A GENERAL FORMALISM FOR THE TRANSITION MATRIX
OF NUCLEAR REACTION THEORY¹

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In this past decade there has been an increased activity in the development of new methods to compute resonant cross sections.³⁻⁶ The usual approach deals with the solution of a set of coupled radial Schrödinger equations (the multichannel equations), involving matrix elements of the nuclear Hamiltonian in the channel eigenfunction representation.⁷ The multichannel equations are solved by expansion in either R-matrix states or shell-model eigenfunctions.⁸⁻¹⁰ In the first instance, the series obtained shows a poor rate of convergence and several prescriptions have to be introduced to compensate for truncation effects.^{8,9} Once the pertinent R-matrix is obtained, one has to perform a matrix diagonalization to obtain the collision matrix. The results obtained depend strongly on the values chosen for the channel radii and the boundary condition numbers.⁵ The second method of solution suffers from the difficulty that the shell model eigenfunctions do not satisfy the appropriate boundary conditions.¹⁰

To obviate these problems, we have developed a general formalism for the transition T-matrix based on the use of Bloch's L-operator¹¹ and invariant imbedding techniques.¹² The result is a matrix-integro-differential equation for the T-matrix as a function of τ , where τ is any of the parameters entering in the nuclear reaction formalism.

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We have

$$\begin{aligned}
 \frac{d}{d\tau} T_{cc'}(r_\alpha | r_\beta, \tau) &= \sum_{c''} \left[i\eta_c \eta_{c'} \left(\frac{2M_{c''}}{\hbar^2} \right) \frac{dr_\beta}{d\tau} \right. \\
 &\quad + \left[\frac{d}{d\tau} \ln(\eta_c \eta_{c'}) \right] T_{c''c'}(r_\alpha | r_\beta, \tau) \delta_{c''c} \\
 &\quad - \left(\frac{2M_{c''}}{\hbar^2} \right) B_{c''} \left[\frac{\eta_c}{\eta_{c'}} T_{c''c}(a_{c''} | r_\beta, \tau) \frac{dr_\beta}{d\tau} + \frac{\eta_c}{\eta_{c''}} T_{c'c''}(r_\alpha | a_{c''}, \tau) \frac{dr_\alpha}{d\tau} \right] \\
 &\quad + \sum_{c'''} \left\{ \left(\frac{2M_{c'''}}{\hbar^2} \right) \left(\frac{\eta_{c'}}{\eta_{c'''}} \right) \int_{r_\alpha}^{a_{c'''}} dr [E_{c'''} \delta_{cc'''} - U_{c''c'''}(r, \tau)] T_{c''c'}(r | r_\beta, \tau) \frac{dr_\beta}{d\tau} \right. \\
 &\quad \left. + \frac{dr_\alpha}{d\tau} \frac{\eta_c}{\eta_{c'''}} \int_{r_\beta}^{a_{c''}} dr [E_{c'''} \delta_{cc'''} - U_{c''c'''}(r, \tau)] T_{c''c'}(r | r_\alpha, \tau) \right\} \\
 &\quad - i \sum_{c'''} \int_0^{a_{c''}} dr \frac{T_{cc''}(r_\alpha | r, \tau)}{\eta_{c''}(r_\alpha)} \left\{ \frac{d}{d\tau} [E_{c'''} \delta_{cc'''} - U_{c''c'''}(r, \tau)] \right\} \frac{T_{c''c'}(r | r_\beta, \tau)}{\eta_{c'''}(r_\beta)} \\
 &\quad - i \sum_{c'''} (\eta_{c''} \eta_{c'''})^{-1} T_{cc''}(r_\alpha | a_{c''}, \tau) \left\{ \left[\left(\frac{2M_{c''}}{\hbar^2} B_{c''}^2 + E_{c'''} \right) \delta_{c''c'''} - U_{c''c'''}(a_{c''} | \tau) \right] \frac{da_{c''}}{d\tau} \right. \\
 &\quad \left. + \frac{dB_{c''}}{d\tau} \right\} T_{c''c'}(a_{c''} | r_\beta, \tau) \Bigg] , \tag{1}
 \end{aligned}$$

where $r_>$ is the largest of the two radial coordinates, r_α and r_β , and B_c is the complex, momentum dependent Kapur-Peierls¹³ boundary conditions, and

$$\eta_c = \left(\frac{\hbar^2 P_c}{M_c a_c} \right)^{1/2} . \quad (2)$$

The sums are carried out over the intermediate channels; P_c is the penetration factor, a_c is the channel radius, and $U_{c''c}(r, \tau)$ is the channel potentials. By discretization of the radial integrals in Eq. (1), one obtains a set of Ricatti equations which, together with the proper initial conditions, defines an initial value problem for the transition matrix. Alternatively one can expand the T-matrix in shell-model eigenfunctions. In this case one makes $\tau = B_c$, and one marches the solution from τ_0 equal to the shell-model logarithmic derivative at the channel radius to the correct boundary conditions, B_c .

As one of the many applications of the present formalism, we show a method to generate the Kapur-Peierls resonance parameters from a set of R-matrix parameters. The poles and residues of the R-matrix derive from an eigenvalue problem in which the boundary conditions, b_c , are real numbers. The corresponding magnitudes in the Kapur-Peierls theory arise from complex momentum dependent boundary conditions. Again we make $\tau = B_c$, $\tau_0 = b_c$, and expand the T-matrix in terms of its residues, $g_{\lambda c}$,

and poles $\varepsilon_\lambda \equiv \mu_\lambda - iV_\lambda$. Introduction of this expansion into Eq. (1) yields:

$$\frac{d}{dB_c} \varepsilon_{\lambda c} = \frac{1}{2} \sum_{c''} \sum_{\lambda' \neq \lambda} (\varepsilon_{\lambda'} - \varepsilon_\lambda)^{-1} (\eta_c \eta_{c''})^{-1} [\varepsilon_{\lambda c''} \varepsilon_{\lambda' c} + \varepsilon_{\lambda c} \varepsilon_{\lambda' c''}] \varepsilon_{\lambda' c} \quad , \quad (3)$$

and

$$\frac{d}{dB_c} \varepsilon_\lambda = \sum_{c''} (\eta_{c''} \eta_c)^{-1} \varepsilon_{\lambda c} \varepsilon_{\lambda c''} \quad , \quad (4)$$

with the initial conditions

$$\varepsilon_{\lambda c} (B_c = b_c) = \left(\frac{P_c}{ka_c} \right)^{1/2} \Gamma_{\lambda c}^{1/2} \quad (k = \text{momentum, cm}^{-1}) \quad (5)$$

and

$$\varepsilon_\lambda (E_c = b_c) = E_\lambda \quad . \quad (6)$$

Numerical solutions can be obtained easily by the Runge-Kutta technique for any value of the angular momentum. To obtain useful analytical approximations, one can expand residues and poles in Taylor series around $B_c = b_c$. The derivatives $[d(n)/dB_c^n]_{b_c}$ are then computed from Eqs. (3) and (4). As a check this procedure has been applied for S-wave neutrons ($b_c = 0$), yielding the Adler-Adler¹⁴ formulae for the poles and residues of the collision matrix.

The main advantages of the present nuclear reaction formalism are:

- (a) It deals directly with "observable" quantities such as the T-matrix or its residues and poles. The solution of Eq. (1) by discretization preserves the unitarity of the collision matrix,
- (b) One has a large degree of flexibility in the choice of the boundary conditions. Hence, one can use shell-model function or R-matrix states indistinctively,
- (c) It does not involve time-consuming iterative calculations, and
- (d) It is very suitable for the performance of a parameter search procedure.

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