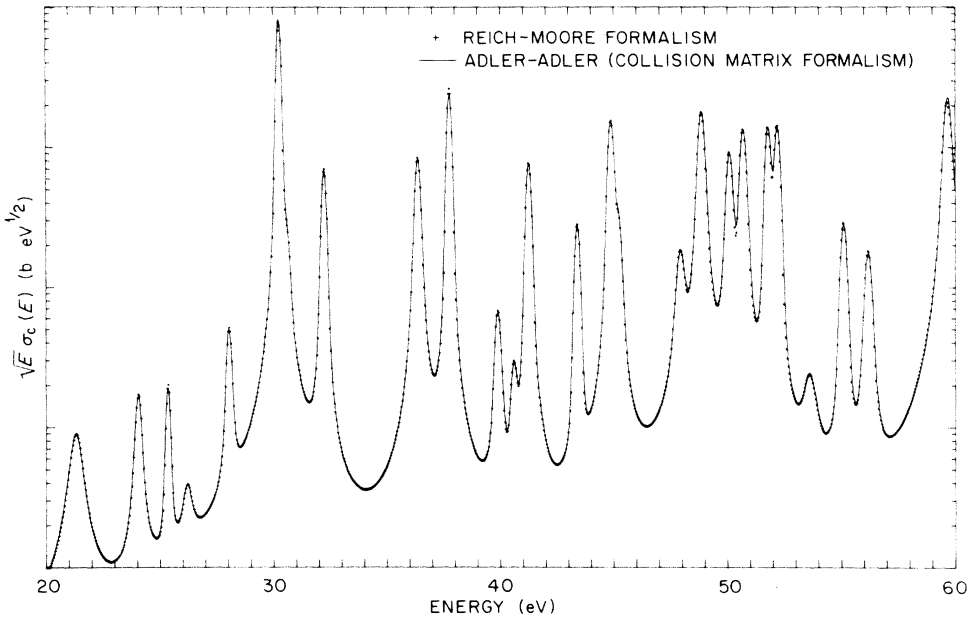

FIG. 4. Comparison of the capture cross section for ^{247}Cm, between 20 and 60 eV, computed by the Reich-Moore formalism (R-matrix parameters) and by the Adler-Adler formalism, with the equivalent set of collision matrix parameters obtained by the method developed in this work.

sults, Eqs. (57) and (59), are valid for $r \geq r'$. For the case $r \leq r'$, the same relations apply with the exchange of primed and unprimed space variables, r, r'.

The next step is to "march" from the R-matrix boundary conditions, Eq. (47), to the U-matrix boundary conditions, Eq. (2). This is done by computing the term $dB_c/d\tau$ in the general Eq. (9) from Eq. (46) and introducing the result into (9). One obtains

$$\frac{d}{d\tau} T^{(0)}_{Rcc}(r \mid r') = T^{(0)}_{Lcc}(r \mid a_c) d_c T^{(0)}_{Rcc}(a_c \mid r'), \tag{60}$$

where

$$d_c = \eta_c^{-2}[B_c - B_{0c}] = -\frac{i}{2P_c}[(S_c - b_c) + iP_c] \tag{61}$$

after use if made of Eqs. (2), (4), (8), and (47). Also the subindexes L (left), and R (right) were introduced to describe the situation in which $r \leq r'$, and $r \geq r'$, respectively. We first make $r = r' = a_c$ in Eq. (60), and make the substitution

$$T^{(0)}_{cc}(a_c \mid a_c) = Y_c^{-1}(a_c \mid a_c) \tag{62}$$

yielding

$$\frac{d}{d\tau} Y_c(a_c \mid a_c) = -d_c; \tag{63}$$

hence

$$Y_c(a_c \mid a_c) = Y_{0c}(a_c \mid a_c) - d_c\tau \tag{64}$$

and

$$T^{(0)}_{cc}(a_c \mid a_c) = [1 - \tau d_c T^{(00)}_{cc}(a_c \mid a_c)]^{-1} T^{(00)}_{cc}(a_c \mid a_c). \tag{65}$$

This first step for the computation of $T^{(0)}_{cc}(a_c \mid a_c)$ is necessary so that $T^{(0)}_{Lcc}(r \mid a_c)$ and $T^{(0)}_{Rcc}(a_c \mid r')$ can in turn be computed by Eq. (60) and again introduced in this equation, now written for $T^{(0)}_{Rcc}(r \mid r')$, for the final determination of the uncoupled problem T matrix. To this end make successively $r = a_c$ and $r' = a_c$ in Eq. (60) to obtain

$$T^{(0)}_{Rcc}(a_c \mid r') = \frac{T^{(00)}_{cc}(a_c \mid a_c)}{T^{(00)}_{Rcc}(a_c \mid r') T^{(0)}_{cc}(a_c \mid a_c)}, \tag{66}$$

$$T^{(0)}_{Lcc}(r \mid a_c) = \frac{T^{(00)}_{cc}(a_c \mid a_c)}{T^{(00)}_{Lcc}(r \mid a_c) T^{(0)}_{cc}(a_c \mid a_c)}. \tag{67}$$

Now introduce the results, Eqs. (66) and (67) into Eq. (60), integrate, and set $\tau = 1$ to obtain

$$T^{(0)}_{Rcc}(r \mid r') = \{T^{(00)}_{cc}(r \mid r') + d_c[T^{(00)}_{Lcc}(r \mid a_c) T^{(00)}_{Rcc}(a_c \mid r') - T^{(00)}_{cc}(a_c \mid a_c) T^{(00)}_{Rcc}(r \mid r')]\}[1 - d_c T^{(00)}_{cc}(a_c \mid a_c)]^{-1} \tag{68}$$

which after utilization of the relation (57) yields

$$T^{(0)}_{Rck}(r \mid r') = \left(\frac{2iP_c}{K_c a_c}\right) \left\{ \frac{Q_c(r) + (2iP_c/K_c a_c) d_c Q_c(a)[Q_c(a) j_{1c}(r) - Q_c(r) n_{1c}(r)] j_{1c}(r')}{[1 - (2iP_c/K_c a_c) d_c Q_c(a) j_{1c}(a)] D_{cu}} \right\} \delta_{ck}. \tag{69}$$

For s-wave neutrons the relation (69) becomes

$$T^{(0)}_{Rck}(r|r') = (2k_c/K_c)\frac{[i\cos(K_c(a_c-r)) + (k_c/K_c)\sin(K_c(a_c-r))]\sin(K_c r')}{\cos(K_c a_c) - i\,(k_c/K_c)\sin(K_c a_c)}\delta_{ck}\,. \tag{70}$$

The Eqs. (69) and (70) illustrate once more the use of the present formalism to relate the results of two boundary value problems with different boundary conditions. Although conceptually equivalent, it is much easier from the numerical viewpoint to solve boundary value problems associated with constant, real boundary conditions, rather than with the momentum-dependent, complex boundary conditions of the collision-matrix formalism.

The final step in the calculation is to turn "on," the coupling and residual potentials. To this end we write

$$V'_{ck}(r,\tau) = \tau V_{ck}(r)\,, \tag{71}$$

where τ goes again between zero and unity. In this case Eq. (9) for the T matrix becomes

$$\frac{d}{d\tau}T_{ck}(r|r') = \tfrac{1}{2}i\sum_{ij}\left[(C_iC_j)^{-1}\int_0^{a_i} r''dr''T_{ci}(r|r'')\left(\frac{V_{ij}(r'')}{[P_i(r'')P_j(r'')]^{1/2}}\right)T_{jk}(r''|r')\right], \tag{72}$$

where Eq. (8) was used.

To illustrate the use of the present T-matrix formalism, embodied in Eq. (72), we have studied the two coupled s-wave neutron channel problem propounded by Tobocman,[26] which has been widely used as testing grounds for various nuclear reaction theories by Purcell,[5] Romo,[27] Schmittroth and Tobocman,[28] and Fu[29] among others. In this model the channel potentials as well as the interaction potential are of the square-well type. The second channel has a threshold at $Q = 3.5$ MeV. All the channel radii are taken to be equal ($a_c = 6$ fm). The depths of the potential wells for the first and second channel are 32 and 39 MeV, respectively. For s-wave neutrons, $P_i(r'') = k_i r''$ and taking the values of all the reduced channel masses equal, Eq. (72) becomes

$$\frac{d}{d\tau}T_{ck}(r|r') = \left(\frac{iC_c^{-2}}{2}\right)\sum_{ij}\int_0^{a_c} dr''T_{ci}(r|r'')\times\left(\frac{V_{ij}(r'')}{(k_ik_j)^{1/2}}\right)T_{jk}(r''|r')$$

$$(c,k,i,j = 1,2)\,. \tag{73}$$

In order to eliminate the singularities at the various channel thresholds one makes the transformation

$$T_{ck}(r|r') = a_c(k_ck_k)^{1/2}t_{ck}(r|r') \tag{74}$$

which after substitution in Eq. (73) yields the following result

$$\frac{d}{d\tau}t_{ck}(r|r') = \left(\frac{iC_c^{-2}a_c}{2}\right)\sum_{ij}\int_0^{a_c} dr''t_{ci}(r|r'')\times V_{ij}(r'')t_{jk}(r''|r')\,, \tag{75}$$

where $t_{ck}(r|r')$ is a reduced T matrix.

The integrodifferential Eq. (75) is converted into a set of first order differential equations of the Ricatti-type by Gaussian integration:

$$\frac{d}{d\tau}t_{ck}(\xi_\alpha,\xi_\beta) = \epsilon_c\sum_{lm}\sum_{s} t_{cl}(\xi_\alpha,\xi_\gamma)\omega_{l,m}(\xi_s)t_{mk}(\xi_\gamma,\xi_\beta) \tag{76}$$

with

$$\epsilon_c = \tfrac{1}{4}iC_c^{-2}a_c^2\,, \tag{77}$$

$$\omega_{lm}(\xi_\alpha) = g_\alpha V_{lm}\,, \tag{78}$$

where we introduced the new "radial" variable

$$\xi = 2r/a_c - 1 \tag{79}$$

and the Gaussian weights, g_α. Care has to be exercised in the handling of Eq. (76) whenever $\xi_\gamma > \xi_\alpha$ or $\xi_\gamma < \xi_\beta$. Then one has to use the relation indicated previously between the T matrix to the right and to the left. The set of Ricatti equations, Eq. (76), can then be solved by the Runge-Kutta technique and the collision matrix, U, computed from Eqs. (74) and (7).

The exact solution to this problem has been given by Purcell[5] (see also Romo[27]). In Fig. 5 we show the results for an interaction potential $V_{12} = 1$ MeV. For the strong coupling case, $V_{12} = 4$ MeV, the results are shown in Fig. 6. In this instance we show a comparison between a three-point Gaussian integration and a 17-point Gaussian quadrature. The latter yields results within a fraction of a percent of the exact answer.

Table IV shows the effect of increasing strength of the coupling potential on the number of Gaussian integration points to be used in the numerical solution of Eq. (75).

At each value of the energy of the incident parti-

cle, the unitarity condition, $\sum_c U_{1c}U_{c1}=1$ is computed at the end of the process. In a particular instance, two calculations were performed with the same number of Runge-Kutta steps and of Gaussian points, but changing the interaction potential from 1 to 4 MeV. For the weaker potential, the elastic cross section was accurate to 0.02%, and the unitarity check was good up to 36 parts per million. For $V_{12}=4$ MeV the accuracy was only 1.0% in the elastic cross section with a corresponding unitarity check of 255 parts per million.

The present method avoids the calculation of the radial matrix elements and the diagonalization of relatively large order matrices. On the other

TABLE IV. Comparison of the results obtained by the direct integration method with the exact results for the case of strong channel coupling.

Coupling potential (MeV)	Exact EL [c]	Exact INEL [d]	T-matrix [a] method EL	T-matrix [a] method INEL	T-matrix [b] method EL	T-matrix [b] method INEL
4	0.6564	0.12720	0.6577	0.12736	0.6571	0.12736
10	0.2713	0.01587	0.2750	0.01611	0.2713	0.01581

[a] 17 points Gaussian quadrature.
[b] 34 points Gaussian quadrature.
[c] $\mathrm{EL} \equiv (k^2/4\pi)\sigma_{\text{elastic}}$.
[d] $\mathrm{INEL} = (k^2/4\pi)\sigma_{\text{inelastic}}$.

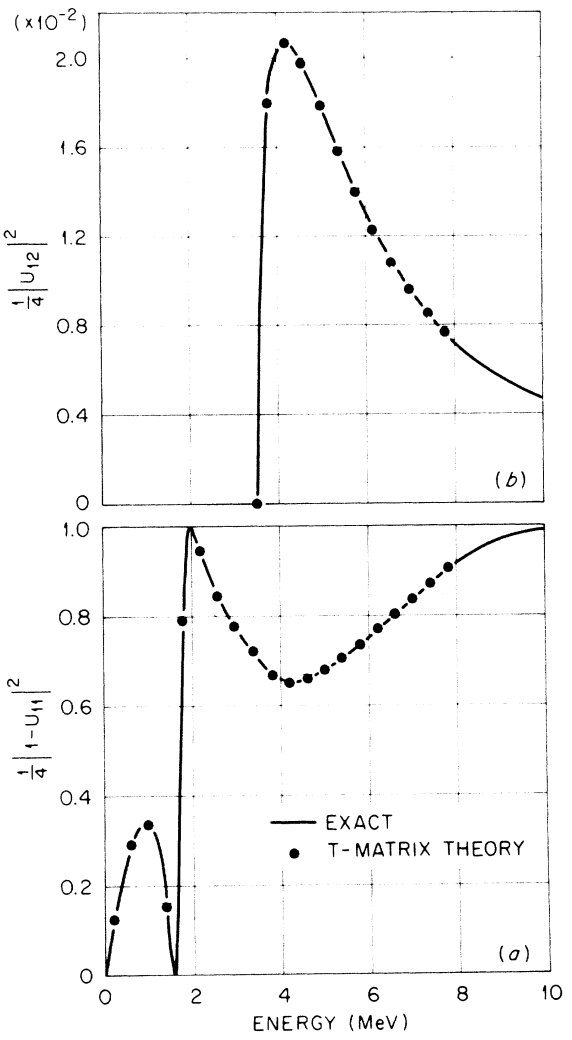

FIG. 5. Comparison between exact and approximate calculations of $k^2/4\pi$ times the cross section for (a) elastic scattering and (b) for inelastic scattering for weak coupling ($V_{12}=1$ MeV). See text for other parameters.

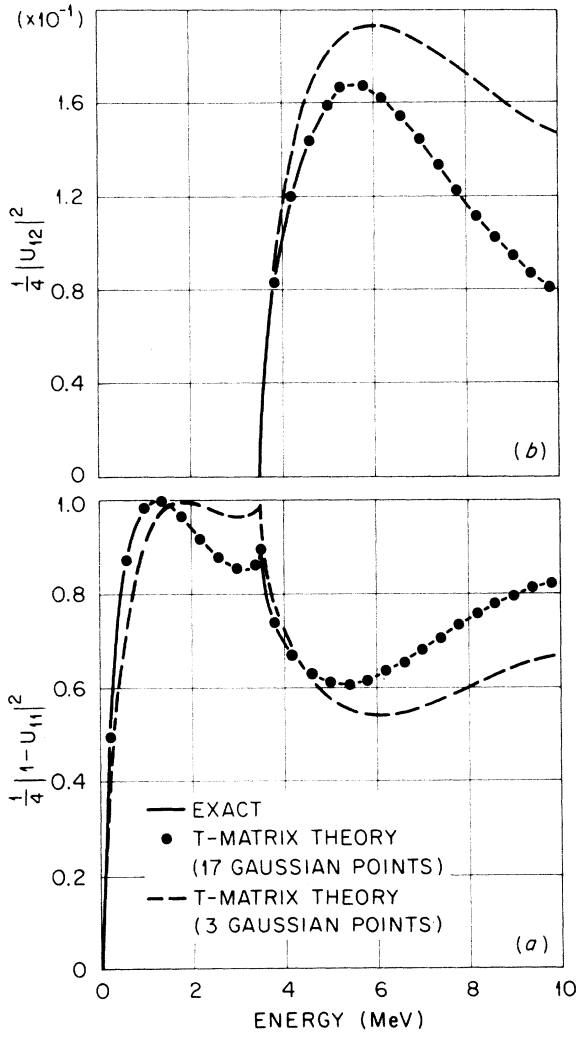

FIG. 6. Comparison between exact and approximate calculations of $k^2/4\pi$ times the cross section for (a) elastic scattering and (b) for inelastic scattering for strong coupling ($V_{12}=4$ MeV). See text for other parameters.

hand the solution of the initial value problem involved here is performed by a step-wise procedure such as the Runge-Kutta algorithm, which for very large perturbations may require many steps.

Hence, the final outcome of a comparison of this method with others, from the viewpoint of practical computational aspects, will depend on the nature of the problem at hand.

VII. DISCUSSION

In Sec. III we have presented a method to compute the collision matrix in terms of a set of unperturbed R-matrix states. This technique has been extended in Sec. IV to determine the widths and poles of either the R-matrix or the U-matrix formalisms under a variety of circumstances such as boundary condition perturbations, and deformed potentials among others. In particular, identification of the parameter τ with the channel orbital angular momentum l would provide a set of first order differential equations defining trajectories which map the variation of widths and poles as a function of a continuous varying angular momentum. The points in the trajectory associated with integer values of the parameter τ will then determine the physical values of the resonance parameters.

The introduction of the matrix functional $\underline{P}$, together with the use of the random-phase approximation for the capture channels, forms a basis for the treatment of fissile nuclei. The method has been tested successfully in Sec. V for the conversion of a given set of R-matrix parameters into its equivalent U-matrix parameters set.

The method presented in Sec. VI for the calculation of the transition matrix has several interesting features:

(a) One avoids the calculation of the radial matrix elements of the channel potentials.

(b) In dealing with the T matrix directly one avoids the singularities found in the R matrix along the real energy axis.

(c) Unitarity is conserved within the limits of the numerical approximations used. Keeping track of this magnitude properly affords a useful check on the accuracy of the calculation.

The present transition matrix theory offers many other possibilities. For example, one can compute the T matrix at a given energy by "marching" the potential, as shown in Sec. VI, and then identify the parameter τ with the bombarding energy, in order to compute the transition matrix along a given range of energies. Identification of the parameter τ with a deformation parameter, will allow calculations pertaining to deformed nuclei, starting initially from spherically symmetric configurations. In general for any physical parameter of the system, the formalism developed here is ideally suited for parameter search procedures, since at every step in the "marching" of the initial value one obtains the answer for a new value of the parameter of interest.

APPENDIX A: TRANSITION MATRIX FOR THE UNCOUPLED MULTICHANNEL CASE

In this instance, the off-diagonal elements of the transition matrix vanish, while each individual component along the diagonal is given in terms of the Green's function by the relation (6). In a given channel, c, of radial coordinate $r_c \equiv r$, the Green's function satisfies the equation

$$\left(\frac{d^2}{dr^2} + K_c^2 - \frac{l_c(l_c+1)}{r^2}\right) G_c(r|r') = \frac{\delta(r-r')}{r}\left(\frac{2Mc}{\hbar^2}\right) \tag{A1}$$

with

$$K^2 = \frac{2M}{\hbar^2}(E_c - V_c)\,. \tag{A2}$$

Because of the discontinuity in the derivative of the Green's function at $r = r'$ one has to split this function into a right and a left Green's function, $G_{cR}(r|r')$ and $G_{cL}(r|r')$, respectively. The values of the derivative on both sides of the discontinuity are related by

$$\left(\frac{d}{dr} G_{cR}(r|r')\right)_{r'} - \left(\frac{d}{dr} G_{cL}(r|r')\right)_{r'} = -\left(\frac{2M_c}{\hbar^2}\frac{1}{r'}\right). \tag{A3}$$

The pertinent boundary conditions are

$$G_{cL}(0|r') = 0\,, \tag{A4}$$

$$G_{cL}(r'|r') = G_{cR}(r'|r')\,, \tag{A5}$$

$$a_c\left(\frac{d}{dr} G_{cR}(r|r')\right)_{a_c} = b_c G_{cR}(a_c|r')\,, \tag{A6}$$

where b_c is a real momentum independent number (R-matrix boundary conditions). One has then to solve Eq. (A.1) subject to the constraints (A3), (A4), (A5), and (A6). This is a straightforward boundary value problem which can easily be solved by the variation of constants method. One

obtains the following results:

$$G_{cL}(r\,|\,r') = (rr')D_{cu}^{-1}[D_{cw}j_{lc}(r') - D_{cu}n_{lc}(r')] \times \left[\frac{2M_c}{h^2K_c}\right] j_{lc}(r) \quad r<r' , \tag{A7}$$

$$G_{cR}(r\,|\,r') = (rr')D_{cu}^{-1}[D_{cw}j_{lc}(r) - D_{cu}n_{lc}(r)] \times \left[\frac{2M_c}{h^2K_c}\right] j_{lc}(r') \quad r>r' , \tag{A8}$$

where

$$D_{cu} = \left(\frac{d}{dr}[rj_{lc}(r)]\right)_{a_c} - b_c j_{lc}(a_c) , \tag{A9}$$

$$D_{cw} = \left(\frac{d}{dr}[rn_{lc}(r)]\right)_{a_c} - b_c n_{lc}(a_c) , \tag{A10}$$

and $j_l(r)$, $n_l(r)$ are the usual spherical Bessel functions.

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