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Fission in nuclear reaction theory

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Abstract. Nuclear fission is incorporated in a formal way into the R matrix reaction theory. Definitions of suitable variables to describe fission deformation in terms of individual nucleon coordinates are first of all described. The kinetic energy operator of the many-particle Schrödinger equation is then cast into a form that explicitly displays its dependence on the new fission deformation variable. A term in the potential energy that similarly displays a dependence only on the fission deformation variable is then defined, and so the Hamiltonian is broken up into a deformation term, an 'intrinsic' term (depending on the other degrees of freedom) and a coupling term. This break-up allows the definition of fission channels; with the choice of channel boundaries close to maxima in the fission potential energy curve these correspond physically to A Bohr's more intuitive definition of fission channels. This formalism is applied to the treatment of the intermediate structure in fission reactions that appears to be a result of the secondary well in the fission potential barrier. A development of the formalism is also made in which an intermediate region of configuration space is introduced, in addition to the usual internal and channel regions that normally appear in R matrix theory. If this intermediate region is defined to include the secondary well of the barrier, the dispersion effects that correspond to intermediate structure appear in the extended penetration and shift factors (the logarithmic derivative of the outgoing waves in the fission channel) rather than in the R matrix of the internal region. This allows a particularly simple treatment of the so-called vibrational resonances of fission reactions.

1. Introduction

Nuclear fission is a complex phenomenon. Most discussions of reactions involving fission lean heavily on explicit models of the process, such as the original liquid drop model of Bohr and Wheeler (1939). A later important step in such discussions was the recognition by A Bohr (1956) that 'internal' quantum states of the nucleus as it passes over the liquid drop barrier can play a vital role in determining fission properties. More recently, Strutinsky (1967) investigated the influence of nucleon shell effects in determining the form of the potential energy surface of the deforming nucleus and concluded that important modifications to the fission barrier could result. In particular, the actinide nuclei, the commonest low energy fissioners, can exhibit a double-humped barrier, according to this theory. It was quickly realized that such a barrier can give rise to striking effects in nuclear reactions involving fission and thus explain some of the dramatic experimental results that had recently appeared (Lynn 1968a, b, Weigmann 1968). Much of the discussion of such effects has been based on phenomenological theories (eg Bjornholm and Strutinsky 1969) of the fission reaction. Attempts have been made to include fission in reaction theories of a more formal nature, however, and this paper constitutes a fuller and more definitive version of one of these (Lynn 1968b).

2. The nuclear Hamiltonian with explicit reference to deformation

2.1. The deformation variable

A suitable variable that will describe overall elongation of the fissioning nucleus (of mass number A) continuously from its near-spherical form to its division into two fragments and their increasing separation must first be defined. We choose here a statistical description of deformation in terms of the individual nucleon coordinates. For example, if the coordinate system is body-fixed a parameter of the type $L = \sqrt{\Sigma_i \bar{z}_i^2}$ is adequate, provided that the (body-fixed) z axis is chosen to maximize L. Here, the $\bar{z}_i$ are z coordinates referred to the centre of mass. For small prolate spheroidal deformations of the kind normally described by a quadrupole dependence of the nuclear radius, $R = R_0(\alpha_0 + \beta Y_{20}(\theta, \phi))$ (α_0 being adjusted to preserve constancy of nuclear volume), the parameter $L \simeq R_0(A/5)^{1/2}\{1+\beta(5/4\pi)^{1/2}\}$, while for large distance of separation l of the fissioning nucleus into two fragments of mass number A_1 and A_2

$$L \simeq l\{A_1 A_2/(A_1+A_2)\}^{1/2}. \tag{1}$$

Equation (1) also applies to the choice of parameter $\mathscr{R} = \sqrt{\Sigma_i \bar{r}_i^2}$, but for small spheroidal deformations this parameter approximates to $\mathscr{R} \simeq R_0(3A/5)^{1/2}(1+5\beta^2/8\pi)$.

The quadrupole moment, $Q = \Sigma_i(3\bar{z}_i^2 - \bar{r}_i^2)$ is also a perfectly adequate parameter. Its limiting form for small spheroidal deformations is $Q \sim 3AR_0^2(1/5\pi)^{1/2}\beta$ and its asymptotic extended form is $Q \sim 2A_1A_2l^2/A$.

2.2. Form of the kinetic energy operator

With the use of a statistical parameter for the deformation one can transform directly the kinetic energy part of the Schrödinger equation for the system as already written in terms of the individual particle coordinates

$$-\frac{\hbar^2}{2m}\sum_i\left(\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}+\frac{\partial^2}{\partial z_i^2}\right)\psi + V\psi = E\psi$$

where m is the individual nucleon mass. The general equation for transforming the second derivative in a particular coordinate x_i into the second derivatives of a new set of coordinates ξ_j is

$$\frac{\partial^2\psi}{\partial x_i^2} = \sum_j\left\{\frac{\partial^2\psi}{\partial\xi_j^2}\left(\frac{\partial\xi_j}{\partial x_i}\right)^2+\frac{\partial\psi}{\partial\xi_j}\frac{\partial^2\xi_j}{\partial x_i^2}\right\}+\sum_{j\neq k}\frac{\partial^2\psi}{\partial\xi_j\,\partial\xi_k}\left(\frac{\partial\xi_j}{\partial x_i}\right)\left(\frac{\partial\xi_k}{\partial x_i}\right).$$

The desirable limitation on the new set ξ_j is that on summing $\partial^2\psi/\partial x_i^2$ over all i, the cross derivative terms in $\partial^2\psi/\partial\xi_j\,\partial\xi_k$ should vanish.

Kinetic energy operators in terms of the new parameters are thus straightforwardly obtained. For example, for the parameter $L = \sqrt{\Sigma_i \bar{z}_i^2}$, the new term, referring only to L, is

$$T_L = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial L^2}+\frac{A-1}{L}\frac{\partial}{\partial L}\right) = -\frac{\hbar^2}{2mL^{A-1}}\frac{\partial}{\partial L}\left(L^{A-1}\frac{\partial}{\partial L}\right) \tag{2}$$

and the 'inertial parameter' B_L is just the nucleon mass m. For $\mathscr{R} = \sqrt{\Sigma_i \bar{r}_i^2}$ it is

$$T_{\mathscr{R}} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\mathscr{R}^2}+\frac{3A-1}{\mathscr{R}}\frac{\partial}{\partial\mathscr{R}}\right) = -\frac{\hbar^2}{2m\mathscr{R}^{3A-1}}\frac{\partial}{\partial\mathscr{R}}\left(\mathscr{R}^{3A-1}\frac{\partial}{\partial\mathscr{R}}\right). \tag{3}$$

These two forms of the kinetic energy operator become, for asymptotically large values of L or $\mathscr{R}$,

$$T_{L,\mathscr{R}} \sim -\frac{\hbar^2}{2m_c}\frac{\partial^2}{\partial l^2} \tag{4}$$

by equation (1), where m_c is the reduced mass A_1A_2m/A for the two separated product nuclei. The kinetic energy operator for the quadrupole moment is

$$T_Q = -\frac{\hbar^2(4Q+8A\overline{r^2})}{2m}\frac{\partial^2}{\partial Q^2} \equiv -\frac{\hbar^2}{2B_Q}\frac{\partial^2}{\partial Q^2}. \tag{5}$$

This transforms into equation (4) for asymptotically large Q. For small spheroidal deformations the inertial parameter is $B_Q \sim (5m/24AR_0^2)\{1-(5/4\pi)^{1/2}\beta\}$. If, in this limit, we transform the kinetic energy operator into its form for β we find $T_\beta = -(\hbar^2/2B_\beta)\partial^2/\partial\beta^2$ with the 'inertial parameter' B_β having just the irrotational liquid drop form $B_\beta = 3AmR_0^2/8\pi$.

2.3. Hamiltonian operator with explicit reference to the deformation mode

We are now in a position to rearrange the Hamiltonian operator of the fissioning nucleus to best advantage. We have seen how the kinetic energy operator can be transformed to give a component T_η that refers only to a suitably defined deformation variable η. The remainder of the kinetic energy operator, for the $3A-4$ 'intrinsic' degrees of freedom (the three centre of mass degrees of freedom are considered already separated out) denoted by ξ will, in general, depend on η and is therefore written $T_\xi(\eta)$.

The Hamiltonian is thus written $H = T_\eta + T_\xi + V(\eta, \xi)$. The eigenvalues of the operator $(T_\xi(\eta) + V(\eta, \xi))$, for fixed η, are labelled $\varepsilon_\mu(\eta)$. Let us now write $\mathscr{V}(\eta) = \varepsilon_0(\eta)$ and $H = T_\eta + \mathscr{V}(\eta) + T_\xi(\eta) + V(\eta, \xi) - \varepsilon_0(\eta)$. An 'intrinsic' Hamiltonian term H_{int} can now be defined for some chosen value of deformation η_0, and a 'coupling' Hamiltonian term H_c from the remainder. Thus

$$H = H_\eta + H_{\text{int}}(\xi, \eta_0) + H_c(\eta, \xi; \eta_0) \tag{6}$$

where

$$H_\eta = T_\eta + \mathscr{V}(\eta) \tag{6a}$$

$$H_{\text{int}}(\eta_0) = T_\xi(\eta_0) - \varepsilon_0(\eta_0) + V(\eta_0, \xi) \tag{6b}$$

$$H_c = T_\xi(\eta) - \varepsilon_0(\eta) + V(\eta, \xi) - H_{\text{int}}(\eta_0). \tag{6c}$$

It is useful to generalize the intrinsic Hamiltonian to any other value of deformation η. The eigenvalues and eigenfunctions of $H_{\text{int}}(\eta)$ are denoted by $\mathscr{E}_\mu(\eta)$ and $\chi_\mu(\eta)$. From the definition of H_{int} the eigenvalues $\mathscr{E}_\mu(\eta)$ are just $\varepsilon_\mu(\eta) - \varepsilon_0(\eta)$, that is, the intrinsic excitation energies with respect to 'ground' at the fixed deformation η. The eigenfunctions and eigenvalues of H_η are denoted by $\Phi_\nu(\eta)$ and ϵ_ν.

2.4. Expansion formulae for the intrinsic wavefunctions

It is useful to be able to expand the intrinsic wavefunctions defined at one deformation η in terms of those defined at some special deformation η_0. We define the expansion

coefficients as follows:

$$\chi_\mu(\eta) = \sum_{\mu'} b_{\mu\mu'}(\eta, \eta_0)\chi_{\mu'}(\eta_0). \tag{7a}$$

The inverse expansion is

$$\chi_\mu(\eta_0) = \sum_{\mu'} b^\dagger_{\mu\mu'}(\eta, \eta_0)\chi_{\mu'}(\eta). \tag{7b}$$

We have the usual relations

$$b_{\mu\mu'}(\eta, \eta_0) = \langle \chi_{\mu'}(\eta_0) | \chi_\mu(\eta) \rangle$$

$$b^\dagger_{\mu\mu'}(\eta, \eta_0) = b_{\mu\mu'}(\eta_0, \eta) = \langle \chi_{\mu'}(\eta) | \chi_\mu(\eta_0) \rangle$$

and, from the complex conjugate expansions

$$b^\dagger_{\mu'\mu}(\eta, \eta_0) = b^*_{\mu\mu'}(\eta, \eta_0)$$

$$b_{\mu'\mu}(\eta, \eta_0) = b^{\dagger *}_{\mu\mu'}(\eta, \eta_0).$$

3. Inclusion of fission in *R* matrix theory

With the decomposition of the Hamiltonian given in equation (6) it is formally straightforward to include fission in R matrix reaction theory.

The channel structure of the A particle system is defined in the usual way for the simpler channels in which the system separates into two composite particles, with radial separation r_c, one being very small compared to the other (eg is a nucleon or α particle). Each channel c in this case is labelled by the internal state of excitation of the large particle (the residual nucleus), their relative orbital angular momentum and their total internal angular momentum (channel spin); the quantum state (channel function) comprising these quantities is denoted by φ_c. The channel regions of configuration space are delineated from the internal region by a channel radius α_c denoting the minimum radial separation of the two particles in the channel. The fission channels are defined similarly by the state of intrinsic excitation μ of the system and the channel entrances are specified by a channel deformation η_0.

In the internal region of configuration space thus defined by the totality of channel radii and deformations, eigenstates X_λ (with eigenvalues E_λ) of the system can be defined as solutions of the Schrödinger equation with appropriate boundary conditions at each channel entrance for the logarithmic derivatives of the wavefunction for motion in the channel. For consideration of fission channels an appropriate expansion of such an internal eigenfunction is in terms of product pairs of the quasi-vibrational functions $\Phi_\nu(\eta)$ and the intrinsic functions χ_μ defined at the channel deformation η_0. Thus

$$X^\lambda = \sum_{\nu\mu} C_{\lambda(\nu\mu)} \Phi^{(\mu)}_\nu \chi_\mu. \tag{8}$$

Here the superscript μ on the vibrational function indicates that a separate set of vibrational states can be defined for every deformation channel labelled by the intrinsic state χ_μ; this allows the imposition of a different (energy independent) boundary condition on Φ for every channel μ

$$\frac{1}{f(\eta_0)\Phi^{(\mu)}_\nu(\eta_0)} \left(\frac{\partial f \Phi^{(\mu)}_\nu}{\partial \eta} \right)_{\eta_0} = \mathscr{B}_\mu. \tag{9}$$

Here $f(\eta)$ depends on the particular choice of form for η; for $\eta \equiv L$ it is $L^{(A-1)/2}$, and for $\eta \equiv \mathscr{R}$ it is $\mathscr{R}^{(3A-1)/2}$.

The integral for products of pairs of general solutions Ψ of the Hamiltonian over the internal region can now be deduced by Green's theorem. For the usual particle channels the procedure and notation is given by Lane and Thomas (1958) with the result

$$(E_2 - E_1)\int_\tau d\tau \Psi_2^* \Psi_1 = \sum_c (V_{2c}^* D_{1c} - V_{1c} D_{2c}^*) \tag{10}$$

where

$$V_c = \left(\frac{\hbar^2}{2m_c a_c}\right)^{1/2} \int_{r_c = a_c} d\mathscr{S} \varphi_c^* \Psi \tag{10a}$$

$$D_c = \left(\frac{\hbar^2}{2m_c a_c}\right)^{1/2} \int_{r_c = a_c} d\mathscr{S} \varphi_c^* \operatorname{grad}_n (r_c \Psi) \tag{10b}$$

are the 'value' and 'derivative' quantities of the wavefunction Ψ at the entrance to channel c and $\int d\mathscr{S}$ denotes the surface integral over the internal region of configuration space.

The extension of this kind of result to the fission channels is straightforward. The extra contribution to the right-hand side of equation (10) is

$$\sum_\mu \frac{\hbar^2}{2B_\eta}\left\{ f(\eta_0)\Phi_{(2)}^{(\mu)*}(\eta_0)\left(\frac{\partial f \Phi_{(1)}^{(\mu)}}{\partial \eta}\right)_{\eta_0} - f(\eta_0)\Phi_{(1)}^{(\mu)}(\eta_0)\left(\frac{\partial f \Phi_{(2)}^{(\mu)*}}{\partial \eta}\right)_{\eta_0}\right\} \tag{11}$$

where we use the expansion $\Psi_n = \Sigma_\mu \Phi_{(n)}^{(\mu)} \chi_\mu$ (see Appendix).

The value and derivative quantities corresponding to equations (10*a*) and (10*b*) above are thus defined as

$$V_\mu = \left(\frac{\hbar^2}{2B_\eta f(\eta_0)}\right)^{1/2} \int_{\eta = \eta_0} d\mathscr{S} \chi_\mu^* f^{-1} \Psi \tag{11a}$$

$$D_\mu = \left(\frac{\hbar^2}{2B_\eta f(\eta_0)}\right)^{1/2} \int_{\eta = \eta_0} d\mathscr{S} \chi_\mu^* f^{-1} \frac{\partial (f\Psi)}{\partial \eta}. \tag{11b}$$

By reason of the boundary conditions (9) (and the corresponding ones for the particle channels) the orthogonality of the X_λ is established. This allows the expansion of a physical wavefunction Ψ in the internal region in terms of the X_λ, and hence, following Lane and Thomas (1958), the deduction of the R matrix relation between value and derivative quantities at the surface,

$$V_{c'} = \sum_c R_{c'c}(D_c - \mathscr{B}_c V_c). \tag{12}$$

Here the sum over channels c is generalized to include the fission channels η. The R matrix element is

$$R_{c'c} = \sum_\lambda \frac{\gamma_{\lambda(c')}\gamma_{\lambda(c)}}{E_\lambda - E}.$$

The reduced-width amplitude quantities occurring here are the value quantities of equations (10*a*) and (11*a*) applied specifically to the basis states X_λ. The deduction of the collision matrix of the system by matching of incoming and outgoing waves in the channels to the internal wavefunction through equation (12) and the logarithmic

derivatives of the outgoing waves, and hence the deduction of cross sections, are then achieved by the standard methods. The logarithmic derivatives of outgoing waves (defined as the radial solution, with asymptotic character of increasing separation, of the radial Schrödinger equation in the channel) in the particle channels have the usual notation

$$L_c = \left[\left(\frac{\rho_c}{O_c}\right)\left(\frac{\partial O_c}{\partial \rho_c}\right)\right]_{r_c=a_c} = S_c + iP_c.$$

Here ρ_c is the product of wavenumber k_c in the channel and radial separation r_c, and S_c and P_c, the shift and penetration factors, are both real quantities. The corresponding quantities for the fission channels are defined as

$$L_\mu = \left[\frac{1}{f\Phi^{(\mu)}}\frac{\partial(f\Phi^{(\mu)})}{\partial \eta}\right]_{\eta=\eta_0} = S_\mu + iP_\mu \tag{13}$$

the wavefunctions $\Phi^{(\mu)}$ being the (outgoing-type) solutions of

$$H_\eta \Phi^{(\mu)} = (E - \mathscr{E}_\mu)\Phi^{(\mu)} \tag{14}$$

beyond the channel deformation η_0. The relationship between the collision matrix $\mathbf{U}$ and the R matrix deduced from matching is

$$\mathbf{U} = \boldsymbol{\Omega}\mathbf{P}^{1/2}\{1 - \mathbf{R}(\mathbf{L} - \boldsymbol{\mathscr{B}})\}^{-1}\{1 - \mathbf{R}(\mathbf{L}^* - \boldsymbol{\mathscr{B}})\}\mathbf{P}^{-1/2}\boldsymbol{\Omega}. \tag{15}$$

The elements of the diagonal matrix $\boldsymbol{\Omega}$ are the ratios of incoming wave to outgoing wave (I_c/O_c) evaluated at $r_c = a_c$. The total cross sections for particular processes bear the well known relation to the collision matrix,

$$\sigma_{ab} = \pi \lambda\!\!\!^{-2}_a g_J |\delta_{ab} - U_{ab}|^2. \tag{16}$$

The collision matrix can also be expressed as a function of a reciprocal level matrix $\mathbf{A}$ that incorporates the properties of the R matrix states X_λ,

$$U_{ab} = \Omega_a \Omega_b \left(\delta_{ab} + 2iP_a^{1/2} \sum_{\lambda\lambda'} \gamma_{\lambda(a)}\gamma_{\lambda'(b)} A_{\lambda\lambda'} P_b^{1/2}\right).$$

The matrix $\mathbf{A}$ is the inverse of the level matrix $\mathbf{C}$, which has elements

$$\begin{aligned} C_{\lambda\lambda'} &= (E_\lambda - E)\delta_{\lambda\lambda'} - \sum_c (L_c - \mathscr{B}_c)\gamma_{\lambda(c)}\gamma_{\lambda(c')} \\ &= (E_\lambda - E)\delta_{\lambda\lambda'} - \Delta_{\lambda\lambda'} + \tfrac{1}{2}i\Gamma_{\lambda\lambda'}. \end{aligned} \tag{17a}$$

The level shift and width quantities introduced in the last equation are

$$\Delta_{\lambda\lambda'} = \sum_c (S_c - \mathscr{B}_c)\gamma_{\lambda(c)}\gamma_{\lambda(c')} \tag{17b}$$

$$\Gamma_{\lambda\lambda'} = 2\sum_c P_c \gamma_{\lambda(c)}\gamma_{\lambda(c')} \tag{17c}$$

and in the narrow level approximation, for which all such quantities must be less than the level spacings, the diagonal quantities Γ_λ and Δ_λ give the widths and positions of the resonances that appear in the cross section,

$$\sigma_{ab} \sim \pi \lambda\!\!\!^{-2}_a g_J \sum_\lambda \frac{\Gamma_{\lambda(a)}\Gamma_{\lambda(b)}}{(E_\lambda - \Delta_\lambda - E)^2 + \frac{1}{4}\Gamma_\lambda^2} \tag{18}$$

the partial widths being $\Gamma_{\lambda(c)} = 2P_c\gamma^2_{\lambda(c)}$.

The collision matrix may also be expanded about its poles $E_l^{(H)} - \frac{1}{2}i\Gamma_l^{(H)}$ in the complex energy plane,

$$U_{ab} = \delta_{ab} + \mathscr{P}_a\mathscr{P}_b\left(Q_{ab} - i\sum_l \frac{G_{l(a)}G_{l(b)}\exp\{i(\xi_{l(a)}+\xi_{l(b)})\}}{|\mathscr{P}_a(E_l)\mathscr{P}_b(E_l)|(E-E_l^{(H)}+\frac{1}{2}i\Gamma_l^{(H)})}\right) \tag{19}$$

where $\mathscr{P}_a$, $\mathscr{P}_b$ are threshold factors, $G_{l(a)}$, $G_{l(b)}$ are partial width amplitudes and $\xi_{l(a)}$, $\xi_{l(b)}$ are associated phase factors. The numerator of each term in the sum of equation (19) is the residue of the pole at $E_l^{(H)} - \frac{1}{2}i\Gamma_l^{(H)}$.

In the narrow-level approximation there is an obvious relation between these poles and the R matrix parameters, that is, $E_l^{(H)} \sim E_\lambda - \Delta_\lambda$, $\Gamma_l^{(H)} \sim \Gamma_\lambda$, $G_{l(a)}^2 \sim \Gamma_{\lambda(a)}$ and $\xi_{l(a)} \sim n\pi$.

When the narrow level approximation is not valid there is no such simple correspondence between the poles and the R matrix parameters. Diagonalization of the level matrix **C** is necessary to determine these poles and hence the resonance properties in the cross section.

4. Specialization of the reaction theory to the double-humped fission barrier

Further development of the reaction theory requires the input of physical models. In the case of a fission barrier with a single maximum, like the liquid-drop barrier, the development can only be of a quantitative kind, giving the values of the reduced widths and derivatives of the internal eigenstates and the detailed energy dependence of the shift and penetration factors. The Strutinsky theory of a double-humped barrier allows further development of a more qualitative kind however. The emphasis in this development can be placed either on classification of the properties of the internal states (as in §§ 4.1 and 4.2 below), or on dispersion characteristics of the shift and penetration factors (as in § 4.3).

4.1. Properties of the internal (R matrix) states in the presence of a double-well deformation potential

4.1.1. 'Vibrational' states of the double well. The nature of the eigensolutions of $H_\eta = T_\eta - V(\eta)$ (equation (6*a*)) for the case in which V has the Strutinsky double-well behaviour is considered first. Qualitatively, it is anticipated that for eigenvalues ϵ_ν below the intermediate barrier of the two wells (at η_A in figure 1), the eigenfunctions Φ_ν will fall into one of two classes; class I eigensolutions will be those with predominant amplitude in the well corresponding to lower deformation, and class II solutions are those of opposite behaviour. The class of vibrational state will be denoted by use of a superscript Roman numeral on Φ, or a subscript Roman numeral on the subscript ν. For their use in the description of internal states of the system they will be discrete states, boundary conditions being imposed in the region of, or beyond, the outer barrier at η_B.

The quantitative description of the class I and class II vibrational states, with particular reference to their relative amplitudes, is described elsewhere (Lynn 1968b). The characteristics of the potential have been found by analysis of fission data to be such that for energy eigenvalues one half MeV or more below the potential at η_A, the ratios of wavefunction amplitudes in the two minima are normally very different from unity and permit a marked separation of class I and class II vibrational states.

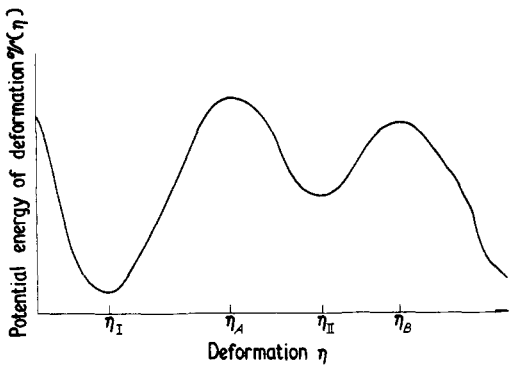

Figure 1. Schematic diagram of Strutinsky form of potential energy $\mathscr{V}$ of deformation.

4.1.2. The internal compound states: basic treatment. The internal states X_λ can be expanded in the manner of equation (8). Substitution of this expansion into the Schrödinger equation with the Hamiltonian in the form (6) followed by multiplication by $(\Phi_{\nu'}^{(\mu')}\chi_{\mu'})^*$ and integration over the internal region, gives

$$(\epsilon_{\nu'}^{(\mu')} + \mathscr{E}_{\mu'} - E_\lambda)C_{\lambda(\nu'\mu')} + \sum_{\nu\mu} C_{\lambda(\nu\mu)}\langle\Phi_{\nu'}^{(\mu')}\chi_{\mu'}|H_c|\Phi_\nu^{(\mu)}\chi_\mu\rangle = 0.$$

The elements of the Hamiltonian matrix that must be diagonalized to give the eigenvalues E_λ and the coefficients $C_{\lambda(\nu\mu)}$ (from the unitary transformation matrix) are therefore

$$H_{\nu'\mu',\nu\mu} = (\epsilon_{\nu'}^{(\mu')} + \mathscr{E}_{\mu'})\delta_{\nu\mu,\nu'\mu'} + \langle\Phi_{\nu'}^{(\mu')}\chi_{\mu'}|H_c|\Phi_\nu^{(\mu)}\chi_\mu\rangle.$$

The Hamiltonian matrix **H** can be partitioned into four submatrices that classify the elements of **H** according to the class of the vibrational states specified in these elements. Thus, the submatrix $\mathbf{H}_{I,I}$ has elements

$$H_{\nu_I'\mu',\nu_I\mu} = (\epsilon_{\nu_I'}^{(\mu')} + \mathscr{E}_{\mu'})\delta_{\nu_I\mu,\nu_I'\mu'} + \langle\Phi_{\nu_I'}^{(\mu')}\chi_{\mu'}|H_c|\Phi_{\nu_I}^{(\mu)}\chi_\mu\rangle,$$

the elements of $H_{I,II}$ are

$$H_{\nu_I'\mu',\nu_{II}\mu} = \langle\Phi_{\nu_I'}^{(\mu')}\chi_{\mu'}|H_c|\Phi_{\nu_{II}}^{(\mu)}\chi_\mu\rangle$$

and so on. Because of the weak overlap of class I and class II vibrational functions at any given deformation η it is expected that the elements of $\mathbf{H}_{I,II}$ and $\mathbf{H}_{II,I}$ will be very small. The submatrices $\mathbf{H}_{I,I}$ and $\mathbf{H}_{II,II}$ may be separately diagonalized by transformation with the unitary matrices **S** and **T** respectively, and we can obtain

$$\mathbf{W}^{-1}\mathbf{H}\mathbf{W} = \begin{pmatrix}\mathbf{S}^{-1} & 0\\ 0 & \mathbf{T}^{-1}\end{pmatrix}\begin{pmatrix}\mathbf{H}_{I,I} & \mathbf{H}_{I,II}\\ \mathbf{H}_{II,I} & \mathbf{H}_{II,II}\end{pmatrix}\begin{pmatrix}\mathbf{S} & 0\\ 0 & \mathbf{T}\end{pmatrix} = \begin{pmatrix}\mathbf{S}^{-1}\mathbf{H}_{I,I}\mathbf{S} & \mathbf{S}^{-1}\mathbf{H}_{I,II}\mathbf{T}\\ \mathbf{T}^{-1}\mathbf{H}_{II,I}\mathbf{S} & \mathbf{T}^{-1}\mathbf{H}_{II,II}\mathbf{T}\end{pmatrix}$$

where $\mathbf{S}^{-1}\mathbf{H}_{I,I}\mathbf{S}$ and $\mathbf{T}^{-1}\mathbf{H}_{II,II}\mathbf{T}$ are diagonal with eigenvalues E_{λ_I} and $E_{\lambda_{II}}$ respectively. The corresponding eigenstates of $\mathbf{H}_{I,I}$ and $\mathbf{H}_{II,II}$ are termed respectively class I and class II internal compound states (denoted by $X_{\lambda_I}^{(I)}$, $X_{\lambda_{II}}^{(II)}$) and their expansion coefficients are given by elements of **S** and **T**:

$$X_{\lambda_I}^{(I)} = \sum_{\nu_I\mu}\langle\nu_I\mu|\lambda_I\rangle\Phi_{\nu_I}^{(\mu)}\chi_\mu = \sum_{\nu_I\mu} S_{\lambda_I(\nu_I\mu)}\Phi_{\nu_I}^{(\mu)}\chi_\mu \tag{20a}$$

$$X_{\lambda_{II}}^{(II)} = \sum_{\nu_{II}\mu}\langle\nu_{II}\mu|\lambda_{II}\rangle\Phi_{\nu_{II}}^{(\mu)}\chi_\mu = \sum_{\nu_{II}\mu} T_{\lambda_{II}(\nu_{II}\mu)}\Phi_{\nu_{II}}^{(\mu)}\chi_\mu. \tag{20b}$$

The nondiagonal submatrices have the elements,

$$(S^{-1}H_{\mathrm{I,II}}T)_{\lambda_{\mathrm{I}}\lambda_{\mathrm{II}}} = \sum_{\nu_{\mathrm{I}}\mu', \nu_{\mathrm{II}}\mu''} \langle\lambda_{\mathrm{I}}|\nu_{\mathrm{I}}\mu'\rangle\langle\nu_{\mathrm{I}}\mu'|H_c|\nu_{\mathrm{II}}\mu''\rangle\langle\nu_{\mathrm{II}}\mu''|\lambda_{\mathrm{II}}\rangle = \langle X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}}|H_c|X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}}\rangle \tag{21a}$$

$$(T^{-1}H_{\mathrm{II,I}}S)_{\lambda_{\mathrm{II}},\lambda_{\mathrm{I}}} = \langle X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}}|H_c|X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}}\rangle. \tag{21b}$$

For compound states below the intermediate barrier it is expected that the admixture of vibrational states (with large amplitude in both wells) from above the barrier will be very small. The matrix elements of equation (21) thus demonstrate the expected property that the interaction of class I and class II compound states below the barrier is very weak. Even though the matrix $\mathbf{W^{-1}HW}$ still has to be diagonalized to obtain the internal states X_λ used in reaction theory, the properties of the individual class I and class II states will be strongly localized in the ultimate cross sections.

4.1.3. Examples of the use of the class I and class II internal state description. (i) *Perturbation coupling of class I and class II states.* We normally expect, both from the qualitative features of the Strutinsky theory (an 'oscillating' shell correction superimposed on a liquid-drop barrier) and the detailed calculations, that the secondary well at larger deformations will be shallower than the first. Consequently, at a given excitation energy the density of class II states is expected to be considerably less than that of class I states. For weak enough values of the interaction matrix elements the diagonalization of the matrix $\mathbf{W^{-1}HW}$ will result, to a good approximation, in the mixing of each class II state with its immediate class I neighbours. The limiting case of very weak coupling is described by first-order perturbation theory (Lynn 1968a, b). In the neighbourhood of a given class II state there will be one state that is, in zero order, the class II state with eigenvalue

$$E_{\lambda''} \simeq E_{\lambda_{\mathrm{II}}} + \sum_{\lambda_{\mathrm{I}}} \frac{|\langle X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}}|H_c|X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}}\rangle|^2}{E_{\lambda_{\mathrm{II}}} - E_{\lambda_{\mathrm{I}}}}$$

and eigenfunction

$$X_{\lambda''} \simeq X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}} + \sum_{\lambda_{\mathrm{I}}} \frac{\langle X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}}|H_c|X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}}\rangle X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}}}{E_{\lambda_{\mathrm{II}}} - E_{\lambda_{\mathrm{I}}}}$$

while the other states have the properties

$$E_{\lambda'} \simeq E_{\lambda_{\mathrm{I}}} + \frac{|\langle X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}}|H_c|X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}}\rangle|^2}{E_{\lambda_{\mathrm{I}}} - E_{\lambda_{\mathrm{II}}}}$$

and

$$X_{\lambda'} \simeq X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}} + \frac{\langle X^{(\mathrm{I})}_{\lambda_{\mathrm{I}}}|H_c|X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}}\rangle X^{(\mathrm{II})}_{\lambda_{\mathrm{II}}}}{E_{\lambda_{\mathrm{I}}} - E_{\lambda_{\mathrm{II}}}}.$$

Second-order perturbation expansions are also quoted in the above reference as are the results for the case in which there is accidental near-degeneracy of the class II state and one of the class I states.

(ii) *Lorentzian coupling of class I and class II states.* In the more general case of coupling between a single class II state and its class I neighbours the resultant mixing is stronger than a simple perturbation; no single resultant state can be described as predominantly class II in character. The eigenfunction X_λ can be expanded thus

$$X_\lambda = \sum_{\lambda_{\mathrm{I}}} C_{\lambda(\lambda_{\mathrm{I}})} X_{\lambda_{\mathrm{I}}} + C_{\lambda(\lambda_{\mathrm{II}})} X_{\lambda_{\mathrm{II}}}$$

and the expansion coefficients and eigenvalues are obtained from the coupled equations

$$C_{\lambda(\lambda_I)}(E_{\lambda_I}-E_\lambda)+C_{\lambda(\lambda_{II})}\langle\lambda_I|H_c|\lambda_{II}\rangle = 0 \tag{22a}$$

$$\sum_{\lambda_I} C_{\lambda(\lambda_I)}\langle\lambda_{II}|H_c|\lambda_I\rangle+(E_{\lambda_{II}}-E_\lambda)C_{\lambda(\lambda_{II})} = 0 \tag{22b}$$

and the normalization condition $\Sigma_{\lambda_I}C^2_{\lambda(\lambda_I)}+C^2_{\lambda(\lambda_{II})} = 1$. The result from equation (22*a*)

$$C_{\lambda(\lambda_I)} = -\frac{\langle\lambda_I|H_c|\lambda_{II}\rangle C_{\lambda(\lambda_{II})}}{E_{\lambda_I}-E_\lambda},$$

substituted into equation (22*b*) gives the eigenvalue relation

$$\sum_{\lambda_I}\frac{|\langle\lambda_I|H_c|\lambda_{II}\rangle|^2}{E_{\lambda_I}-E_\lambda} = E_{\lambda_{II}}-E_\lambda. \tag{23}$$

Further algebraic manipulation leads to the result (Lynn 1968b)

$$C^2_{\lambda(\lambda_{II})} = \left(\sum_{\lambda_I}\frac{|\langle\lambda_I|H_c|\lambda_{II}\rangle|^2}{(E_{\lambda_I}-E_\lambda)^2}+1\right)^{-1}. \tag{24}$$

In the uniform model, in which the class I states are equally spaced at intervals D_I and have equal values H_c^2 of the squared matrix element $|\langle\lambda_I|H_c|\lambda_{II}\rangle|^2$, this can be transformed to

$$C^2_{\lambda(\lambda_{II})} = \frac{H_c^2}{(E_{\lambda_{II}}-E_\lambda)^2+(\pi^2H_c^4/D_I^2)+H_c^2}. \tag{25}$$

This is a lorentzian form with halfwidth (at half-maximum), $W_c = \sqrt{(\pi^2H_c^4/D_I^2+H_c^2)}$.

In practice the matrix elements $\langle\lambda_I|H_c|\lambda_{II}\rangle$ are far from being uniformly distributed. Hence the lorentzian profile for the admixture coefficients given by equation (25) can only be an ideal, about which the individual values will be scattered. The quantitative aspects of this distribution are discussed elsewhere (Lynn 1969, 1972). Other aspects of the detailed shape of the admixture profile can be treated by this shape-classified eigenstate method; for example, the background reduced fission width term due to the class I levels and possible interference between the lorentzian and background term are discussed in another report (Lynn 1973).

4.1.4. Discussion of the coupling matrix element. (i) *Illustration with a simple model.* Some aspects of the behaviour of H_c can be made explicit by use of the expansions (7). From these and the form of H_c as given in equation (6*c*) we can obtain

$$\langle\nu\mu|H_c|\nu'\mu'\rangle = \langle\nu|\sum_{\mu''}b_{\mu''\mu}(\eta)b^*_{\mu''\mu'}(\eta)\mathscr{E}_{\mu''}(\eta)|\nu'\rangle-\delta_{\nu\nu'}\delta_{\mu\mu'}\mathscr{E}_{\mu'}(\eta_0) \tag{26}$$

which enables us to calculate the coupling matrix elements for chosen models of the behaviour of the intrinsic states χ_μ as a function of deformation.

A very simple model that illustrates the use of equation (26) and at the same time provides some insight into aspects of H_c that may affect correlations and interference in the class II resonance behaviour of reduced widths, comprises two single-particle states with energies $\mathscr{E}'_0$, $\mathscr{E}'_1$ which depend on deformation and intersect at a given deformation η_1 (see figure 2). These Nilsson-type levels are assumed to have the same set of good quantum numbers and a residual interaction between them that is described by a matrix element v independent of deformation. The separation of $\mathscr{E}'_1$ and $\mathscr{E}'_0$ is assumed to be linear, $\mathscr{E}'_1-\mathscr{E}'_0 = |a(\eta-\eta_1)|$. The separation of the diagonalized states is therefore

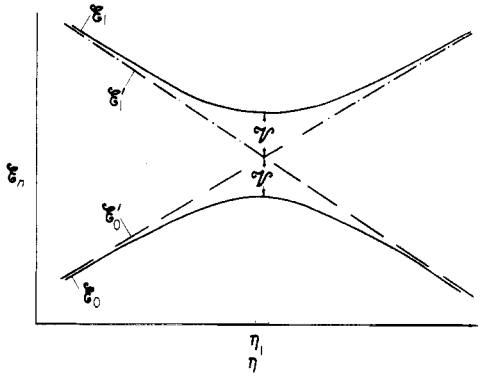

Figure 2. Schematic diagram of two intersecting Nilsson states, energies $\mathscr{E}'_0$ and $\mathscr{E}'_1$, with residual interaction (matrix element v) between them. Final state energies are $\mathscr{E}_0$ and $\mathscr{E}_1$.

$\mathscr{E}_1 - \mathscr{E}_0 = \{a^2(\eta-\eta_1)^2+4v^2\}^{1/2}$ while their eigenfunctions in terms of the single particle states at large separation ($\eta \to \infty$) are

$$\chi_0(\eta) = \frac{v}{\mathscr{D}(\eta)}\chi_0(\infty)+\frac{\mathscr{E}'_0(\eta)}{\mathscr{D}(\eta)}\chi_1(\infty) \tag{27a}$$

$$\chi_1(\eta) = -\frac{\mathscr{E}'_0(\eta)}{\mathscr{D}(\eta)}\chi_0(\infty)+\frac{v}{\mathscr{D}(\eta)}\chi_1(\infty) \tag{27b}$$

(where $\mathscr{D}(\eta) = (\mathscr{E}'^2_0+v^2)^{1/2}$ and $\mathscr{E}'_0 = 0{\cdot}5[\{a^2(\eta-\eta_1)^2+4v^2\}^{1/2}-\{a^2(\eta-\eta_1)^2\}^{1/2}]$) for $\eta \geqslant \eta_1$. For $\eta < \eta_1$ the right-hand sides of equations (27*a* and *b*) are interchanged. From these equations the overlap coefficients b, and hence the coupling matrix elements, are easily calculated.

Examples of the matrix elements are shown in figure 3 for a few different conditions. The matrix element $\langle\chi_1(\eta_0)|H_c|\chi_0(\eta_0)\rangle$ and the combination

$$\Delta E = \mathscr{E}_1+\langle\chi_1(\eta_0)|H_c|\chi_1(\eta_0)\rangle-\langle\chi_0(\eta_0)|H_c|\chi_0(\eta_0)\rangle$$

are shown for $v = 0{\cdot}1$, $a = 1{\cdot}0$, $\eta_1 = 0{\cdot}3$ and $\eta_0 = 0{\cdot}3$, $0{\cdot}6$ and $3{\cdot}0$. As an illustration of the implications of these consider the second example. Suppose that the lowest vibrational wavefunction is centred about $\eta = 0$ and is narrowly confined to this region so that $\langle\Phi_0\chi_1|H_c|\Phi_0\chi_0\rangle \simeq -0{\cdot}17$ and $\langle\Phi_0|\Delta E|\Phi_0\rangle \simeq -0{\cdot}14$. Diagonalization of just the states $\Phi_0\chi_0$ and $\Phi_0\chi_1$ yields an eigenvalue separation for the eigenstates Ψ_0 and Ψ_1 of $0{\cdot}35$ and expansion coefficients $T^2_{0(00)} = 0{\cdot}3$, $T^2_{0(01)} = 0{\cdot}7$ for the lower state. The implication of these numbers is that there is a degree of mismatch between the ground state of this simple system with zero-point vibration about $\eta = 0$ and the lowest 'channel state' at η_0 ; the fission-reduced width of the ground state through the lowest channel is not the value $(\hbar^2/2Bf(\eta_0))\Phi^{(0)2}_0(\eta_0)$ that might be expected intuitively, but the smaller value $(\hbar^2/2Bf(\eta_0))T^2_{0(00)}\Phi^{(0)2}_0(\eta_0)$. This model has obvious qualitative relevance to the problem of the relative spontaneous fission halflives of neighbouring odd, odd-mass and even nuclei.

This illustration can be extended with the assumption of an intermediate barrier at, say, $\eta = -0{\cdot}6$ and no more level crossings in the region $\eta = -0{\cdot}6$ to $\eta = 0$. If the eigenstates at $\eta = 0$ are expanded in terms of basic intrinsic states set up at $\eta = -0{\cdot}6$, the new expansion coefficients are $T^2_{0(00)} = 0{\cdot}966$, $T^2_{0(01)} = 0{\cdot}034$. These can be taken as a

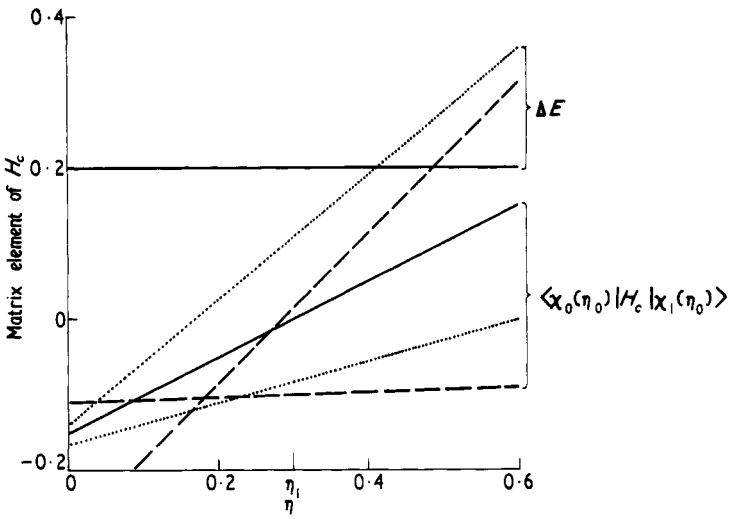

Figure 3. Calculated behaviour of energy difference

$\Delta E = \mathscr{E}_1 + \langle\chi_1(\eta_0)|H_c|\chi_1(\eta_0)\rangle - \langle\chi_0(\eta_0)|H_c|\chi_0(\eta_0)\rangle$

and matrix element of interaction $\langle\chi_1(\eta_0)|H_c|\chi_0(\eta_0)\rangle$ as function of deformation for $a = 1{\cdot}0$, $v = 0{\cdot}1$. Basis states χ for these curves are taken at $\eta_0 = 0{\cdot}3$ (full curves), $\eta_0 = 0{\cdot}6$ (dotted curves), $\eta_0 = 3{\cdot}0$ (broken curves).

measure of coupling into class I states at still lower values of η; it is obvious that the coupling through the lowest 'channel state' at η_A is not correlated with the fission width through the lowest channel at η_0. A more explicit calculation of the coupling matrix elements can be made with the introduction schematically of a class I and class II vibrational state, the wavefunctions of which are confined closely around $\eta_I = -1{\cdot}2$ and $\eta_{II} = 0$. The amplitudes of the tails of these functions in the opposite well are denoted as $c \times$ (amplitude of opposite class vibrational state). The coupling matrix elements can be expanded thus,

$$\langle\Phi_{\nu_I}\chi_n|H_c|\Psi_m\rangle = \langle\Phi_{\nu_I}\chi_n|H_c|\Phi_{\nu_{II}}\chi_0\rangle T_{m(\nu_{II}0)} + \langle\Phi_{\nu_I}\chi_n|H_c|\Phi_{\nu_{II}}\chi_1\rangle T_{m(\nu_{II}1)}.$$

Using values of $\langle\chi_0|H_c|\chi_0\rangle \simeq 1{\cdot}3$, $\langle\chi_0|H_c|\chi_1\rangle \simeq -0{\cdot}5$ and $\langle\chi_1|H_c|\chi_1\rangle \simeq -1{\cdot}3$, which are appropriate for the centre of the class I region ($\eta \simeq -1{\cdot}2$) in our model, we find that

$$\langle\Phi_{\nu_I}\chi_0|H_c|\Psi_0\rangle \simeq -0{\cdot}27c \quad \text{and} \quad \langle\Phi_{\nu_I}\chi_0|H_c|\Psi_1\rangle \simeq -1{\cdot}2c.$$

(ii) *Useful expressions for the coupling matrix element.* For the purpose of deriving estimates of the coupling matrix elements, the deformation η_0 at which the basic intrinsic states χ_μ are defined, is chosen to be at the intermediate barrier η_A. The region of deformation lower than this is called region I while region II comprises deformations greater than η_A, and partial matrix elements confined to integration over a particular region of η are denoted by a subscript. The matrix element is now split as follows:

$$\begin{aligned}\langle\lambda_I|H_c|\lambda_{II}\rangle &= \langle\lambda_I|H_c|\lambda_{II}\rangle_{\text{region I}} + \langle\lambda_I|H_c|\lambda_{II}\rangle_{\text{region II}} \\ &= \sum_{\nu_{II}\mu''} \langle\lambda_I|H_c|\nu_{II}\mu''\rangle_{\text{region I}} T_{\lambda_{II}(\nu_{II}\mu'')} + \sum_{\nu_I\mu'} S_{\lambda_I(\nu_I\mu')}\langle\nu_I\mu'|H_c|\lambda_{II}\rangle_{\text{region II}} \\ &\simeq \sum_{\nu_{II}\mu''} \langle\lambda_I|H_c|\nu_I\mu''\rangle_{\text{region I}} c_{\nu_{II}(\nu_I)} T_{\lambda_{II}(\nu_{II}\mu'')} + \sum_{\nu_I\mu'} S_{\lambda_I(\nu_I\mu')} c_{\nu_I(\nu_{II})}\langle\nu_{II}\mu'|H_c|\lambda_{II}\rangle_{\text{region II}}\end{aligned}$$

in which we write the vibrational wavefunction $\Phi_{\nu_{II}}$ in region I as $c_{\nu_{II}(\nu_I)}\Phi_{\nu_I}$, the state Φ_{ν_I} being that one closest to $\Phi_{\nu_{II}}$ in energy, and similarly for Φ_{ν_I} in region II. The coefficients T, S can now be written as lorentzian-type functions (equation (25)) with damping halfwidths $W_{\nu_{II}\mu'',\lambda_{II}}$, $W_{\nu_I\mu',\lambda_I}$ of modes $\nu\mu$ into the class II and class I states respectively, while the quantities $\langle\lambda_I|H_c|\nu_I\mu''\rangle$, $\langle\nu_{II}\mu'|H_c|\lambda_{II}\rangle$ can be expressed in terms of the damping halfwidths $W_{\nu_I\mu'',\lambda_I}$, $W_{\nu_{II}\mu',\lambda_{II}}$. The final expression for the expectation value of $\langle\lambda_I|H_c|\lambda_{II}\rangle^2$ is

$$\mathrm{Exp}(\langle\lambda_I|H_c|\lambda_{II}\rangle^2) \simeq \sum_{\nu_{II}\mu''} c^2_{\nu_{II}(\nu_I)} \frac{D_I W_{\nu_I\mu'',\lambda_I}}{\pi^2} \frac{D_{II} W_{\nu_{II}\mu'',\lambda_{II}}}{(E_{\lambda_{II}} - E_{\nu_{II}\mu''})^2 + W^2_{\nu_{II}\mu'',\lambda_{II}}}$$

$$+ \sum_{\nu_I\mu'} c^2_{\nu_I(\nu_{II})} \frac{D_{II} W_{\nu_{II}\mu',\lambda_{II}}}{\pi^2} \frac{D_I W_{\nu_I\mu',\lambda_I}}{(E_{\lambda_I} - E_{\nu_I\mu})^2 + W^2_{\nu_I\mu,\lambda_I}}.$$

In sub-barrier fission only one significant term (with ν high and μ low) is expected in each of the sums. On average, the second term is expected to be smaller than the first because the lower excitation energy for intrinsic states in the secondary well implies that the damping halfwidth $W_{\nu_{II}\mu',\lambda_{II}}$ is considerably lower than $W_{\nu_I\mu'',\lambda_I}$. The expression thus demonstrates the existence of vibrational resonance structure in the coupling elements. The energy averaged value of the coupling is (assuming $2W_{\nu_I\mu'',\lambda_I} \simeq \hbar\omega_I$)

$$\overline{\langle\lambda_I|H_c|\lambda_{II}\rangle^2} \simeq \frac{c^2_{\nu_{II}(\nu_I)} D_I D_{II}}{2\pi}. \tag{28}$$

The coefficient $c_{\nu_{II}(\nu_I)}$ can be calculated numerically, given the potential and inertial parameters of the intermediate barrier.

4.2. Cross section properties for double-humped fission barrier

In the above the channel deformation η_c has been assumed to be at or close to the outer barrier η_B. For deformations beyond η_B and up to the scission point, a range of deformation formally included in the channel, it is certain that strong nuclear interactions will operate and mix the wavefunctions formally defined above as separate fission channels. However, since it is the sum of cross sections over all the channels that lead to fission that is being sought at this stage, this mixing is only important insofar as it affects the effective shift and penetration factors at the channel boundaries. The detailed way in which these are affected can be discussed by using an extension of the methods described in § 4.3.

In this paper we are mainly concerned with sub-barrier fission. Hence, only one formal channel for a particular intrinsic state χ_μ defined at η_B will normally be important: this is the state of lowest energy appropriate to the total angular momentum and parity quantum numbers (and any other quantum numbers that may happen to be good) of the compound nucleus. The discussion will therefore be conducted for one such fission channel; it can be generalized to more than one channel by simply summing the cross sections obtained for each.

4.2.1. Narrow class II states. When the total widths associated with the class II R matrix states (as well as the class I states) are small, by which is meant in a general sense that they are less than the spacings among all coupled R matrix states, there is no difficulty in calculating or interpreting the cross section to be expected. A resonance will be associated with each coupled R matrix state, and the resonance parameters (in

the single-level approximation) will be simply related to the parameters of that R matrix state by equations (17*a*), (17*b*) and (18).

4.2.2. Broad class II states. The single-level shapes described above become very distorted when the total widths associated with the R matrix states approach the level spacings, and if the total widths exceed the spacings the cross section pattern bears no easily recognizable relation to the R matrix parameters.

The simplest case to treat in this last category is the one in which a class I and class II state are accidentally degenerate and their widths are greater than the spacing of the final eigenvalues (Lynn 1968a, b). Of more importance is the case in which the fission width of the class II state overlaps many class I states. When the coupling between the class II and class I states is very weak a method for treating this case has already been given (Lynn 1968b).

For rather stronger coupling a perturbation treatment involving continuum states can be made. From R matrix theory an expression for the internal wavefunction of the nucleus in the presence of unit incoming flux in only one entrance channel e can be obtained (Lane and Thomas 1958):

$$\Psi^{(e)}(E) = -\mathrm{i}\hbar^{1/2}\,\mathrm{e}^{-\mathrm{i}\phi_e}\sum_{\lambda\lambda'} A_{\lambda\lambda'}\Gamma^{1/2}_{\lambda(e)}X_{\lambda'} \tag{29}$$

in which the matrix $\mathbf{A}$ is the reciprocal level matrix of equation (17). Equation (29) can be applied to either class I or class II eigenstates, X^{I}_{λ} or $X^{\mathrm{II}}_{\lambda}$, for all the quantities on the right-hand side, to give the zero-order wavefunctions $\Psi^{\mathrm{I}(e)}(E)$, $\Psi^{\mathrm{II}(e')}(E')$ in the absence of coupling between class I and class II states. For the perturbation treatment the channel e of the class I function is specialized to the neutron channel n while channel (e') in the class II function is specialized to the fission channel μ. At the same time the complex conjugate of the latter wavefunction is used; this corresponds to the internal wavefunction when there is an outgoing wave in only the fission channel. These wavefunctions can be made discrete though dense by containing them in boxes (with specific boundary conditions) of very large dimension. These dimensions are a_n for the neutron channel and η_μ for the fission channel. The normalization factors are $v_n^{1/2}/a_n^{1/2}$ for the class I wavefunction and $v_\mu^{1/2}/a_\mu$ for the class II wavefunction, v_n and v_μ being the relative velocities associated with the (asymptotic) waves in the neutron and fission channels. The densities of class I and class II states thus defined are $a_n/v_n h$ and $\eta_\mu/v_\mu h$ respectively. By perturbation theory the first-order approximation to the actual wavefunction can be either

$$\Psi^{(n)}(E) \simeq \Psi^{\mathrm{I}(n)}(E) + \frac{\eta_\mu}{v_\mu h}\int \mathrm{d}E'\,\frac{v_\mu^{1/2}}{\eta_\mu^{1/2}}\,\frac{\langle\Psi^{\mathrm{II}(\mu)\dagger}(E')|H_{\mathrm{int}}|\Psi^{\mathrm{I}(n)}(E)\rangle}{E-E'}\,\frac{v_\mu^{1/2}}{\eta_\mu^{1/2}}\Psi^{\mathrm{II}(\mu)\dagger}(E') \tag{30}$$

or $\Psi^{(\mu)}(E)$ written in a perfectly analogous way. The matrix element here is

$$\langle\Psi^{\mathrm{II}(\mu)\dagger}|H_{\mathrm{int}}|\Psi^{\mathrm{I}(n)}\rangle = -\hbar\exp\{-\mathrm{i}(\phi_n+\phi_\mu)\}\sum_{\lambda_{\mathrm{II}}\lambda'_{\mathrm{II}}} A_{\lambda_{\mathrm{II}}\lambda'_{\mathrm{II}}}\Gamma^{1/2}_{\lambda_{\mathrm{II}}(\mu)}\sum_{\lambda_{\mathrm{I}}\lambda'_{\mathrm{I}}} A_{\lambda_{\mathrm{I}}\lambda'_{\mathrm{I}}}\Gamma^{1/2}_{\lambda_{\mathrm{I}}(n)}\langle X_{\lambda'_{\mathrm{II}}}|H_{\mathrm{int}}|X_{\lambda'_{\mathrm{I}}}\rangle.$$

If a pole expansion (as in equation (19)) is applied to

$$\exp(-\mathrm{i}\phi_\mu)\sum_{\lambda_{\mathrm{II}}\lambda'_{\mathrm{II}}} A_{\lambda_{\mathrm{II}}\lambda'_{\mathrm{II}}}\Gamma^{1/2}_{\lambda_{\mathrm{II}}(\mu)}X_{\lambda'_{\mathrm{II}}},$$

the contour integration of equation (30) can be performed. When the levels are well

separated, in the neighbourhood of any one of them we obtain

$$\Psi^{(n)}(E) \simeq \Psi^{\mathrm{I}(n)}(E) + \mathrm{i}\hbar^{1/2} \exp(-\mathrm{i}\phi_n) \sum_{\lambda_\mathrm{I}\lambda_\mathrm{i}} A_{\lambda_\mathrm{I}\lambda_\mathrm{i}} \Gamma^{1/2}_{\lambda_\mathrm{I}(n)} \frac{\langle X_{\lambda_\mathrm{II}} | H_{\mathrm{int}} | X_{\lambda_\mathrm{i}} \rangle X_{\lambda_\mathrm{II}}}{E_{\lambda_\mathrm{II}} - E + \frac{1}{2}\mathrm{i}\Gamma_{\lambda_\mathrm{II}}}$$

and is valid if $|\langle X_{\lambda_\mathrm{II}} | H_{\mathrm{int}} | X_{\lambda_\mathrm{i}} \rangle| \ll \frac{1}{2}\Gamma_{\lambda_\mathrm{II}}$. This wavefunction can be written in just the form (29) for levels λ_I, provided that the basis wavefunctions X_λ are taken to be

$$X_\lambda \simeq X_{\lambda_\mathrm{I}} - \frac{\langle X_{\lambda_\mathrm{II}} | H_{\mathrm{int}} | X_{\lambda_\mathrm{I}} \rangle X_{\lambda_\mathrm{II}}}{E_{\lambda_\mathrm{II}} - E_{\lambda_\mathrm{I}} + \frac{1}{2}\mathrm{i}\Gamma_{\lambda_\mathrm{II}}}.$$

Thus, for narrow resonances, fission widths $\Gamma_{\lambda(\mu)}$ are introduced; the fission width amplitudes are

$$\Gamma^{1/2}_{\lambda(\mu)} \simeq -\frac{\langle X_{\lambda_\mathrm{II}} | H_{\mathrm{int}} | X_{\lambda_\mathrm{I}} \rangle \Gamma^{1/2}_{\lambda_\mathrm{II}(\mu)}}{E_{\lambda_\mathrm{II}} - E_{\lambda_\mathrm{I}} + \frac{1}{2}\mathrm{i}\Gamma_{\lambda_\mathrm{II}}}. \tag{31}$$

Similarly, the first-order form for $\Psi^{(\mu)}$ turns out to be

$$\Psi^{(\mu)}(E) = \Psi^{\mathrm{II}(\mu)}(E) - \hbar^{1/2}\, \mathrm{e}^{-\mathrm{i}\phi_\mu} \frac{\Gamma^{1/2}_{\lambda_\mathrm{II}(\mu)}}{E_{\lambda_\mathrm{II}} - E - \frac{1}{2}\mathrm{i}\Gamma_{\lambda_\mathrm{II}}} \sum_{\lambda_\mathrm{I}\lambda_\mathrm{i}} \frac{\Gamma^{1/2}_{\lambda_\mathrm{I}(n)} \langle X_{\lambda_\mathrm{II}} | H_{\mathrm{int}} | X_{\lambda_\mathrm{I}} \rangle}{E_{\lambda_\mathrm{i}} - E + \frac{1}{2}\mathrm{i}\Gamma_{\lambda_\mathrm{i}}}$$
$$\times \frac{\Gamma^{1/2}_{\lambda_\mathrm{i}(n)} X_{\lambda_\mathrm{i}}}{E_{\lambda_\mathrm{i}} - E_{\lambda_\mathrm{I}} + \frac{1}{2}\mathrm{i}(\Gamma_{\lambda_\mathrm{I}} + \Gamma_{\lambda_\mathrm{i}})}$$

for non-interfering class I levels. Here the expression is written for only one channel (n) of the class I states but can obviously be extended to others. This form corresponds to a very broad resonance in the cross section with fission width essentially $\Gamma_{\lambda_\mathrm{II}(\mu)}$ and neutron width amplitude given by

$$\Gamma^{1/2}_{(n)} \simeq -\sum_{\lambda_\mathrm{I}} \frac{\langle X_{\lambda_\mathrm{II}} | H_{\mathrm{int}} | X_{\lambda_\mathrm{I}} \rangle \Gamma^{1/2}_{\lambda_\mathrm{I}(n)}}{E_{\lambda_\mathrm{I}} - E_{\lambda_\mathrm{II}} + \frac{1}{2}\mathrm{i}(\Gamma_{\lambda_\mathrm{II}} + \Gamma_{\lambda_\mathrm{I}})}. \tag{32}$$

Strictly speaking the width amplitudes of equations (31) and (32), being complex, should be interpreted as the partial width and phase amplitudes $G_{l'(\mu)} \exp(\mathrm{i}\xi_{l'(\mu)})$ and $G_{l''(n)} \exp(\mathrm{i}\xi_{l''(n)})$ of the S matrix pole expansion in equation (19).

4.3. The extended penetration factor: channel dispersion effects

In circumstances in which the widths of R matrix states are greater than their spacings, the S matrix poles and hence the cross section resonances bear no simple relation to the R matrix parameters. In addition, the matrix element of the coupling term in the Hamiltonian, which plays a central role in the theory presented above, is often a very difficult quantity to survey; this particularly applies to its energy variation, and to obtain in cross sections the long-range energy variation expected by physical intuition it is often required to include 'distant levels' in the formal expressions. It can be more convenient in these circumstances to define the internal and channel regions in such a way that the physical content of the situation is carried more by the shift and penetration factors. This idea is often utilized in a crude way for the case of 'pure vibrational resonances'—zero damping in the secondary well; a transmission coefficient is calculated for a wave traversing the entire double-humped barrier, and this is used loosely as the penetration factor. In this section we examine this method more closely, beginning with just this 'zero-damping' case.

4.3.1. Zero damping in the secondary well. (i) *Construction of logarithmic derivative.* If no damping of the vibrational wavefunctions in the secondary-well region is assumed, it is very simple to introduce the extended penetration and shift factor method. The channel deformation parameter η_c is chosen at a smaller deformation than the intermediate barrier at η_A. The internal states for the R matrix are introduced with a real energy-independent boundary condition $\mathscr{B}_\mu$ for each channel labelled by an intrinsic state χ_μ at η_c. There is now no question of classifying the vibrational states within the internal region. Outgoing wavefunctions satisfying equation (14) are now calculated right through the secondary-well region and their logarithmic derivatives are calculated at η_c to give the shift and penetration factors as defined in equation (13).

(ii) *Numerical examples for rectangular barriers.* The shift and penetration factors are easily computed in the case of a barrier composed of constant sections as in figure 4.

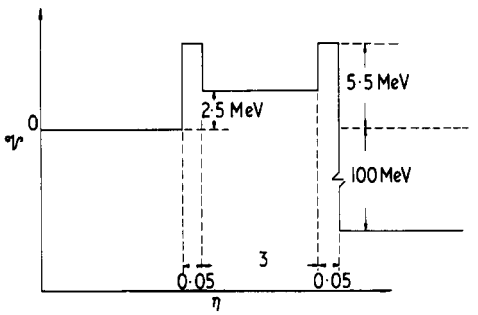

Figure 4. Double-humped barrier with rectangular elements used for calculating results of figures 5 and 6. The mass parameter employed here is $B = 4{\cdot}065 \times 10^{-46}$ g cm^2.

The outgoing wave in the final region η_3 to ∞ has the form $\exp(ik_0\eta)$. In the other regions it is $c_n \exp(ik_n\eta) + b_n \exp(-ik_n\eta)$ or $c_n \exp(-\kappa_n\eta) + b_n \exp(\kappa_n\eta)$ depending on the sign of $E - \mathscr{E}_\mu - \mathscr{V}(\eta)$. From the matching of these waveforms and the values of the (complex) coefficients c_0, b_0 at η_c the logarithmic derivative of the outgoing wave $\Phi^{(\mu)}$ can be obtained. In addition, the transmission coefficient, $T = 1 - 1/|c_4|^2$, of a wave with kinetic energy $E - \mathscr{E}_0 - \mathscr{V}_0$ proceeding from $\eta = -\infty$ to $\eta = +\infty$, can be obtained.

An overall plot of the transmission coefficient as a function of energy for a barrier with parameters that are of the order of magnitude of those expected in actinide fission is shown in figure 5. It is well known that such a plot shows peaks, the vibrational resonances, that correspond closely to the positions of eigenstates in the secondary well of the barrier. It is commonly assumed in the phenomenological theory of fission that the fission strength function is simply proportional to this transmission coefficient, $\Gamma_{(\mu)}/\bar{D} = T/2\pi$.

Close to the positions of the vibrational resonances in the transmission coefficient the shift and penetration factors undergo anomalies. These are shown for just one vibrational resonance in figure 6.

4.3.2. Interpretation of shift and penetration factor behaviour. (i) *One-dimensional case.* The behaviour of the shift and penetration factors as shown in figure 6 can be discussed within the framework of an extended version of R matrix theory. This is confined first to the one-dimensional case in which we consider only the deformation degree of freedom. This potential energy $\mathscr{V}$ is shown schematically in figure 1, and now two channel

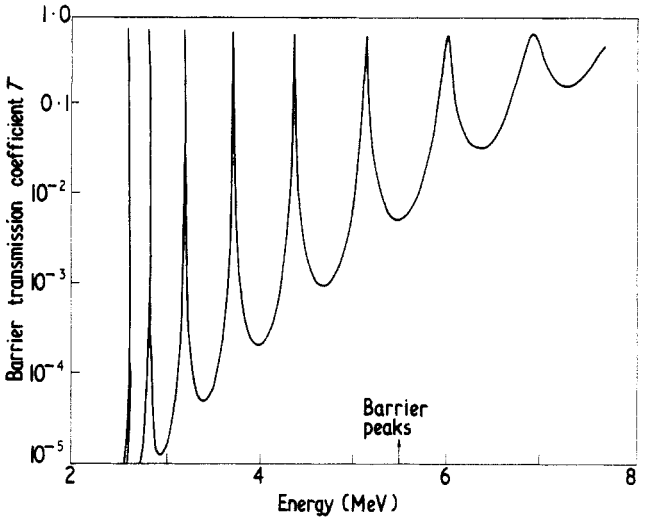

Figure 5. Transmission coefficient through barrier of figure 4.

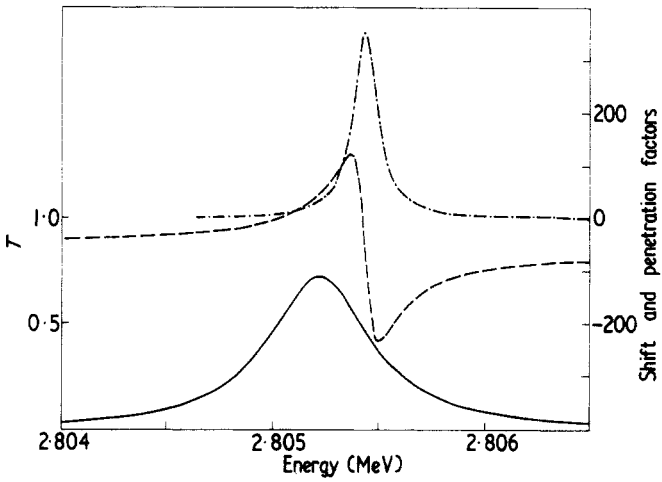

Figure 6. Transmission coefficient (full curve) over a single vibrational resonance at 2·805 MeV in figure 5 and corresponding shift (chain curve) and penetration (broken curve) factors.

deformation parameters η_c and η_d are chosen, one in the region of each potential energy maximum. Solutions of the Schrödinger equation (equation (6*a*)) are now found with a boundary condition that is real and energy independent at the inner boundary η_c, and at η_d is equal to the logarithmic derivative of the outgoing wave proceeding beyond η_d with chosen energy ϵ:

$$(T_\eta + \mathscr{V}(\eta))\Phi_\nu = \epsilon_\nu \Phi_\nu \tag{33}$$

$$\frac{1}{f(\eta_c)\Phi_\nu(\eta_c)}\left(\frac{\partial f \Phi_\nu}{\partial \eta}\right)_{\eta_c} = \mathscr{B} \tag{34}$$

$$\frac{1}{f(\eta_d)\Phi_\nu(\eta_d)}\left(\frac{\partial f \Phi_\nu}{\partial \eta}\right)_{\eta_d} = S(\eta_d) + iP(\eta_d).$$

The eigenvalues ϵ_ν are complex (as in the theory of Kapur and Peierls 1938). The Green's theorem relation for the eigenfunctions Φ in the intermediate region η_c to η_d is just

$$(\epsilon_2-\epsilon_1)\int_{\eta_c}^{\eta_d} d\eta\Phi_2\Phi_1 = \frac{\hbar^2}{2B_\eta}\left\{f(\eta_d)\Phi_2(\eta_d)\left(\frac{\partial f\Phi_1}{\partial\eta}\right)_{\eta_d} - f(\eta_d)\Phi_1(\eta_d)\left(\frac{\partial f\Phi_2}{\partial\eta}\right)_{\eta_d}\right.$$
$$\left. - f(\eta_c)\Phi_2(\eta_c)\left(\frac{\partial f\Phi_1}{\partial\eta}\right)_{\eta_c} + f(\eta_c)\Phi_1(\eta_c)\left(\frac{\partial f\Phi_2}{\partial\eta}\right)_{\eta_c}\right\}. \tag{35}$$

This establishes orthogonality for the solutions of equations (33) and (34). Expansions of solutions (between η_c and η_d) of the Schrödinger equation at real energy ϵ are made in terms of these (complex) intermediate states Φ_ν, $\Phi_\epsilon(\eta) = \Sigma_\nu A_\nu\Phi_\nu(\eta)$, the coefficients in which are $A_\nu = \int_{\eta_c}^{\eta_d}\Phi_\nu\Phi_\epsilon\, d\eta$. By means of equations (35) and (34) this leads to a relationship for the logarithmic derivative of Φ_ϵ at η_c,

$$\frac{1}{f\Phi_\epsilon(\eta_c)}\left(\frac{\partial f\Phi_\epsilon}{\partial\eta}\right)_{\eta_c} \equiv S(\eta_c)+iP(\eta_c) = \mathscr{B} - \left(\sum_\nu \frac{\gamma_\nu^2(\eta_c)}{\epsilon_\nu-\epsilon}\right)^{-1}.$$

If the intermediate eigenstates ν are to have reasonably uniform properties the poles of this expression for the logarithmic derivative must be located approximately midway between the eigenvalues ϵ_ν. In a uniform model for the eigenstates ν, the poles occur at energies $\epsilon_n \simeq \frac{1}{2}(\epsilon_\nu+\epsilon_{\nu+1})$ and their residues are $D_\nu^2/\pi^2\gamma_\nu^2(\eta_c)$. The imaginary component w_n of the pole ϵ_n is just the mean of that of the eigenvalues ϵ_ν and $\epsilon_{\nu+1}$. Because of the Kapur–Peierls type of boundary condition imposed at η_d it follows that this is just the halfwidth for decay of an intermediate state at energy ϵ through the outer barrier B. In the region of the pole $\epsilon_n = e_n - iw_n$ the logarithmic derivative at η_c thus has the form

$$S+iP \simeq \mathscr{B} + \frac{D_\nu^2}{\pi^2\gamma_\nu^2(\eta_c)}\frac{(e_n-\epsilon)}{(e_n-\epsilon)^2+w_n^2} + i\frac{D_\nu^2}{\pi^2\gamma_\nu^2(\eta_c)}\frac{w_n}{(e_n-\epsilon)^2+w_n^2} \tag{36}$$

the width of the resonance term in P being given by the decay width through the outer barrier.

The poles ϵ_n can be identified with the 'natural' vibrational states of the secondary well in the following manner. At η_c the wavefunction of such a vibrational state will be exponentially increasing (exponentially decreasing towards smaller deformation) with attenuation wavenumber κ. On the other hand an outgoing wave from the primary well region will, in the absence of resonance conditions, be exponentially decreasing. Thus the boundary condition to be chosen for the intermediate eigenstates, according to equation (34) is the latter one, $\mathscr{B} = -\kappa$. The effect of change of boundary condition on the eigenvalues and reduced widths has been discussed by Teichmann (1950). The new eigenvalue $\epsilon_\nu^{(a)}$ resulting from a change of boundary condition from $\mathscr{B}$ to $\mathscr{B}^{(a)}$ is given in the present case by

$$\sum_\nu \frac{\gamma_\nu^2(\eta_c)}{\epsilon_\nu-\epsilon_\nu^{(a)}} = \frac{1}{\mathscr{B}-\mathscr{B}^{(a)}} \tag{37}$$

and the new reduced widths amplitudes $\gamma_\nu^{(a)}(\eta_c)$ by

$$\gamma_\nu^{(a)}(\eta_c) = \sum_\nu \frac{\gamma_\nu^2(\eta_c)}{\epsilon_\nu-\epsilon_\nu^{(a)}}\left(\sum_\nu \frac{\gamma_\nu^2(\eta_c)}{(\epsilon_\nu-\epsilon_\nu^{(a)})^2}\right)^{-1/2}.$$

Relation (37) results in the eigenvalues $\epsilon_\nu^{(a)}$ being pushed to almost midway between the

ϵ_v (ie very close to the poles ϵ_n) on changing the boundary condition to $\mathscr{B}^{(a)} = \kappa$, for large κ, while in the uniform case the new reduced widths for the vibrational states become

$$\gamma_v^{(a)2}(\eta_c) = \frac{1}{4\kappa^2}\frac{D^2}{\pi^2\gamma_v^2(\eta_c)}.$$

The logarithmic derivative at η_c is thus

$$S+iP \simeq \mathscr{B} + \frac{4\kappa^2\gamma_v^{(a)2}(\eta_c)(e_n-\epsilon)}{(e_n-\epsilon)^2+w_n^2} + i\frac{4\kappa^2\gamma_v^{(a)2}(\eta_c)w_n}{(e_n-\epsilon)^2+w_n^2}. \tag{38}$$

(ii) *Many degrees of freedom.* The result for the logarithmic derivative at the inner surface of the intermediate region can be generalized to the case of many degrees of freedom. The discussion is confined to the deformation channel for simplicity. The Green's theorem relation for the intermediate region, denoted by τ(int) ranging from η_c to η_d, is now written in the form

$$\begin{aligned}(E_2-E_1)\int_{\tau(\mathrm{int})} d\tau\Psi_2^\dagger\Psi_1 = \sum_\mu \Bigg[&\frac{\hbar^2}{2B(\eta_d)}\Bigg\{ f(\eta_d)\Phi_{(2)}^{(\mu)}(\eta_d)\left(\frac{\partial f\Phi_{(1)}^{(\mu)}}{\partial\eta}\right)_{\eta_d} \\ &- f(\eta_d)\Phi_{(1)}^{(\mu)}(\eta_d)\left(\frac{\partial f\Phi_{(2)}^{(\mu)}}{\partial\eta}\right)_{\eta_d}\Bigg\} - \frac{\hbar^2}{2B(\eta_c)}\Bigg\{ f(\eta_c)\Phi_{(2)}^{(\mu)}(\eta_c)\left(\frac{\partial f\Phi_{(1)}^{(\mu)}}{\partial\eta}\right)_{\eta_c} \\ &- f(\eta_c)\Phi_{(1)}^{(\mu)}(\eta_c)\left(\frac{\partial f\Phi_{(2)}^{(\mu)}}{\partial\eta}\right)_{\eta_c}\Bigg\}\Bigg]\end{aligned} \tag{39}$$

where $\Psi_n = \Sigma_\mu\Phi_{(n)}^{(\mu)}\chi_\mu$, $\Psi_n^\dagger = \Sigma_\mu\Phi_{(n)}^{(\mu)}\chi_\mu^*$. This expression can be generalized further by recognizing that the intrinsic states χ_μ for the wavefunction expansions do not need to be the same at different deformations. Two sets of intrinsic states can be defined, one set at η_d and the other at η_c. The existence of these two sets is assumed implicitly in the argument below. The value and derivative quantities at η_c and η_d are denoted by

$$V_\mu(\eta_c) = \left(\frac{\hbar^2}{2B(\eta_c)f(\eta_c)}\right)^{1/2}\int_{\eta=\eta_c} d\mathscr{S}\chi_\mu^* f^{-1}(\eta)\Psi$$

$$D_\mu(\eta_c) = \left(\frac{\hbar^2}{2B(\eta_c)f(\eta_c)}\right)^{1/2}\int_{\eta=\eta_c} d\mathscr{S}\chi_\mu^* f^{-1}(\eta)\frac{\partial(f\Psi)}{\partial\eta}$$

(and similarly for η_d). Eigenstates for the intermediate region are denoted by Z_λ; they are solutions of the nuclear Hamiltonian with boundary conditions

$$\begin{aligned}\frac{D_{\lambda\mu}(\eta_c)}{V_{\lambda\mu}(\eta_c)} &= \mathscr{B}_\mu \\ \frac{D_{\lambda\mu}(\eta_d)}{V_{\lambda\mu}(\eta_d)} &= \frac{1}{f(\eta_d)\Phi_{\epsilon^{(\mu)}}(\eta_d)}\left(\frac{\partial f\Phi_{\epsilon^{(\mu)}}}{\partial\eta}\right)_{\eta_d} \equiv S_\mu(\eta_d)+iP_\mu(\eta_d)\end{aligned} \tag{40}$$

in which $\Phi_{\epsilon^{(\mu)}}$ is an outgoing-wave type solution of the Schrödinger equation with the deformation Hamiltonian $(T_\eta+\mathscr{V}(\eta))\Phi_{\epsilon^{(\mu)}} = \epsilon^{(\mu)}\Phi_{\epsilon^{(\mu)}}$, the energy being that available to the deformation mode, $\epsilon^{(\mu)} = E-\mathscr{E}_\mu(\eta_d)$. With these boundary conditions (and normalization) orthonormality can be established from equation (39) in the sense that $\int_{\tau(\mathrm{int})} d\tau Z_\lambda^\dagger Z_{\lambda'} = \delta_{\lambda\lambda'}$. Eigenvalues of these states are denoted by F_λ, and they are complex, the imaginary component representing the halfwidth for decay through channels μ open at η_d and leading to fission.

A general solution Ψ of the Schrödinger equation at energy E can now be expanded in terms of the Z_λ, $\Psi(E) = \Sigma_\lambda A_\lambda Z_\lambda$ and the coefficients A_λ determined through the Green's theorem relationship,

$$A_\lambda = \int_{\tau(\text{int})} \mathrm{d}\tau Z_\lambda^\dagger \Psi = \frac{1}{F_\lambda - E} \sum_\mu [V_{\lambda\mu}(\eta_d)\{D_\mu(\eta_d) - (S_\mu(\eta_d) + \mathrm{i}P_\mu(\eta_d))V_\mu(\eta_d)\}$$

$$- V_{\lambda\mu}(\eta_c)(D_\mu(\eta_c) - \mathscr{B}_\mu V_\mu(\eta_c))].$$

If $\Psi(E)$ is the continuation of outgoing waves in the channels μ it must have the boundary conditions (40) at η_d, and therefore its expansion becomes

$$\Psi(E) = -\sum_\lambda \frac{Z_\lambda}{F_\lambda - E} \sum_\mu V_{\lambda\mu}(\eta_c)(D_\mu(\eta_c) - \mathscr{B}_\mu V_\mu(\eta_c))$$

from which the logarithmic derivative of $\Psi(E)$ at η_c in the channel μ is

$$\frac{D_\mu(\eta_c)}{V_\mu(\eta_c)} \equiv S_\mu(\eta_c) + \mathrm{i}P_\mu(\eta_c) = \mathscr{B}_\mu - \sum_{\mu'} (R_{\text{int}}^{-1})_{\mu\mu'} \frac{V_{\mu'}(\eta_c)}{V_\mu(\eta_c)}. \tag{41}$$

Here, the intermediate R matrix element is $R_{\text{int},\mu\mu'} = \Sigma_\lambda V_{\lambda\mu}(\eta_c)V_{\lambda\mu'}(\eta_c)/(F_\lambda - E)$. The poles of the right-hand side of equation (41) are the complex energies for which $\det R_{\text{int}} = 0$. The poles are denoted by $\mathscr{F}_l - \mathrm{i}\mathscr{W}_l$ and the residues of $(R_{\text{int}}^{-1})_{\mu\mu'}$ at the poles by $G_{l(\mu\mu')}$. Thus the logarithmic derivative in channel μ can be expanded

$$\frac{D_\mu(\eta_c)}{V_\mu(\eta_c)} = \mathscr{B}_\mu - \sum_l \frac{1}{\mathscr{F}_l - E - \mathrm{i}\mathscr{W}_l} \sum_{\mu'} \frac{G_{l(\mu\mu')}V_{\mu'}(\eta_c)}{V_\mu(\eta_c)}. \tag{42}$$

When there is essentially only one intrinsic state μ (or 'channel' over the intermediate barrier) contributing to this expression, it reduces essentially to the form of equation (38) with $\mathscr{F}_l$, $\mathscr{W}_l$ and $G_{l(\mu\mu)}$ replacing e_n, w_n and $4\kappa^2\gamma_v^{(a)2}(\eta_c)$.

4.3.3. Treatment of cross sections by channel dispersion method. (i) *The absorption cross section and fission strength function.* As shown above the logarithmic derivative of an outgoing wave transmitted through the secondary well (even in the presence of 'mixing' forces) has, in the neighbourhood of a virtual state E_l associated with the secondary well, a dispersion form

$$L_\mu = S_\mu + \mathrm{i}P_\mu = S_{b\mu} + \frac{G_l}{\mathscr{F}_l - E - \mathrm{i}\mathscr{W}_l} \tag{43}$$

where $S_{b\mu}$ is a real, slowly varying background term. This is used to determine the collision matrix and cross sections through equations (15) and (16) in which the R matrix has now to be constructed for an internal region that comprises only the primary well in the deformation coordinate. It is convenient in many applications to determine the fission strength function, and this can be assessed by calculating the absorption cross section when the system is entered through the fission channel (or channels) μ. For this purpose one-channel reduced R matrix theory (Thomas 1955) can be used, provided that the widths in all the exit channels are small ($\Gamma_{\lambda(e)} \ll D_\lambda$) and uncorrelated. The collision function is just $U_{\mu\mu} = \mathrm{e}^{2\mathrm{i}\phi_\mu}(1 - \hat{L}_\mu^* R)/(1 - \hat{L}_\mu R)$ where $\hat{L}_\mu = \hat{L}_\mu - \mathscr{B}_\mu$

($\mathscr{B}_\mu$ is now the boundary condition at η_c for the internal region) and

$$R = \sum_\lambda \gamma^2_{\lambda(\mu)}/(E_\lambda - E - \mathrm{i}W_\lambda),$$

with $W_\lambda = \frac{1}{2}\Sigma_e \Gamma_{\lambda(e)}$.

(*a*) *Overlapping R matrix levels.* In the approximation of uniform, overlapping R matrix levels ($W_\lambda \gg D$) the R function is just $\mathrm{i}\pi s_\mu$, where the reduced strength function $s_\mu = \gamma^2_{\lambda(\mu)}/D$. The absorption cross section is proportional to $1-|U_{\mu\mu}|^2$, which, in this approximation, becomes

$$1-|U_{\mu\mu}|^2 = \frac{4\pi s_\mu P_\mu}{|1-\hat{L}_\mu R|^2}.$$

With the introduction of equation (43) for P_μ and $\hat{L}_\mu$,

$$1-|U_{\mu\mu}|^2 = \frac{4\pi s_\mu G_l \mathscr{W}_l (1+\hat{S}^2_{b\mu}\pi^2 s^2_\mu)^{-1}}{\{\mathscr{F}_l + \pi^2 G_l \hat{S}_{b\mu} s^2_\mu/(1+\pi^2\hat{S}^2_{b\mu}s^2_\mu) - E\}^2 + \{\mathscr{W}_l + \pi G_l s_\mu/(1+\pi^2\hat{S}^2_{b\mu}s^2_\mu)\}^2}$$

where $\hat{S}_{b\mu} = S_{b\mu} - \mathscr{B}_\mu$. The absorption cross section (for specific total angular momentum J) is $\pi\lambda\!\!\!^{-2} g(J)$ times this, but is also commonly written as a local average over a sequence of (assumed) non-interfering states. In the uniform model (Lane and Thomas 1958)

$$\sigma_{\mathrm{abs}} = 2\pi^2 \lambda\!\!\!^{-2} g(J) \frac{\bar{\Gamma}_{\lambda(\mu)}}{\bar{D}_\lambda} \frac{1-\exp(-4\pi W_\lambda/D_\lambda)}{1-\exp(-4\pi W_\lambda/D_\lambda)(1-2\pi\bar{\Gamma}_{\lambda\mu}/\bar{D}_\lambda)}. \tag{44}$$

Since $4\pi W_\lambda/D_\lambda \gg 1$ the fission strength function becomes

$$\frac{\bar{\Gamma}_{\lambda(\mu)}}{\bar{D}_\lambda} = \frac{1}{2\pi} \frac{\Gamma_{l(c)}\Gamma_{l(\mu)}}{(\mathscr{F}_l + \Delta_l - E)^2 + \frac{1}{4}(\Gamma_{l(c)} + \Gamma_{l(\mu)})^2} \tag{45}$$

with

$$\Gamma_{l(\mu)} = 2\mathscr{W}_l, \qquad \Gamma_{l(c)} = 2\pi s_\mu G_l/(1+\pi^2\hat{S}^2_{b\mu}s^2_\mu), \qquad \Delta_l = \pi^2 s^2_\mu G_l \hat{S}_{b\mu}/(1+\pi^2\hat{S}^2_{b\mu}s^2).$$

It is of interest to compare this formula with some of the numerical examples given above. Let us assume that the 'internal region' is simply a square well extended indefinitely towards decreasing deformation. The eigenvalues of the states in this well have spacing $D_\lambda = 2\pi(\hbar^2 E_\lambda/2B_\mu\eta_1^2)^{1/2}$ where η_1 is the range of the well, and the reduced widths of these states are $\gamma^2_{\lambda(\mu)} = \hbar^2/(B_\mu\eta_1)$, so that the reduced strength function is $s_\mu = 1/\pi k_\lambda$ where k_λ is the wavenumber of the state E_λ in the well. With a numerical value of $s_\mu = 5{\cdot}6\times10^{-3}$ (for $E_\lambda = 2{\cdot}805$ MeV), $\Gamma_{l(c)} = 0{\cdot}4497$ keV, $\Delta_l = -0{\cdot}2171$ keV and $\mathscr{W}_l = 0{\cdot}225$ keV (from the penetration factor curve). These values are in agreement with the transmission curve shown in figure 6, as we would expect. However, this also reveals the rigidity in the phenomenological transmission factor approach to determining fission strength functions; departures of the reduced strength function from the 'infinite' square well value lead to deviations of the fission strength function from the calculated transmission factor.

(*b*) *Narrow R matrix levels.* Numerical calculations of the absorption cross section can be used to study the behaviour of the fission strength function when $W_\lambda < D$. Local averages of such calculated cross sections are defined as the uniformly averaged cross section over an energy interval D. The fission strength function is extracted from this with the use of equation (44) and reveals that it is still very well approximated by equation (45). Examples of such cross sections are shown in figure 7; in these examples the coupling width $\Gamma_{l(c)}$ and decay width $\Gamma_{l(\mu)}$ of the intermediate state l are equal.

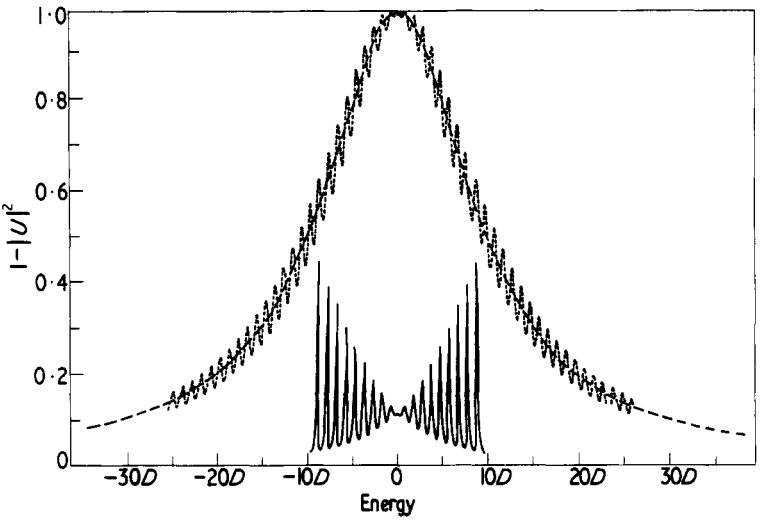

Figure 7. Fine structure cross section in the uniform-level model across a vibrational resonance with equal coupling width and decay width ($\Gamma_{l(\mu)} = 10D_\lambda, \Gamma_{l(c)} = 10D_\lambda$). The full curve represents $\Gamma_{\lambda(e)} = 0{\cdot}01\ D_\lambda$, the long-dashed curve is for $\Gamma_{\lambda(e)} = 1{\cdot}6\ D_\lambda$ and the short-dashed curve for $\Gamma_{\lambda(e)} = 0{\cdot}4\ D_\lambda$.

(ii) *Fine structure.* The fine structure of a cross section is often described schematically by presenting the poles of the S matrix. In the one-channel case the S matrix is just

$$S_{\mu\mu} = 1 - U_{\mu\mu} = \frac{-2iP_\mu R}{1-\hat{L}_\mu R}.$$

With the dispersive form of equation (43) for $\hat{L}$, this becomes

$$S_{\mu\mu} = \frac{-2iG_l \mathscr{W}_l R}{(\mathscr{F}_l - E + i\mathscr{W}_l)\{(1-\hat{S}_{b\mu})(\mathscr{F}_l - E - i\mathscr{W}_l) - G_l R\}}$$

which has poles $\mathscr{E}$ given by

$$(\mathscr{F}_l - \mathscr{E} - i\mathscr{W}_l)(1-\hat{S}_{b\mu}R) - G_l R = 0. \tag{45}$$

Further discussion will be simplified by the assumption that $\hat{S}_{b\mu} = 0$.

(*a*) *Discrete R matrix states; broad intermediate state.* The broad intermediate state is defined by the conditions that $2G_l\gamma_\lambda^2/\mathscr{W}_l D_\lambda \ll 1$ and $\mathscr{W}_l \gg D_l$. The complicated many-level interference can then be ignored, and the fine-structure resonances appear at energies $\mathrm{Re}\,\mathscr{E} = E_\lambda + \Delta_\lambda$, the level shifts Δ_λ being

$$\Delta_\lambda \simeq \frac{G_l\gamma_{\lambda(\mu)}^2(\mathscr{F}_l - E_\lambda)}{(E_\lambda - \mathscr{F}_l)^2 + \mathscr{W}_l^2}$$

and with widths

$$-2\,\mathrm{Im}\,\mathscr{E} \simeq \frac{2G_l\mathscr{W}_l\gamma_{\lambda(\mu)}^2}{(E_\lambda - \mathscr{F}_l)^2 + \mathscr{W}_l^2}. \tag{46}$$

With the above-mentioned conditions the level shifts and widths are always much less than the level spacings D_λ. In the uniform model, with one of the E_λ coinciding with $\mathscr{F}_l$, the real part of equation (45) is, by symmetry, satisfied by $\mathrm{Re}\,\mathscr{E} = \mathscr{F}_l$. In this instance the approximate solutions of $\mathrm{Im}\,\mathscr{E}$ are $\mathrm{Im}\,\mathscr{E} \simeq -G_l\gamma_\lambda^2/\mathscr{W}_l$ agreeing with equation (46) above, for one pole, and $\mathrm{Im}\,\mathscr{E} \simeq -\mathscr{W}_l$ for the other.

(*b*) *Discrete R matrix states; narrow intermediate state.* In the limit of vanishingly narrow intermediate state the poles of $S_{\mu\mu}$ are real, satisfying the equation

$$\mathscr{F}_l - \mathscr{E} = G_l \sum_\lambda \frac{\gamma_{\lambda(\mu)}^2}{E_\lambda - \mathscr{E}}. \tag{47}$$

This is identical in form with equation (23) and allows us to make the quasi-identification: $\mathscr{F}_l \simeq E_{\lambda_{\mathrm{II}}}$, $E_\lambda \simeq E_{\lambda_{\mathrm{I}}}$, $G_l\gamma_{\lambda(\mu)}^2 \simeq \langle\lambda_{\mathrm{I}}|H_c|\lambda_{\mathrm{II}}\rangle^2$. For non-zero, but still very small $\mathscr{W}_l$ equation (47) is still approximately true (for $\mathrm{Re}\,\mathscr{E}$) and we can use the solution of $\mathrm{Re}\,\mathscr{E}$ implied therein to give a first order result for $\mathrm{Im}\,\mathscr{E}$:

$$\mathrm{Im}\,\mathscr{E} \simeq \frac{-\mathscr{W}_l}{G_l\Sigma_\lambda\gamma_\lambda^2/(E_\lambda - \mathrm{Re}\,\mathscr{E})^2 + 1}. \tag{48}$$

This is perfectly analogous to equation (24).

(*c*) *Discrete R matrix states; moderately broad intermediate level.* The intermediate case has to be studied through direct numerical calculations. A typical example is shown in figure 8. Here $\mathscr{W}_l/D_\lambda = 5$, $G_l/D_\lambda = 159{\cdot}16$ and $\gamma_{\lambda(\mu)}^2/D_\lambda = 0{\cdot}01$ (giving $\Gamma_{l(c)}/D_\lambda = 10$).

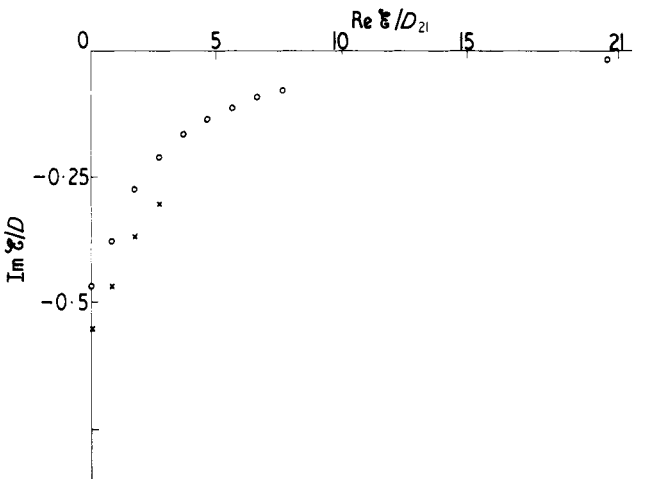

Figure 8. *S* matrix poles for the cross sections in the family of figure 7 ($\Gamma_{l(\mu)} = \Gamma_{l(c)} = 10D_\lambda$). Open circles represent poles for $\Gamma_{\lambda(e)}/D_\lambda = 0$, crosses are for $\Gamma_{\lambda(e)}/D_\lambda = 0{\cdot}2$.

As is well known in this type of intermediate coupling (see Lejeune and Mahaux 1968) the pole widths do not follow a lorentzian form despite the fact that the fission strength function, as deduced from the locally-averaged absorption cross section, does. The corresponding absorption cross section for various values of $\Gamma_{\lambda(e)}/D_\lambda$ has been shown in figure 7. For small values of $\Gamma_{\lambda(e)}/D_\lambda$ the poles of the *S* function do not differ much from

those shown in figure 8 but for large values they have wandering paths; one of them is shown in figure 9.

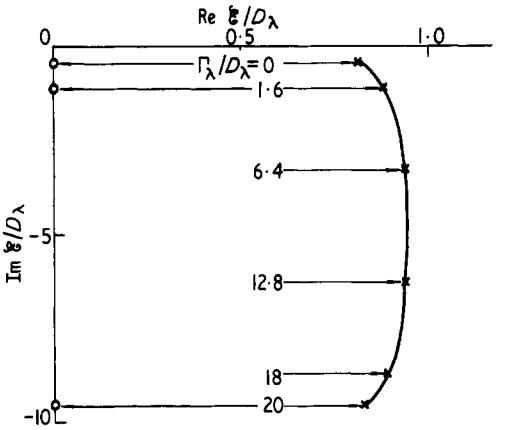

Figure 9. Paths of poles for changing $\Gamma_{\lambda(e)}/D_\lambda$.

5. Conclusion

In this paper a formal method for incorporating fission in R matrix nuclear reaction theory has been proposed, the discussion centring on suitable definitions of the kinetic energy and potential energy operators for the fission degree of freedom. From these basic points detailed application of the theory to the phenomenon of the Strutinsky double-humped fission barrier has been made, two possible treatments being considered. In the first of these the secondary well of the barrier (as well as the primary well) has been incorporated in the internal region, and this is reflected by the possibility of constructing the formal basis states of the internal region by coupling two distinct types of auxiliary state, class I and class II states, characterized by very different probabilities for localization within the primary and secondary wells. This method is particularly useful when the widths associated with these basis states, particularly the class II states, are small compared with the overall spacing. In the other method the secondary well is made part of the external region and must be taken into account in the construction of effective shift and penetration factors for the fission channels. These factors show dispersion characteristics which account for intermediate structure in the fission cross sections. The method is particularly applicable when the width of the intermediate structure resonances is many times the fine structure spacing.

Although the two methods are particularly simple to use in extreme conditions of opposite kind they are both quite general in principle and can be applied to conditions other than the ideal ones. Such application, a few examples of which have been indicated in the text, require detailed numerical treatment, however.

Acknowledgment

I wish to thank Dr A M Lane for his critical reading of the manuscript and for valuable discussions on the conditions for choice of channel boundaries.

Appendix. Validity of Green's theorem application to interior surfaces

Equation (11) of § 3 requires some justification. This must start with some discussion of the nature of the other variables that describe degrees of freedom other than that of extended deformation. For this purpose let us assume that we have taken $\mathscr{R} = \sqrt{\Sigma_i \bar{r}_i^2}$ as the deformation variable. A suitable set of forms for the remaining variables $\xi_j, j = 2$ to $3A$, that satisfies the conditions $\partial^2\psi/\partial\xi_j\partial\xi_k$ is

$$\xi_2 = \arcsin\left(\frac{u_{3A}}{\sqrt{\Sigma_{i=1}^{3A} u_i^2}}\right)$$

$$\xi_3 = \arcsin\left(\frac{u_{3A-1}}{\sqrt{\Sigma_{i=1}^{3A-1} u_i^2}}\right)$$

$$\ldots$$

$$\xi_j = \arcsin\left(\frac{u_{3A+2-j}}{\sqrt{\Sigma_{i=1}^{3A+2-j} u_i^2}}\right)$$

$$\ldots$$

$$\xi_{3A} = \arcsin\left(\frac{u_2}{\sqrt{(u_1^2+u_2^2)}}\right). \tag{A.1}$$

(For simplicitly of expression, the inclusion of the centre of mass degrees of freedom has been neglected here.) The quantities u_i are simply the $3A$ cartesian coordinates of the A nucleons of the system.

Some cross sections through $3A$ dimensional configuration space are shown in figures 10 and 11. In figure 10 the plane shown is that of the deformation parameter $\mathscr{R}$ and the parameter ξ_2. The areas of different cross-hatching indicate different kinds of constraints on the remaining parameters ξ_3 to ξ_{3A} (ie different planes are shown on the same diagram). The main areas shown comprise single nucleon channels and general deformation channels as well as the internal region of interaction of all A nucleons. In the first case one channel is defined by u_{3A} as the nucleon variable while all other coordinates are confined within a residual nucleus volume constrained to deformations lying between $\beta = 0{\cdot}2$ and $0{\cdot}3$; this is shown again for $\beta = 0{\cdot}55$ to $0{\cdot}65$ (the upper curve). The third nucleon channel shown is for u_1 (or some coordinate other than u_{3A}) as the nucleon parameter (β between $0{\cdot}2$ and $0{\cdot}3$ for the residual nucleus). In the general deformation channel u_{3A} represents a typical nucleon coordinate within the deforming nucleus or within one of the ultimate product nuclei typical of fission. All the other coordinates u, and hence ξ_3 to ξ_{3A}, take on a typical set of values that correspond to the nuclear shapes followed in the course of fission; they are thus generally increasing with increasing deformation $\mathscr{R}$. Similar regions are shown for the plane $\mathscr{R}$ against ξ_{3A} in figure 11.

Because of the constraints on ξ_3 to ξ_{3A} (or, in figure 11, ξ_2 to ξ_{3A-1}), the areas of apparent overlap, in these figures, of different regions of configuration space do not in fact overlap. Thus, along the lines A, B that correspond to the deformations at the two maxima in the Strutinsky model of the fission barrier the ξ_3 to ξ_{3A} parameters for the internal region correspond to all nucleons being confined to a volume with roughly spheroidal shape and β values of the order of $0{\cdot}45$ and $0{\cdot}75$ respectively. Where the nucleon channel areas cross A and B, ξ_3 to ξ_{3A}, in two cases, and ξ_2 to ξ_{3A-1} in the other case, correspond to the $A-1$ nucleons of the residual nucleons confined to volumes with

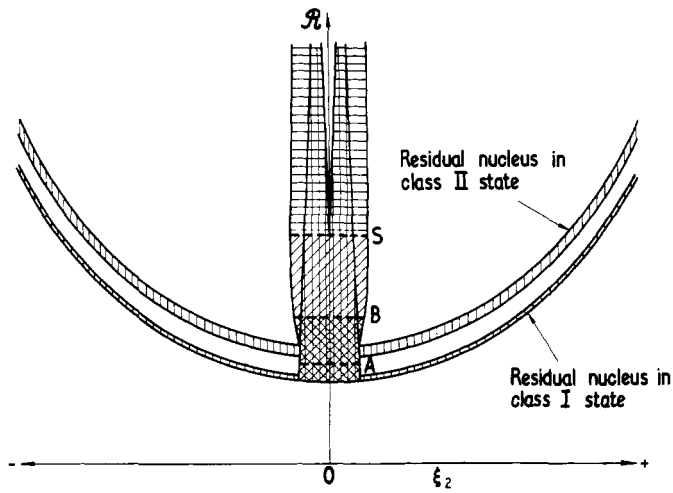

Figure 10. Schematic diagram of configuration space projected against two parameters $\mathcal{R}$ and ξ_2. Areas of vertical shading correspond to single nucleon channels with the residual nucleus in low excited states with different deformations. Areas of horizontal shading correspond to separated fission product channels (shown in this case for symmetric mass division only). The cross-shaded area //// shows the internal region defined with fission channel boundaries set at the scission point (indicated by the line S), and cross-shading \\\\ shows the internal region defined with fission channel set at the Strutinsky outer barrier B. The Strutinsky inner barrier A is indicated by line A.

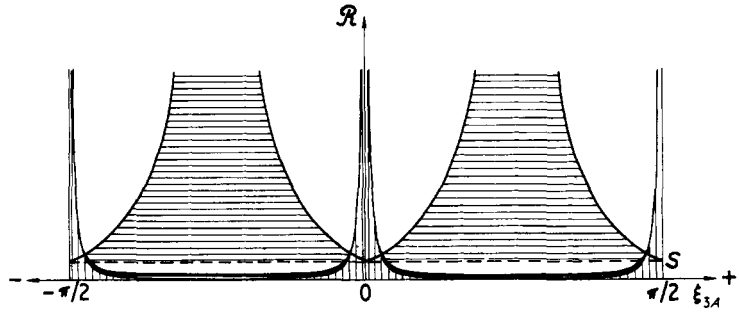

Figure 11. Schematic diagram of configuration spacing against parameters $\mathcal{R}$ and ξ_{3A}. Shading has the same significance as in figure 10.

deformations corresponding to the Strutinsky minima I and II ($\sim$0·25 and 0·6 respectively) and one nucleon far outside this volume. So long as the excitation energy of the system is such that the energetically possible states of the residual nucleus do not have (with appreciable probability) a range of deformation that extends to the Strutinsky maxima, this separation of the regions is physically distinct.

Because of the physical separation of these regions it is very convenient to draw the boundary of the internal region through the conventional entrances to the single nucleon channels (and the other light particle channels) where the system has comparatively small values of $\mathcal{R}$. Outside such channels the boundary can be drawn in a more or less arbitrary fashion through regions of vanishing wavefunction until it reaches a larger value corresponding to a deformation $\mathcal{R}_C$ close to either $\mathcal{R}_A$ or $\mathcal{R}_B$ (at the Strutinsky

maxima) along which value the boundary can be taken to mark the division between the internal region and the deformation channel.

Just within this last part of the boundary the internal wavefunction of the system can be expanded in the form

$$\Psi_k = \sum_{\mu} \Phi_{(k)}^{(\mu)}(\mathscr{R})\chi_{\mu}(\xi) \tag{A.2}$$

where the $\Phi_{(k)}^{(\mu)}$ satisfy the Schrödinger equation for the deformation potential, (equation (6*a*)), and the $\chi_{\mu}(\xi)$ satisfy equation (6*b*) for the remaining degrees of freedom at fixed deformation $\mathscr{R}_A$ or $\mathscr{R}_B$. The gradient of Ψ normal to the surface is

$$\text{grad}_n \Psi_k = \frac{\partial \Psi}{\partial \mathscr{R}} = \sum_{\mu} \frac{\partial \Phi_{(k)}^{(\mu)}}{\partial \mathscr{R}} \chi_{\mu}. \tag{A.3}$$

The reasonable physical assumption is made now that, for the low to medium excitation energies at which R matrix theory is useful, the states χ_{μ} appearing in expansions (A.2) and (A.3) are discrete and bound, vanishing along lines of $\mathscr{R}_C$ just outside the deformation channel region. The states χ_{μ} do, in general, form a complete set and are thus capable in principle of describing a residual nucleus and a light particle in free space in the other channel regions. We now consider the integral

$$(E_2 - E_1) \int_{\tau} d\tau \Psi_2^* \Psi_1 = \int_{\tau} d\tau \{(T\Psi_2^*)\Psi_1 - \Psi_2^*(T\Psi_1)\}, \tag{A.4}$$

the potential energy terms of the nuclear system being assumed to be self-adjoint as usual. The volume integral is taken over the internal region of configuration space as defined above. The volume element $d\tau$ is given by

$$d\tau = h_{\mathscr{R}}\, d\mathscr{R} h_{\xi_2} d\xi_2 \ldots h_{3A}\, d\xi_{3A}$$

and the scaling factors are

$$h_{\mathscr{R}} = 1$$

$$h_j = \mathscr{R}\left(1 - \sum_{i=2}^{j-1} \cos^2 \xi_2 \ldots \cos^2 \xi_{j-1} \sin^2 \xi_{j+1-i}\right)^{1/2}.$$

With the separation of the kinetic energy term as in § 2.2 and the substitution of equation (A.2) the integral on the right-hand side of (A.4) becomes

$$\sum_{\mu\mu'} \int \left(\frac{h_2}{\mathscr{R}}\right) d\xi_2 \ldots \left(\frac{h_{3A}}{\mathscr{R}}\right) d\xi_{3A} \chi_{\mu}^* \chi_{\mu'} \int d\mathscr{R} \mathscr{R}^{3A-1} \{\Phi_{(1)}^{(\mu')}(T_{\mathscr{R}} \Phi_2^{(\mu)*}) - \Phi_2^{(\mu)*}(T_{\mathscr{R}} \Phi_{(1)}^{(\mu')})\}$$

$$+ \sum_{\mu\mu'} \int_{\tau} d\mathscr{R} \left(\frac{h_2}{\mathscr{R}}\right) d\xi_2 \ldots \left(\frac{h_{3A}}{\mathscr{R}}\right) d\xi_{3A} \{\chi_{\mu'}(T_{\xi} \chi_{\mu}^*) - \chi_{\mu}^*(T_{\xi} \chi_{\mu'})\}$$

$$\times \mathscr{R}^{3A-1} \Phi_{(2)}^{(\mu)*} \Phi_{(1)}^{(\mu')}. \tag{A.5}$$

The kinetic energy operators T_{ξ} have the form

$$T_{\xi} = \sum_j -\frac{h^2}{2m}\left(\frac{1}{h_j^2} \frac{\partial^2}{\partial \xi_j^2} + \frac{(j-3A)\mathscr{R} \cos \xi_2 \ldots \cos \xi_{j-1} \sin \xi_j}{h_j^2 h_{j+1}} \frac{\partial}{\partial \xi_j}\right)$$

and the result of the integration over an individual ξ_j in the second integral gives terms involving products of $\chi_{\mu'}(\partial \chi_{\mu}^*/\partial \xi_j)$ etc, evaluated at the limits of ξ_j. By virtue of the physical assumptions made above on the nature of the wavefunctions χ these products

vanish in the deformation channel region. The assumed orthogonality of the χ_μ and the substitution of equation (3) for the explicit form of $T_{\mathscr{R}}$ in the first term of (A.5) gives, finally, for the contribution to $(E_2-E_1)\int_\tau d\tau \Psi_2^* \Psi_1$ in the deformation channel region the term

$$-\frac{h^2}{2m}\sum_\mu \left[\mathscr{R}^{(3A-1)/2}\Phi_{(1)}^{(\mu)} \frac{\partial}{\partial \mathscr{R}} (\mathscr{R}^{(3A-1)/2}\Phi_{(2)}^{(\mu)*}) - \mathscr{R}^{(3A-1)/2}\Phi_{(2)}^{(\mu)*} \frac{\partial}{\partial \mathscr{R}} (\mathscr{R}^{(3A-1)/2}\Phi_{(1)}^{(\mu)}) \right]_{\mathscr{R}=\mathscr{R}_c}$$

that appears as expression (11) in the text.

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