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THE GENERATION OF KAPUR-PEIERLS PARAMETERS FROM R-MATRIX PARAMETERS BY THE INVARIANT IMBEDDING TECHNIQUES[1]

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The Kapur-Peierls[2] dispersion theory leads to a very convenient parameterization of the cross section. This is especially true for the fissile nuclei, where level interference and channel effects are of importance, Adler and Adler.[3] A drawback of these types of cross section parameterizations 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,[4] Moldauer,[5] Garrison,[6] Hwang,[7] Harris,[8] and de Saussure and Perez.[9]

Further work in this area is motivated by the need of generating Kapur-Peierls parameters for p-wave neutrons in order to study the effects of level interference on Doppler coefficients and self-shielding factors in the unresolved energy region.

The residues and poles in the R-matrix formalism arise from an eigenvalue problem associated with real, momentum independent values of the logarithmic derivatives, $B_{o,c}$, at the nuclear surface for each channel, c. In the case of the collision matrix, U, the residues and poles result from an eigenvalue problem in which the logarithmic derivatives, $B_c = -(S_c + iP_c)$, are complex and momentum dependent, where S_c and P_c are the usual shift and penetration factors respectively. In the spirit of the invariant imbedding technique,[10] one can think in terms of a family of eigenvalue problems, with logarithmic boundary conditions, $B_o(\tau)$, defined in the form

$$B_c(\tau) = -[(S_c - B_{o,c}) + iP_c]\,\tau - B_{o,c} \quad , \tag{1}$$

where the parameter, τ, varies between zero and unity. In this case, it has been shown that the transition, T-matrix, as a function of τ is given by the differential equation[11]

$$\frac{d}{d\tau} T_{cc'}(\tau) = -\frac{i}{2} \sum_{c''} P^{-1}_{c''} T^{(\tau)}_{cc''} \left[\frac{d}{d\tau} B^{(\tau)}_{c''}\right] T^{(\tau)}_{c''c'} \quad . \tag{2}$$

The result, Eq. (2), defines the trajectories in configuration space, described by the transition matrix elements as the parameter τ varies between zero and unity. In order to find the corresponding equations for the complex level widths $g_{\lambda c}$ and poles $\varepsilon_\lambda = \mu_\lambda - i\nu_\lambda$, one introduces in Eq. (2) the expression

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

and one uses Eq. (1) to compute the $dB_{c''}/d\tau$ term.

After some manipulations one obtains

$$\frac{d}{d\tau} g_{\lambda c} = \frac{1}{2} \sum_{\lambda' \neq \lambda} (\varepsilon_{\lambda'} - \varepsilon_\lambda)^{-1} g_{\lambda' c} \left[\sum_{c''} P^{-1}_{c''} \beta_{c''} g_{\lambda c''} g_{\lambda' c''}\right] \quad (4)$$

and

$$\frac{d}{d\tau} \varepsilon_\lambda = - \frac{1}{2} \sum_{c''} P^{-1}_{c''} \beta_{c''} g^2_{\lambda c''} \quad (5)$$

with

$$\beta_c = (S_c - B_{o,c}) + iP_c \quad . \quad (6)$$

The results of Eqs. (4) and (5), together with the initial conditions $g_{\lambda c}(0) = \Gamma^{1/2}_{\lambda c}$ and $\varepsilon_\lambda(0) = E_\lambda$, form a Cauchy initial value problem, which lends itself easily to solution.[12]

There are several advantages to the method discussed here. It applies to any value of the angular momentum, and it does not involve iterative techniques or the inversion of matrices.

To demonstrate the feasibility of the method, Eqs. (4) and (5) have been coded for s-wave neutrons and its results compared with some POLLA[9] calculations.

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

3. D. B. Adler and F. T. Adler, ANL-6792, p. 695 (1963).

4. D. B. Adler and F. T. Adler, COO-1546-4 (1967).

5. P. A. Moldauer, Phys. Rev. 135, B642 (1966); also P. A. Moldauer, R. N. Thomas, and B. S. Garbow, ANL-7590 (1969).

6. J. D. Garrison, Ann. Phys. 50, 355 (1968).

7. R. N. Hwang, Nucl. Sci. Eng. 36, 67 (1969).

8. D. R. Harris, LA-4327 (1969).

9. G. de Saussure and R. B. Perez, ORNL-TM-2599 (1969).

10. R. Bellman, R. Kalaba, and M. Wing, J. Math. Phys. 1, 280 (1960).

11. R. B. Perez, ORNL-TM-3778, to be published.

12. F. Ceschino and J. Kuntzmann, Numerical Solution of Initial Value Problems, Prentice-Hall, 1966.