R-MATRIX THEORY*

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**These notes are for five lectures, which the author gave, October 4-8, 2004, at the R-Matrix School of the Joint Institute for Nuclear Astrophysics (JINA) at Notre Dame University, South Bend, Indiana. The five sections of the notes correspond to the five given lectures. The notes are not a review article but are intended to be helpful to the participants of the school and to serve as an introduction to the R-Matrix programs prepared for the School participants by Professor Richard Azuma. These notes are dedicated to Fred Barker who, for half a century, has been more consistent than anyone else in championing the R-Matrix theory.*

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1 INTRODUCTION

1.1 General Introduction

This is again an interesting time for the theory of low-energy nuclear reactions. The new facilities for nuclear astrophysics, including the new radioactive beam facilities, now make it possible to pursue experiments for many of the processes involved in stellar evolution and nuclear astrophysics. These studies are central now to nuclear physics and many of the processes are resonance reactions. The analysis of the data then returns us to an era, almost half a century ago, when nuclear reactions were first studied and analyzed at a time when nuclear physics dominated physics and, indeed, much of science. It is then an interesting turn around in our field, which brings us here to examine, with hindsight, many of the critical issues, which were emerging fifty years ago. As background material each of the participants of this school have been given three quite ancient papers: the encyclopaedic review paper of Lane and Thomas[1] (referred to as Ref. A in the text); two review papers by the present author[2,3] (referred to, respectively, as Ref. B and Ref. C in the text).

As we shall discuss, the R-matrix theory of Wigner and his collaborators turns out to be the most physical and appropriate, among the various alternative frameworks, for the analysis of resonance reactions. These frameworks evolved almost as soon as nuclear physics began. Shortly after the discovery by Chadwick (1932) of the neutron, Fermi and his collaborators in Rome studied the cross sections for neutron bombardment of many elements. They found many resonances, often spaced only a few eV apart, compared to the spacing of many MeV demanded by the mass of the neutron and the known size of nuclei, for single-particle neutron levels in a potential well of nuclear size. The plethora of resonances immediately led to a new concept; the compound nucleus, articulately stated by Bohr. In this picture a neutron entering a nucleus immediately excites the many degrees of freedom of the many-nucleon system and is resonantly absorbed. In essence, the nucleus is “black” for the neutron (“black” means that at the nuclear surface the wave

function of the neutron is given by an incoming wave) and this black-nucleus picture was well described in the famous 1937 review articles on nuclear physics by Bethe[4].
The verdict was in: the nucleus was black and no single-particle motion such as that of the nuclear shell model seemed possible. There had been initial stirrings, in the 1930's, of the single-particle model but the neutron evidence and the great strength and short range of the nuclear force between nucleons set back any serious consideration of the shell model for almost two decades until new evidence led to its rebirth.

The immediate problem, in the mid-1930's, was to describe the closely spaced resonances observed for neutrons and also other beams. The known physics of the nuclear system gave clues about how to proceed. The nucleus was known to have a reasonably well defined radius – deduced from saturation and other properties – and inside the two-body nuclear forces were assumed to thoroughly mix things until, after some length of time (compared to the transit time of a nucleon across the nucleus) something emerged that was energetically permissible. Such a system was not unlike an electromagnetic cavity, driven by wave-guides connected to it. The early frameworks constructed for the description of resonance reactions were based on such analogies.

The first published framework was that of Kapur and Peierls[5]. They viewed the nucleus as a complicated box in the configuration space of all the nucleons and therefore they added boundary condition numbers at the nuclear surface which corresponded to purely incoming waves. As we shall see below, this framework has many beguiling features but its usefulness appears to be limited by the fact that its boundary conditions are complex numbers and also strongly energy dependent.

The R-matrix framework came next (see references A or B for a complete list of the early papers). Eugene Wigner who proposed it had already provided, with Gregory Breit[6], the famous Breit-Wigner formula, which needed a better foundation. The R-matrix formulation provided that foundation. It was begun in 1941, by Wigner but only fully worked out immediately after WWII by Wigner and Eisenbud and others. The R-matrix framework also had its origins in the earlier work pertaining to electromagnetic cavities. It is then amusing that very recently the R-matrix formalism has been applied by Richter and his colleagues[7] to the description of their measurements of the properties of electromagnetic wave guides. This new work was seemingly unaware of its earlier antecedents.

Central to each of these frameworks is the division of the configuration space of the problem into an "internal" region, corresponding to the compound nucleus, and an "external" region, corresponding to the reaction alternatives, or channels, possible to reach the compound nucleus or emerge from it. This division of space is made by a choice of the boundary of the compound nucleus: a nuclear radius is chosen for each reaction alternative. The resonances displayed in the cross sections are those of the compound nucleus and are given by boundary condition numbers chosen at each radius. Such a choice yields a complete set of wave functions, or resonances, for the compound nucleus through the construction of the appropriate boundary value problem. The channel radii and the corresponding boundary condition numbers are auxiliary quantities which are not artificial adjuncts to the framework – as has often been falsely alleged – but may be subject to good physics, as we shall see below. The external region provides us with

the paraphernalia – having nothing to do with the underlying nuclear physics – of scattering theory, such as the collision matrix or phase shifts or penetration factors, etc. The internal region provides the parameters – level energies, level widths and reduced widths (or spectroscopic factors) – pertaining to the nucleus.

The physical reason why such reaction frameworks – with their division of configuration space into external and internal regions – work at all is that the atomic nucleus has a reasonably well defined radius which, in turn, arises from the short range of the nuclear forces. Similarly, the reason why the R-matrix framework has emerged as the best for the description of resonance processes is that the nuclear or internal parameters that it yields are strongly tied to the physics of nuclear spectroscopy.

1.2 A Heuristic Model – S-wave Scattering of a Neutron by a Square-Well Potential

Here we follow, especially for the "internal bits", the treatment of Section II of Ref. C. With this example we encounter all of the quantities of the formal reaction theory including those of the R-matrix.

The radial part of the Schroedinger equation for this problem may be written as:

$$-(\hbar^2/2m)\,d^2\varphi/dr^2 + V_0\varphi = E\varphi \qquad (1)$$

where $V = -V_0$ for $r \leq a$, and $V_0 = 0$ for $r > a$. To be somewhat realistic, relative to the known mean free field for neutrons, we choose the square-well depth to be about $V_0 = -50$ MeV and the square-well radius to be about $a = 1.25\ A^{1/3}$ fm. The square-well is spinless and so we can ignore spin in this heuristic problem.

1.2.1 External Bits

To define and describe the "external bits" (that is, those pieces of the problem which have nothing to do with the potential) of this heuristic problem we follow the treatment of any introductory text for quantum mechanics. We envisage a neutron beam produced by an appropriate source and collimators, incident as a plane wave on a distant scatterer with the scattered waves being observed outside the beam and the scatterer. In all generality we can then write the external wave function as the sum of an incident plane wave, e^{ikz} plus a scattered wave, as follows:

$$\Psi(r, \theta, \varphi) = A\,[e^{ikz} + (1/r)\,f(\theta,\varphi)e^{ikr}] \qquad (2)$$

where k (= mv/h) is the wave number of the neutron. We next insert the expansion of the plane wave into partial waves of given angular momentum, *l,* (this expansion is not without mathematical interest because the plane wave is not square integrable and therefore care must be taken in the expansion):

$$e^{ikz} = e^{ikr\cos\theta} = \Sigma_{\ell=0}^{\infty}\,(2\ell + 1)\,i^{\ell}\,j_{\ell}\,(kr)\,P_{\ell}\,(\cos\theta) \qquad (3)$$

The scattering cross section is defined to be:

$$\sigma\ (\theta,\varphi)\ =\ \left|f(\theta,\varphi)\right|^2 \tag{4}$$

We next note that the incoming plane wave, (3), is a sum of incoming and outgoing spherical waves, for example, for *l*= *0*:

$$j_o\ (kr)\ =\ (1/kr)\ \sin kr = (2i/kr)\ [e^{-ikr} - e^{ikr}]\ \equiv\ (2i/kr)\ (4\pi v)^{½}\ [I - O] \tag{5}$$

where I [$\equiv (4\pi v)^{-1/2}\ e^{-ikr}$] and O [$\equiv (4\pi v)^{-1/2}\ e^{ikr}$] are, respectively, incoming and outgoing waves for *l*=0, both normalized to unit flux.

We next define the phase shift, δ_ℓ, and the collision function, U_ℓ, both of which relate to the external wave function at large distance. Asymptotically the radial solution for any partial wave, *l*, is a sine function which is phase shifted. That is,

$$\text{radial solution}\ (r \to \infty)\ \approx\ A_\ell\ \sin\ (kr + \delta_\ell) \tag{6}$$

which, for $l = 0$ (again dropping the 0 subscript) allows us to write the external wave function as:

$$\varphi\ = [I - e^{2i\delta}\ O] = [I - UO] \qquad r > a \tag{7}$$

which defines the collision function ($U \equiv \exp(2i\delta)$), which may be used as an alternative to the phase shift to parameterize the asymptotic wave function. The corresponding cross section is

$$\sigma = (\pi/k^2)\ \sin^2\ \delta = (\pi/k^2)\ |1 - U|^2 \tag{8}$$

It is the cross section σ – and hence δ or U – which is measured. To relate them to the scattering potential we first need to look at the "internal bits".

1.2.2 Internal Bits

The "internal" ($r < a$) solution for the radial Eqn. (1), of our heuristic problem is

$$\varphi\ (r) = A \sin Kr, \qquad \text{where } K = [(2m/\hbar^2)(E + V_0)]^{1/2} \tag{9}$$

We match the logarithmic derivative of this internal wave function with that of the external wave function, (5):

$$(\varphi' / \varphi)\ \big|_{\text{internal}} = (\varphi' / \varphi)\ \big|_{\text{external}}\ ,\ \text{at}\ r = a \tag{10}$$

where the prime indicates the dimensionless derivative, rd/dr. We then find at once

$$Ka \cos (Ka) / \sin (Ka) = ika\ [-e^{-ika}\ - e^{2i\delta} e^{ika}] / [e^{-ika}\ - e^{2i\delta}\ e^{ika}]$$

which can be solved to yield:

$$\delta = \tan^{-1}\ [\ (ka / Ka) \tan Ka] - ka \tag{11}$$

This completely solves the heuristic problem, if we insert the phase shift into (8), but we shall solve it in another way immediately to achieve its heuristic value. We note, however, that the cross section, (8), has a maximum whenever $\delta = (n + ½)\,\pi$. Does this correspond to resonance? Surprisingly, the answer is no! We shall then enquire about the definition of resonance in this heuristic problem.

1.2.3 The Square-Well as a Resonant Cavity

To exhibit the resonances of the square-well we need to look at what happens inside the well. In the expression for the phase shift, Eqn. (11), the final term, -ka, is a hard sphere scattering phase shift, which pertains to the impact of the change in potential at the nuclear radius but has nothing to do with what happens inside. It depends on k, not on K. Instead, the resonances inside are given by that part of the phase shift which pertains to the wave number, K, inside. This part is (1/Ka) tan Ka. The expansion of this part in terms of resonances needs a definition of resonance and we do this using the radial wave equation inside to which we add an appropriate boundary condition at the nuclear radius to achieve a resonance or stationary state. This is the essence of the R-matrix theory.

We get standing waves, X_λ, with the radial equation,

$$-(\hbar^2 / 2m)\, d^2X_\lambda / dr^2 + V X_\lambda = E_\lambda X_\lambda \tag{12}$$

to which we add the boundary condition, at r = a

$$a\,(d X_\lambda / dr)_{|\, r=a} = b\, X_\lambda\,(a) \tag{13}$$

Where b is a real number, which we choose to be zero for this case – a choice that the physics will justify. We then have

$$X_\lambda = (2 / a)^{1/2} \sin (K_\lambda r) \tag{14}$$

and

$$K_\lambda = (\lambda + ½)\,\pi / a \tag{15}$$

Figure 1 shows the s-wave resonances for a typical nuclear square-well.

Because this is a Hermitian eigenvalue problem the X_λ form a complete set of states in terms of which we can expand any function, in particular, the internal wave function, $\phi(r)$.

$$\varphi\,(r) = \Sigma_\lambda\, C_\lambda\, X_\lambda\,(r) \tag{16}$$

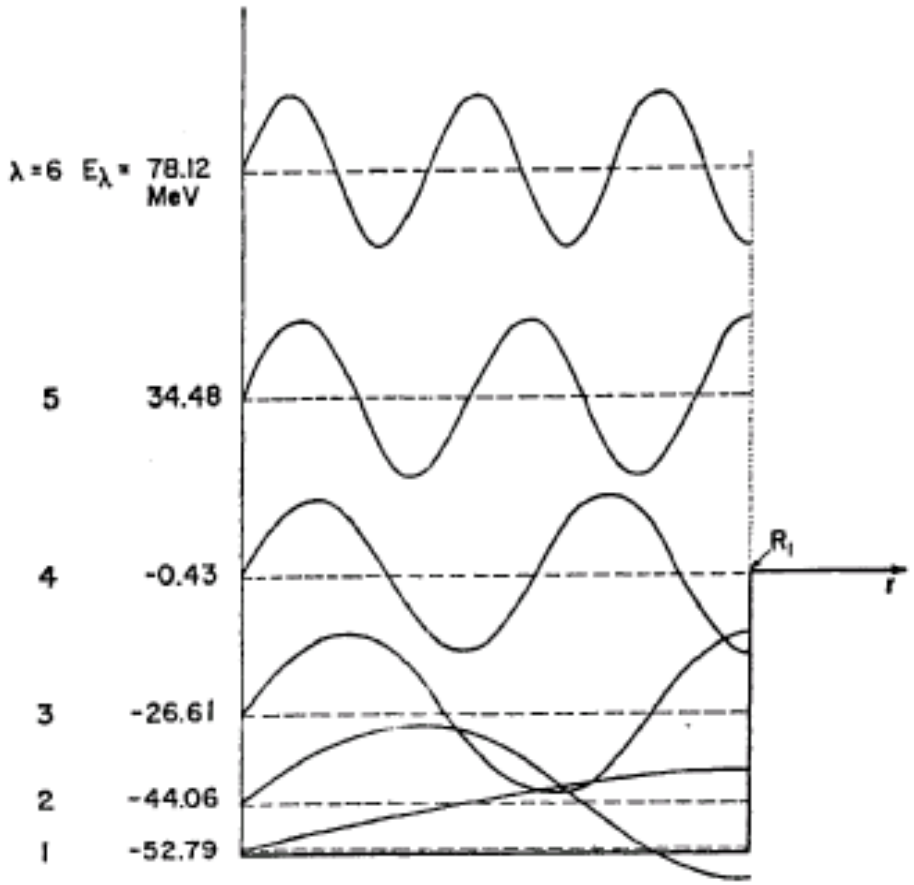

Fig. 1. The first six standing waves of the square well (A = 155) constructed with the natural boundary condition number for s-wave neutrons (b = 0).

with

$$C_\lambda = \int_o^a X_\lambda^*(r)\, \varphi(r)\, dr \qquad (17)$$

A straightforward application of Green's theorem then yields the logarithmic derivative, $r\,\phi'/\phi$, of the internal function evaluated at r = a – it was this logarithmic derivative which we used in constructing the phase shift – as a Fourier series with the stationary states, X_λ. We multiply (1) by $X_\lambda^*(r)$ and the complex conjugate of (12) by $\phi(r)$, subtract and integrate to obtain:

$$(\hbar^2 / 2m)\,[\varphi X_\lambda'^{\,*} - X_\lambda^* \varphi']_{r=a} = (E - E_\lambda) \int_o^a \varphi X_\lambda^*\, dr \qquad (18)$$

yielding

$$C_\lambda = (E_\lambda - E)^{-1} (\hbar^2 / 2ma)\, X_\lambda^*(a)\, [\varphi'(a) - b\varphi(a)] \qquad (19)$$

In both of which, again, the prime indicates, rd / dr. Inserting Eqn. (19) into Eqn. (16) yields:

$$\varphi'(a) / \varphi(a) = (1 + bR) / R \tag{20}$$

for the logarithmic derivative of the internal wave function, where the R-function is:

$$R = \sum_\lambda \gamma^2 / (E_\lambda - E) \tag{21}$$

with

$$\gamma^2 = (\hbar^2 / 2ma) \left| X_\lambda(a) \right|^2, \quad [= (\hbar^2 / ma^2), \text{ if } b = 0] \tag{22}$$

Eqn. (22) defines the reduced width, γ_λ^2. We remember that the logarithmic derivative of the internal wave function, Eqn. (9), of our problem is also given by Ka / tan Ka so that Eqn. (20) then yields:

$$(1/Ka) \tan Ka = R / (1 + bR) \tag{23}$$

which allows us at once to write the phase shift as

$$\delta = \tan^{-1} [ka R / (1 + bR)] - ka \tag{24}$$

in which the R-function is properly embedded. We shall note again, almost immediately, that for our problem b has the value 0.

We can also, instead, solve for the collision function, U, in terms of the R-function. Equating the logarithmic derivative of the external wave function, Eqn. (7) with that of the internal wave function, Eqn. (23), yields:

$$U = O^{-1} (1 - RL)^{-1} (1 - RL^*) I = e^{-2ika} (1+ bR - ikaR)^{-1}(1+ bR + ikaR) \tag{25}$$

which has a form that will be helpful to us later. In (25) all quantities are evaluated at the channel radius, a, and L is defined to be $L = O'O^{-1} - b$.

The new Eqns. (24) and (25), which we have just derived, allows us to display the Breit-Wigner formula for individual resonances. If we approximate the R-function, Eqn. (21), by a single term, λ, $R = \gamma_\lambda^2 / (E_\lambda - E)$, and use this in the phase shift, Eqn. (24), or in the collision function, Eqn. (25), we obtain for the cross section, Eqn. (8).

$$\sigma = (\pi / k^2) \left| 2 \sin ka \, e^{ika} - \Gamma_\lambda / [(E_\lambda - E + \Delta_\lambda) - i\Gamma_\lambda / 2] \right|^2 \tag{26}$$

with

$$\Gamma^\lambda \equiv 2ka \, \gamma^2 \quad \text{and} \quad \Delta_\lambda \equiv b\gamma^2 \tag{27}$$

The first expression in (27) is the level width and the second is the level shift (which vanishes here for b = 0). The factor of ka in the level width is the penetration factor, P.

The square-well resonances are clearly manifested in the single-level Breit-Wigner formula, Eqn. (24). If we are at low neutron energy (say well below 1 MeV so that ka is small) and far from resonance, that is, if E_λ - E is large, then the scattering term of Eqn. (24) dominates and the cross section is equal to πa^2, which is just the geometric cross section of the well. We would expect such a cross section because of the abrupt change in wavelength at r = a, even though we are dealing with a potential well rather than a hard sphere. Apart from the phenomenon of resonance, the external wave function at low energy does not distinguish between a hard sphere and a square-well. On the other hand if we are close to resonance then the second term of the amplitude in Eqn. (24) dominates. The cross section then exhibits the square-well resonances.

However, for s-waves the hard sphere phase shift and, indeed, the penetration factor, P, both have very rapid energy dependence so that the cross section as a function of the neutron energy, for a specific atomic weight, A, does not easily exhibit the natural square-well resonances. To exhibit them properly we choose, on Fig. 2, the artifice of plotting the neutron cross section at a fixed neutron energy (50 keV), as a function of the square-well radius (or, alternatively, as a function of the atomic weight, A). All of the well-known features of the resonance appear and the approximation of the actual cross section by the Breit-Wigner formula is also shown. The figure gives the Breit-Wigner result for several values of the boundary condition number, b. It is found that the "natural" (see below) value of b, (b = 0), for this case works very well.

We remark here also that the phenomenon of the energy dependence of the external quantities (hard sphere phase shift and penetration factors), disguising somewhat the resonances in the cross section, is a well-known effect. For electron scattering by atoms it is called the Ramsauer Effect and it is also prominent in the neutron scattering by nuclei, over the lowest 10 MeV, which gave rise to the nuclear optical potential (see Section 5).

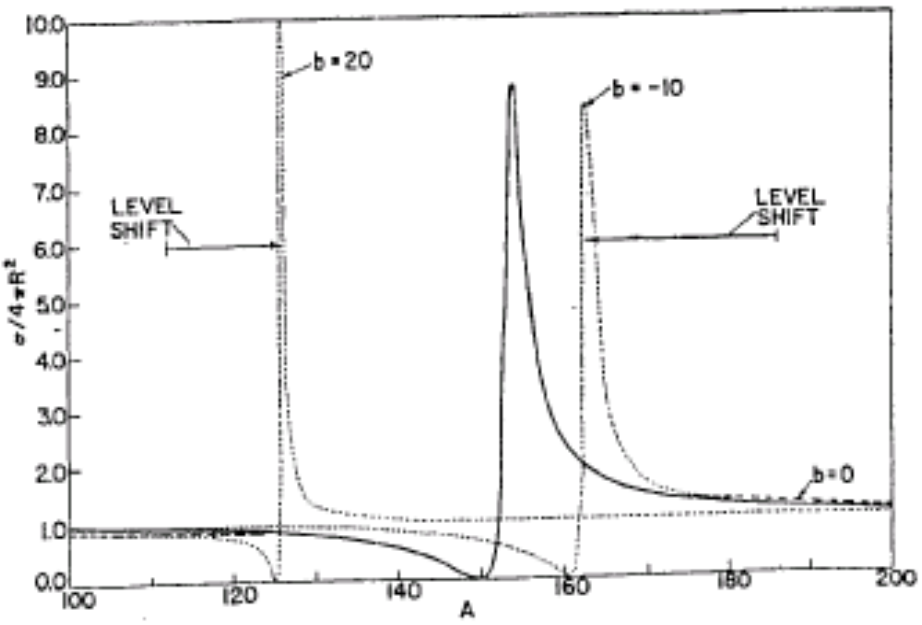

Fig. 2. The s-wave scattering cross sections for a nucleon by a square-well of depth 51 MeV and a radius, $a = 1.25\ A^{1/3}$ F, where A is the atomic weight. The solid line gives the exact cross section (divided by $4\pi a^2$) at 50 keV as a function of A. The broken lines give the one-level approximation to the cross section near the 4s resonance for various values of the boundary condition number, b. The heavy broken line, corresponding to $b = 0$, merges with the solid line near the resonance.

2 A MORE COMPLETE EXAMPLE

2.1 Scattering of a Spinless Particle by a Potential

In a lecture series we can be more discursive than in a review paper. Therefore we shall scale the heights of the R-matrix theory using not only the base camp of the last section (s-wave scattering of neutrons by a square-well) but building first a second camp in which we add further partial waves and also the Coulomb potential and permit a general potential well, V(r), in the internal region, for the interaction between the particle and the nucleus. The interaction potential includes the centrifugal potential for each partial wave. This second camp then pertains to the scattering of charged spinless particles by a nuclear potential well. It is the "base camp" of Ref. A (Section 4 – the didactic nature of this section of Lane and Thomas would be better served if it did not, initially, choose the boundary condition number $b_l = 0$ for all partial waves). The results of this further example not only bring us closer to the final heights but also are sufficiently complete to serve as a vehicle to discuss the relative merits of various frameworks for resonance reactions, including the advantages and disadvantages of R-matrix theory.

We then retrace the steps, which we took in Section 1 adding the effects of partial waves and the Coulomb Potential. "Externally" we now have phase shifts, δ_ℓ, and collision functions, $U_\ell = \exp(2i\delta_\ell)$ for each partial wave and we have the differential cross section:

$$d\sigma / d\Omega = (1/4k^2) \left| \Sigma_\ell (2\ell+1)(1 - U_\ell) P_\ell (\cos\theta) \right|^2 \qquad (28)$$

and the integrated cross section:

$$\sigma = \int (d\sigma / d\Omega)\, d\Omega = (\pi / k^2) \Sigma_\ell \, (2\ell + 1) \left| 1 - U_\ell \right|^2 \qquad (29)$$

which can be compared with (8).

"Internally" we have resonant states, $X_{\lambda\ell}(r)$, for each partial wave, ℓ, resulting from the Schroedinger equation and an imposed boundary condition, as in the preceding section.

The Schroedinger radial equation for the resonant states is identical to (12) [except for the inclusion of the centrifugal potential in V] for each partial wave:

$$-(\hbar^2 / 2m)(d^2 X_{\lambda\ell} / dr^2) + V(r) X_{\lambda\ell} = E_{\lambda\ell} X_{\lambda\ell} \qquad (30)$$

with the boundary condition,

$$a_\ell \, (dX_{\lambda\ell} / dr)|_{r=a} = b_\ell \, X_{\lambda\ell}(a_\ell) \qquad (31)$$

where b_ℓ is the boundary condition number chosen for each partial wave and a_ℓ is the matching radius chosen for each partial wave to separate the "internal' from the "external" regions. If the boundary condition numbers are real we have a proper Hermitian boundary value problem for the resonant states.

The actual internal wave function, ϕ_ℓ (r), at arbitrary energy, E, satisfies the same Schroedinger equation and then, by straightforward application of Green's theorem, as in the preceding section, we get its logarithmic derivative at the matching radius as:

$$(\varphi_\ell' / \varphi_\ell)|_{r=a_\ell} = (1 + b_\ell R_\ell) / R_\ell \qquad (32)$$

where again the prime indicates the dimensionless derivative, $rd\phi_\ell / dr$, and the R-function is defined as:

$$R_\ell = \Sigma_\lambda \gamma_{\lambda\ell}^2 / (E_{\lambda\ell} - E) \qquad (33)$$

with

$$\gamma_{\lambda\ell}^2 = (\hbar^2 / 2ma_\ell) X_{\lambda\ell}^2 (a_\ell) \qquad (34)$$

which corresponds to (21) and (22) of the preceding section. If the internal potential is a square-well (apart from the centrifugal interaction) of radius a, then it is shown in Ref. A that for the natural choice of boundary condition number (see below), $b_\ell = a_\ell \ell$, each reduced width is again given by $\gamma_{\lambda\ell}^2 = (\hbar^2 / ma^2)$, the same common value we had for s-waves.

If, as before, we match the internal and external logarithmic derivatives at the matching radii we obtain the result for the collision function corresponding to (25), that is:

$$U_\ell = O_\ell^{-1} (1 - R_\ell L_\ell)^{-1} (1 - R_\ell L_\ell*) I_\ell \qquad (35)$$

In which the I_ℓ, O_ℓ and L_ℓ pertain to the incoming and outgoing wave functions of the external region, as before, [$L_\ell \equiv O_\ell'/O_\ell - b_\ell$], but the angular momentum and Coulomb barriers in the external region have significantly altered all of these external quantities as we now indicate.

The external radial equation now is:

$$d^2\varphi_\ell / dr^2 - [\ell (\ell + 1) / r^2 + (2m / \hbar^2) (-E + Z_1 Z_2 e^2 / r)] \varphi_\ell = 0 \qquad (36)$$

This equation has regular solutions, F_ℓ, which are finite at r = 0, and irregular solutions, G_ℓ, which are not finite at r = 0. Their asymptotic behaviour at large r is:

$$F_\ell \sim \sin [kr - \eta \log (2kr) - (1/2)\ell\pi + \sigma_\ell] \qquad (37)$$

and

$$G_\ell \sim \cos [kr - \eta \log (2kr) - (1/2)\ell\pi + \sigma_\ell] \qquad (38)$$

where again k = (mv/ħ) and the Coulomb phase shift and the Coulomb parameter are given by:

$$\sigma_\ell = \arg [1 + \ell + i\eta] \tag{39}$$

$$\eta = Z_1 Z_2 e^2 / hv \tag{40}$$

and now we have incoming and outgoing waves:

$$I_\ell = (G_\ell - iF_\ell) \exp (i \omega_\ell) \tag{41}$$

and

$$O_\ell = (G_\ell + i F_\ell) \exp (-i \omega_\ell)$$

with

$$\omega_\ell = \sum_{n=1}^{\ell} \tan (\eta / n) \tag{42}$$

These yield:

$$L_\ell \equiv (O'_\ell / O_\ell) - b_\ell \equiv S_\ell - b_\ell + i P_\ell \tag{43}$$

Thus with these definitions of the regular and irregular wave functions and their asymptotic behaviour we get immediately the standard definitions of penetration factor, P_ℓ, shift functions, S_ℓ, and scattering phase shifts, Ω_ℓ :

$$P_\ell = (kr) / (F_\ell^2 + G_\ell^2) \tag{44}$$

$$S_\ell = (F'_\ell F_\ell + G'_\ell G_\ell) / (F_\ell^2 + G_\ell^2) \tag{45}$$

and

$$O_\ell^{-1} I_\ell = \exp (2i \Omega_\ell)$$

with

$$\Omega_\ell = \omega_\ell - \tan(F_\ell / G_\ell) \tag{46}$$

In the scattering phase shift ω_ℓ is the Coulomb phase shift and – tan (F_ℓ / G_ℓ) is the phase shift of a hard sphere (resulting from the division into external and internal quantities at the matching radius – the internal potential, V(r), doesn't have to be a square-well but we assume that it vanishes in the external region and thus the abrupt change at the matching radius introduces square-well phase shifts).

We now have all the apparatus needed to describe the resonances of all partial waves for the potential scattering of a spinless particle. In particular we can display the garden variety Breit-Wigner formula. If, for partial wave ℓ, we choose the R-function, Eqn. (33) to have a single resonance, λ, and we then insert this one-term R-function as well as the

external functions just described, into the collision function, Eqn. (35), and, in turn, use this collision function in the cross section formula Eqn. (29) we find:

$$\sigma = (\pi / k^2)(2\ell + 1) \mid - \exp(2i\Omega_\ell) \{1 + i\,\Gamma_{\lambda\ell} / [\,(E_{\lambda\ell} - E + \Delta_{\lambda\ell}) - (i/2)\,\Gamma_{\lambda\ell}\,]\,\} \mid^2 \quad (47)$$

Here we have

$$\Gamma_{\lambda\ell} = 2P_\ell\ \gamma^2_{\lambda\ell} \quad (48)$$

and

$$\Delta_{\lambda\ell} = (S_\ell - b_\ell)\ \gamma^2_{\lambda\ell} \quad (49)$$

This cross section contains all of the essential elements of resonance: unlike the s-wave example of the preceding section the resonance can be made as narrow as we wish by choosing its energy (through choice of the potential well depth), $E_{\lambda\ell}$, to be sufficiently far below the Coulomb or angular momentum barrier; it has an energy dependent level shift, $\Delta_{\lambda\ell}$, whose dependence on the choice of boundary condition number is clearly evident; it also has interference between potential and resonance scattering. Thus it has most of the elements of the real nuclear problem other than the complications of a multiplicity of reaction channels (under which the functions of (35) all become matrices, as we show in the next section) and the Clebsch-Gordanerie, which is introduced by the spins, which we have ignored here. These complications of the real nuclear problem are necessary but before introducing them we discuss the various reaction frameworks and the advantages and disadvantages of the R-matrix framework. For that comparison we don't require the complications.

2.2 Comparison of Reaction Frameworks

As we said at the beginning of these lectures, the nuclear forces are short range and this physical fact, combined with the Pauli Principle for nucleons, leads to a nuclear mean field, which is quite deep and has a reasonably well-defined radius. In other words, a cavity not unlike acoustic or electromagnetic cavities. The earliest reaction theory frameworks (Kapur-Peierls and R-matrix) employed the notion of cavities and their physics in the nuclear context. One theory (K-matrix) did not employ this physics. We compare the different frameworks here and comment in more detail on the advantages and disadvantages of R-matrix theory.

2.2.1 K-matrix Framework

The papers of Rosenfeld and Humblet[8] which introduced the K-matrix framework in the early 1960's were instigated by some real (see R-matrix below) and imagined problems with R-matrix theory. Rosenfeld thought that the channel parameters (matching radii and boundary condition numbers) of the R-matrix theory were too artificial. This framework then chose to ignore the mean field attributes of the problem and focus instead on the analytic properties of the scattering matrix and its parameterization in terms of a K-matrix. This followed the fashion of the time – since abandoned – in particle physics of eschewing the direct physics of hadron structure and focusing on the analytic properties

of the scattering matrix instead. In particle physics many interesting concepts emerged, such as Regge poles, but since the introduction of quarks and quantum chromodynamics the interest in these concepts has not been sustained. This approach for the nuclear problem also deserves now to be abandoned, although a number of papers for resonance analysis have used this approach, even recently, and have not encountered any great difficulty in fitting experimental data.

The problem with the K-matrix approach is that it introduces all kinds of analytic properties, such as ghost states, which are not easily related to nuclear structure. More generally, the resonance parameters of this framework also do not relate naturally to the quantities arising out of nuclear structure studies. There seems then little point in dwelling further on this framework here and little point in analyzing data with it. Rosenfeld's concerns did serve to direct attention to the physics of the channel parameters of the R-matrix theory, as we do (below) in Section 2.2.3.

2.2.2 The Kapur-Peierls Framework

In the middle 1930's – the very earliest years of nuclear physics – Kapur and Peierls[5] were the first to develop a comprehensive framework for nuclear resonance reactions. (The R-matrix theory developed a few years later). They divided the configuration space of all the particles into an external and internal region – just as we do for R-matrix theory – but they chose very different boundary condition numbers for the resonances of the internal region. Looking at Eqn. (35), Kapur and Peierls chose L_ℓ (not L_ℓ^*) to be zero by the choice:

$$b_\ell = S_\ell + iP_\ell \tag{50}$$

This special choice brings with it some significant advantages. First, the boundary condition number corresponds to purely outgoing waves: quite naturally, the resonances decay. Second is the enormous advantage, when we change all the functions to matrices as in the next section, that matrix inversion is entirely avoided. Those who struggle with the complicated matrices of the R-matrix theory will wish fervently that the framework of Kapur and Peierls would have triumphed.

It is the significant disadvantages of the framework, which have limited its usefulness. The first of these is that the boundary condition numbers are strongly energy-dependent. As we shall see, the shift functions vary relatively slowly with energy (this is the saving grace of the R-matrix theory) but the penetration factor does not! This easily vitiates any analysis of low energy resonance reactions with this framework. Another disadvantage is that the extracted resonance parameters are not easily connected to the parameters emerging from nuclear structure calculations. Finally, there is a more mathematical disadvantage, namely that the boundary conditions are complex numbers. This means that the eigenvalue problem for the resonance states is not Hermitian and the completeness theorems do not necessarily hold.

This speaker is not aware of many analyses of data, which employ the Kapur and Peierls framework but it has been used for the theory of direct reactions[9].

2.2.3 A General Discussion of the Advantages and Problems of R-Matrix Theory

It will become evident in the sections, which follow that the R-matrix theory is a proper framework for the description of resonance reactions, especially the kind of nuclear reactions, which dominate for astrophysical reaction rates. It is solidly based in our physical knowledge of the atomic nucleus: it relates easily to the ideas associated with the nuclear mean field; its resonance energies relate easily to observed energy levels; its reduced widths correspond to the spectroscopic factors of these levels as calculated with the nuclear shell model; it leads straightforwardly to resonance cross section formulae when one requires approximations involving either a small number of levels or a small number of reaction channels; it is easily employed to derive results for average cross sections at higher energy, such as those needed for the interpretation of the optical model of nuclear reactions. In short, it has a universality of application and a close tie to physics not matched by the other frameworks. It is in this perspective that we discuss the problems of the R-matrix theory.

The first reaction of many people to the R-matrix theory is that it is cumbersome. It is! As we shall find, it usually involves matrix inversion, which makes the written formulae messy and makes the work of diligent programmers, such as our esteemed colleague, Professor Azuma, quite tedious.

Although, formally, the R-matrix theory is all encompassing, the treatment of resonance reactions with the R-matrix usually involves focusing on the data in a small energy interval and then, necessarily, making approximations which throw away all levels or channels not pertinent to that interval. That means that direct reactions – which require contributions from large energy intervals – are thrown away along with the discarded levels in such approximations. Even the scattering phase shifts of the formulae are those of a hard-sphere rather than the appropriate mean-field phase shifts. (We shall comment on this more fully below.) Therefore direct reactions, even direct capture reactions, do not easily emerge from the R-matrix framework and are an add-on because they arise from the distant levels, which were thrown away.

Historically the greatest unease with the R-matrix theory arose from the auxiliary parameters of the theory – the matching radii and the boundary condition numbers, both needed to define the resonant states and thus give body to the theory – which many regarded, initially, as both arbitrary and artificial. This unease was not helped by the fact that almost all of the early papers on R-matrix theory emphasized the arbitrariness of these parameters. Often the boundary condition numbers were simply chosen to be zero for all channels – a good choice if they are indeed arbitrary – and even in Lane and Thomas (Ref. A) the heuristic section on elastic scattering by as spinless potential interaction begins by making this choice of boundary condition number for all partial waves. For such reasons we shall focus here on the physics of these auxiliary parameters and show that there are "natural" definitions well rooted in good physics. This then becomes a strength, not a weakness, of the theory. The initial unease was misplaced. However, we pay a price for such natural definitions. The boundary condition numbers may become modestly energy dependent, not enough so that it vitiates a resonance

analysis of data in a relatively small energy interval. Such natural choices improve the connection to nuclear structure.

2.3 Natural Boundary Conditions and Matching Radii

To preserve the Hermitian nature of the eigenvalue problem for the resonant states the R-matrix theory insists that all the b_ℓ are real. Thus we cannot make the Kapur-Peierls choice, Eqn. (50). What can we do? There is some advantage to making the choice to correspond as closely as possible to that of purely outgoing waves. Therefore it is tempting to alter Eqn. (50) and to make the b_ℓ equal to the real part of the logarithmic derivative of an outgoing wave, namely:

$$b_\ell \equiv S_\ell \tag{51}$$

This can be compared to Eqn. (50). We shall call this the "natural" boundary condition.

The shift functions generally vary slowly with energy (the only real exception pertains to "halo" states, s-wave neutron states which are slightly bound: such states extend very far beyond any normal matching radius and thus require special care, in any case, in any resonance analysis) so that if we make the choice of energy at which the equality Eqn. (51) holds to be in the energy interval in which the data is analyzed then the level shifts, Δ_ℓ, are close to zero for all of the resonances in the interval and we then have the happy circumstance that the resonance energies, $E_{\lambda\ell}$, all nearly coincide with the positions of the states of the nucleus. We also note (see Section IV of Ref. A) that for neutrons at zero energy the natural boundary condition number, Eqn. (51), is $b_\ell = a_\ell\ \ell$, as noted above, and that then all of the single-particle neutron widths have the familiar value ($\gamma_{\lambda\ell}^2 = (\hbar^2 / m a_\ell^2)$ which holds for s-wave neutrons. Thus the natural boundary condition numbers are not only physically compelling but they also make the extracted level energies and level widths as close as possible to those arising from the shell model.

What then should one do about the boundary condition numbers in fitting astrophysical reaction data? We recommend that one choose the boundary condition numbers so that for each reaction channel it is a fixed number chosen so that the level shift vanishes somewhere in the energy interval of interest. Where? This should not matter much. If the choice does matter – as is the case for halo states – then more care must be taken. Perhaps one can say that the very applicability of the R-matrix framework comes into question if the level shifts vary sufficiently with energy to affect the data analysis. This is then like a warning bell.

Having chosen the boundary condition numbers as suggested one should not ignore the level shifts completely, even though they will be quite small. After all, the level shift function is moderately energy-dependent and it is best to include it explicitly in the level formulae. Alternatively, approximate methods exist (see Ref. A) for including the first order energy dependence of the shift function by using its energy derivative to renormalize the reduced widths. Usually this approximate method is more cumbersome to employ than incorporating the proper shift function in the formulae as we have suggested.

The occurrence of a finite but nonzero value of b_ℓ essentially implies that we have an impedance matching problem, a term deliberately meant to convey the kind of situation which one encounters in the analysis of electromagnetic cavities – a classical problem from which the R-matrix theory gained a significant amount of its original impetus. This led us to make some general remarks about boundary conditions.

In order for a wave equation to have solutions, $X_{\lambda\ell}$, which are part of Hermitian boundary value problem we need at the boundaries to have linear homogenous boundary condition such as $rdX_{\lambda\ell}/dr = b_\ell X_\lambda$, where b_ℓ is a real constant. The need for boundary conditions of this kind arises from the same Variation Principle or Action Principle as the wave equation itself.

A classical example familiar to every student of physics pertains to the vibrations of a stretched string under tension, T. To make an analogue with the resonances of neutrons, above, we consider on Fig. 3, a string which has a fixed end at its left end (to simulate the fact that the radial equation must be finite at r = 0) and then enquire about what we are allowed to do at the right end of the string. Usually discussions of stretched strings refer to two specific cases: a fixed end ($b_\ell = \infty$) or a free end ($b_\ell = 0$). But what about the physics of the more general case where b_ℓ is allowed to have any finite or infinite value? For the string, as the figure shows, this physics can be achieved by attaching to the end of the string a vertical, massless spring (restoring force for vertical displacements, y, is $F = sy$, where s is the spring constant). As the end of the string moves the vertical component of the tension, T, is balanced exactly by the restoring force of the spring, that is, $T\, dy/dr = sy$. Thus for this system of string plus spring we have a general boundary condition for the end of the string which is $r\, dy/dr = (rs/T)\, y$, so that we have $b_\ell = sr/T$, an arbitrary constant, and we can achieve arbitrary values of the boundary condition number simply by varying the spring constant. To make an analogue for all partial neutron waves, ℓ, we choose the spring constant to have the value $s = \ell\, T$. In this string-spring system we impedance-match at the right-hand boundary to accommodate the spring, or in the case of the neutron waves, to accommodate the effect of the angular momentum barrier.

Although the natural boundary condition numbers have been discussed for four decades, the choice of matching radii has had much less attention. Even in many recent fits to astrophysical reaction data the matching radius has been left as a free parameter. Yet there is some physics guidance for the choice. If dealing with the potential scattering of neutrons by a square-well interaction only a fool would choose a matching radius different from the square-well radius. But why not be the fool? After all, the framework allows an arbitrary choice. I discussed this in a paper[10] almost a decade ago, and showed that for s-wave neutrons, making a choice different from the square-well radius led to obtaining the wrong level width for the calculation of Fig. 2, just as the choice of the non-natural boundary condition number led to the wrong position of the energy level. Thus, in this case, physics dictates the sensible choice of a. This appears to be more difficult to demonstrate for higher partial neutron waves but still, for square wells, the sensible choice should prevail.

But what should one do for the typical nuclear reaction in which the mean field has a Saxon-Woods shape with a mid-point radius and a surface thickness significantly smaller? Should one choose a large matching radius so that most of the mean field is in

the internal region? Should one leave the radius as a free parameter? There is no easy answer to these questions.

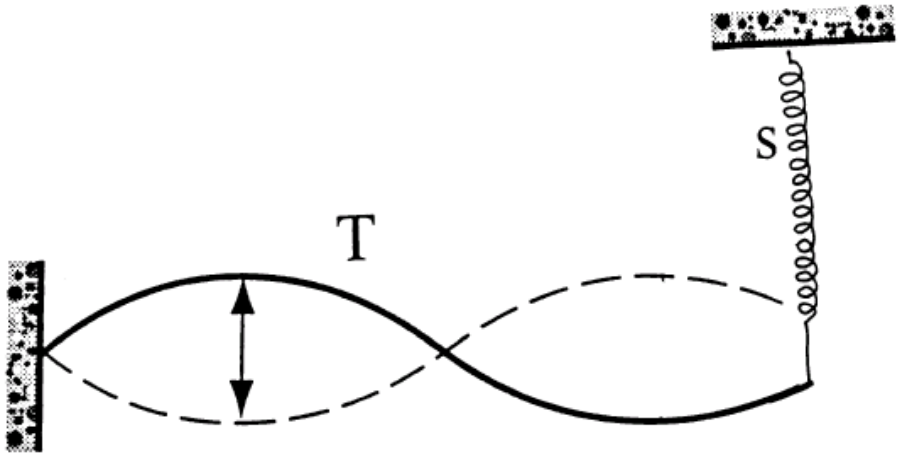

Fig. 3. A mechanical analogue for the general boundary condition, $b = r\,\phi'/\phi$ at $r = a$, of the radial wave function. In the analogue we have a stretched string, with tension T, which is fixed at the left end (to simulate the fact that the radial wave function vanishes at $r = 0$) and at the right hand we have attached the string to a vertical massless spring, of spring constant s. By varying either s or T we can achieve either the usual "fixed" end boundary condition or the usual "free" end boundary condition or any value of b in between these two extremes.

It turns out that the R-matrix fits to data do not generally appear to depend critically on the choice of radius, at least within a sensible range, say from the mid-point radius of the mean field up to a few fermis beyond it. Fred Barker[11] has explored this insensitivity of the framework to choice of radii. Still we should remember that it we move the radius outward, in the presence of significant barriers, then the width may not change but the penetration factor may become much smaller and the reduced width correspondingly larger. It is a matter then of which choice of radius leads to reduced widths, which are readily comparable to the results of nuclear structure calculations. As discussed in Ref. C, the right choice for this purpose appears to be a matching radius approximately one fermi larger than the mid-point radius of the mean field. That makes good common sense but one should also feel free to vary the choice a little about this sensible value.

Any such choice then leads to a troubling matter for the R-matrix framework. Since the mean field falls quickly but reaches zero only at very large radius are we correct in ignoring it completely in the external region? Surprisingly the answer appears to be yes. Strictly speaking, if we are dealing with a reaction problem in which much data has yielded a physical answer to the parameter of the optical potential which applies to the problem we should, after making our choice of radius, use the tail of the real part of the optical potential, which lies beyond the matching radius to modify the external wave functions. The way to do this is straightforward in principle. We choose a radius much

beyond the matching radius at which the real part of the optical potential is negligible and then take the regular and irregular solutions, F_ℓ and G_ℓ, and continue them inward, analytically, up to the matching radius through that part of the external region in which the optical potential cannot be neglected. These modified wave functions will lead to significant modifications of the penetration and shift functions. In particular the level widths will be significantly larger because the Saxon-Woods potential is much less reflective than the square-well embedded in the R-matrix formulation. (In the R-matrix, if we have a potential in the internal region but ignore if outside then, in effect, we make the abrupt change, which pertains to a square-well).

Fortunately there is a fix, which works and, quite generally, allows one to forget about making those analytic continuations of the external quantities. Almost half a century ago Peaslee[12] showed that if one multiplies the reduced widths by a reflection factor given by,

$$f = (2^{1/2}\ \pi\ K\ d)\ \coth\ (2^{1/2}\ \pi K\ d) \qquad (52)$$

where K is the wave number deep inside the optical potential and d is the surface thickness, then the level widths are corrected for reflection. Further, in ref. C it is shown that the usual R-matrix framework with its garden-variety regular and irregular wave functions applies. I would not want to discourage some ambitious theorist in showing how well this approximate procedure works in fitting actual data, compared to making the correct analytic continuations!

3 THE FEW- CHANNEL, MULTI-LEVEL R-MATRIX THEORY

We now tackle the full nuclear problem with its denumerable infinity of reaction channels and its denumerable infinity of energy levels. At first we must enumerate the reaction channels. Then we follow the preceding sections in showing how the collision matrix, whose rows and columns pertain to channels, can be connected to an R-matrix. Of course, in the description of cross section one must make approximations within this framework. In this section we show how, if one retains only a few channels, the implicit matrix inversion is manageable and one is then led directly to the few-channel, many-level approximations of the R-matrix theory. In the next section we show another way in which the approximations can be made manageable. The R-matrix has the felicitous property that the problem of matrix inversion, in a space which pertains to channels, can be transformed into a problem of matrix inversion in a space pertaining instead to levels. In this new space one then obtains the many-channel, few-level approximate formulae, which are required for many applications to astrophysical reactions.

3.1 The Configuration Space for Nuclear Resonances

We first enumerate the reaction channels. If we have A nucleons the configuration space has 3A dimensions and this cannot easily be depicted on a two-dimensional drawing. Ignoring the multitude of dimensions we qualitatively describe the external and internal regions of the space for resonance reactions on Fig. 4, taken from Ref. B. There is an internal region of the compound nucleus (in this case Be^8) in which, perhaps very briefly, all of the A nucleons are together in a resonance state. In the external region are the various possible channels through which the compound nucleus can be formed or decay. The system looks rather like a Scottish bagpipe, which consists of a bag with many pipes protruding from it. If one blows into one pipe rude noises may emerge from any of the others. The physical reason why the space can be divided into such external and internal regions is that the forces between nucleons are rather short range (one of the miracles that emerges from QCD where the underlying gluon forces increase with distance!).

It is the external wave functions, which enumerate the reaction channels. We write the total external wave function as a sum of products, for each channel c, of the radial wave function, ϕ_c, with the channel wave function, ψ_c:

$$\Psi_c = \Sigma_c \; \Psi_c \; \varphi_c \tag{53}$$

in which the channel wave function is:

$$\Psi_c \equiv (1/r_c)\Phi_\alpha \Sigma_{m\ell} \Sigma_{m_s} (ls m_l m_s | J M_J) i^l i_{\ell m_\ell} \; X_{s m_s} \tag{54}$$

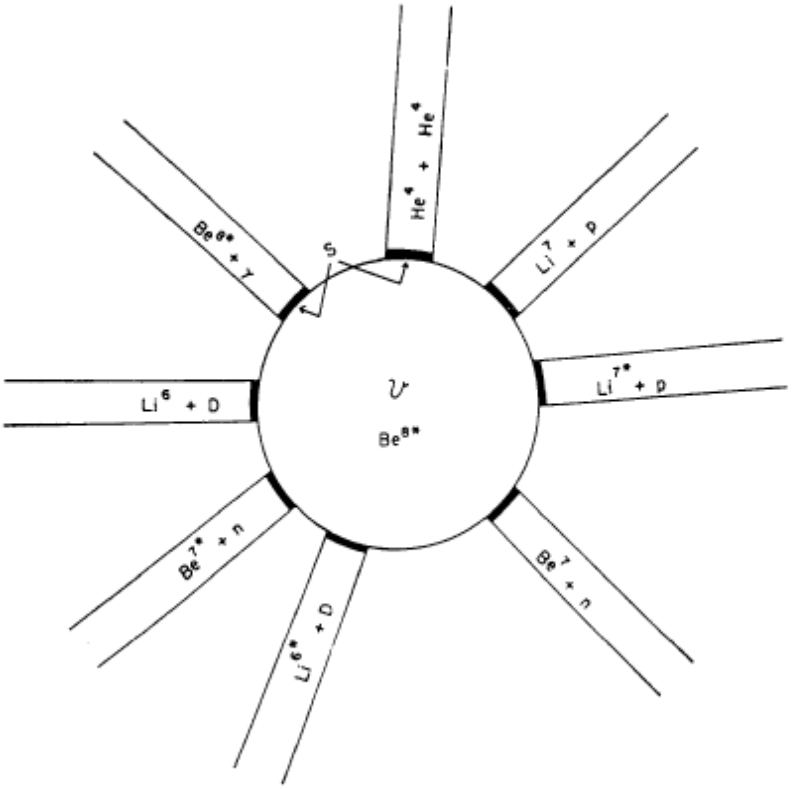

Fig. 4. A rough illustration, in two dimensions, of the various regions in the many-dimensional configuration space pertinent to the theory of resonance reactions. The compound nucleus, say Be^8, is shown by the region marked *V*. A number of channels emerging from *V* are also shown, e.g. Li^7 + p, corresponding to an emitted proton and Li^7 in its ground state, or Be^{7*} + n, corresponding to an emitted neutron and Be^7 in an excited state. Only a few of the reaction alternatives are shown: the angular momentum quantum numbers, which, together with the reaction alternative, define a channel, are not indicated. The surface, *S*, of the compound nucleus is shown by heavy lines.

in which Φ_α represents the state of internal excitation of the two particles in the channel. Thus the reaction channel, c, is specified by the quantum numbers $c \equiv (\alpha, \ell, s, J, M_J)$. We note that for this choice of channel parameters we have recoupled the angular momenta in order to obtain **J.** The vector additions involved are:

$$s = I + i, \qquad J = \ell + s \tag{55}$$

in which I and i are the intrinsic spins of the two particles in the channel.

The ψ_c are a set of unit vectors for the external channel space. At the nuclear surface ($r_c = a_c$), where a_c is the chosen matching radius for the channel, we get a piece, S_c, of the total channel surface, S, of configuration space.

$$S=\Sigma_c S_c \tag{56}$$

In any integration over the total channel surface we must, of course, integrate over all of the angles of the piece, S_c.

The clear separation into external and internal parts of the configuration space holds only if we have a proper orthogonality condition for the channel wave functions, that is:

$$\int_s \Psi_c \Psi_{c'} * dS = \delta_{cc'} \tag{57}$$

This orthogonality condition exerts some constraints on the choice of channel radii: we should not choose the matching radius too close to the internal region of the compound nucleus (in general, the choice of a matching radius about one fermi larger than the mid-point radius should suffice for this purpose).

We are now ready to define the internal and external bits of the problem as we did in the preceding two sections. For no good reason we reverse the previous order and deal with the internal bits first, thus defining the R-matrix, and then in the following subsection we connect the R-matrix to the collision matrix and, in turn, to the cross sections. The derivations in the next two subsections are more in the nature of sketches, relying on the more complete treatment of the simpler problems in the preceding two sections: fuller treatment can be found in either ref A or ref, C.

3.2 The Internal Bits of the Nuclear Problem

In the full configuration space we write down the Schroedinger equation for the full wave function, Ψ,

$$H\Psi = E\Psi \tag{58}$$

as well as for the resonant states, X_λ:

$$HX_\lambda = E_\lambda X_\lambda \tag{59}$$

whose definition requires, in addition to the wave equation, an imposed boundary condition at each piece of the channel surface:

$$\left[\left(r_c \, dX_\lambda / dr_c \right) / X_\lambda \right] |_{r_c = a_c} = b_c \tag{60}$$

The resonant states again form a complete set in terms of which we can expand the full wave function:

$$\Psi = \Sigma_\lambda C_\lambda X_\lambda \tag{61}$$

with expansion coefficients:

$$C_\lambda = \int X_\lambda * \Psi \, dV \tag{62}$$

for which the integration extends over the full volume of the internal configuration space.

Again, we use Green's theorem to find the expansion coefficients of the harmonic analysis, Eqn. (62). This yields:

$$C_\lambda = (E_\lambda - E)^{-1} \Sigma_c \gamma_{\lambda c} (\varphi' - b_c \varphi_c) (\hbar^2 / 2 m_c a_c) \quad (63)$$

where prime again indicates the dimensionless derivative (rd / dr) and the reduced width amplitude is given by:

$$\gamma_{\lambda c} = (\hbar^2 / 2 m_c a_c)^{1/2} \int \Psi_c^* X_\lambda \, dS \quad (64)$$

Evaluating the harmonic analysis on the full surface, S we then find the derivative of the internal wave function on the channel surface in terms of its value at the surface – and, finally, it provides us with the much-sought R-matrix:

$$(\hbar^2 / 2 m_c a_c)^{1/2} \varphi_c = \Sigma_{c'} R_{cc'} [\varphi_{c'}' - b_{c'} \varphi_{c'}] (\hbar^2 / 2 m_{c'} a_{c'}) \quad (65)$$

and

$$R_{cc'} = \Sigma_\lambda \gamma_{\lambda c} \gamma_{\lambda c'} / (E_\lambda - E) \quad (66)$$

We shall comment shortly (Section 5) on the physics of the reduced width amplitudes but first we complete the external bits of the problem.

3.3 The External Bits of the Nuclear Problem

By writing the radial wave function of Eqn. (53) in terms of incoming and outgoing waves the full external wave function is:

$$\Psi = \Sigma_c (1 / v_c)^{1/2} (A_c I_c - B_c O_c) \Psi_c \quad (67)$$

The incoming A_c and B_c are arbitrary coefficients and the incoming and outgoing waves have asymptotic behaviour which follows from Eqn. (37) and Eqn. (38), namely:

$$I_c^* = O_c \approx \exp i [k_c r_c - (1/2) \ell_c \pi_c - \eta_c \ell n (2 k_c r_c)] \quad (68)$$

The collision matrix is then defined by the connection between incoming and outgoing waves:

$$B_c = \Sigma_c U_{cc'} A_c \quad (69)$$

In words, it gives the outgoing waves in each channel from the incoming waves in any channel. If we multiply Eqn. (67) by ψ_{c*} and then integrate over the full channel surface, S, we get:

$$\varphi_c = (1 / v_c)^{1/2} [A_c I_c - \Sigma U_{cc'} A_{c'} O_{c'}] \quad (70)$$

in which we have incoming waves in the channel, c, leading to outgoing waves in all channels. We now take the derivative of the channel wave function Eqn. (70) and divide it by the wave function to obtain its logarithmic derivative. Matching this with the logarithmic derivative of the internal wave function obtained from Eqn. (65) we then get the collision matrix in terms of the R-matrix:

$$U_{cc'} = (k_c\ a_c)^{1/2}\ O_c^{-1}\ \Sigma_{c''}\ [1 - RL\ ]^{-1}_{cc''}\ [\delta_{c''c'} - R_{c''c'}\ L_{c'}^{*}]\ I_{c'}\ (k_{c'}a_{c'})^{-1/2} \quad (71)$$

We have displayed all of the indices of the matrices, which clearly indicates which quantities are column matrices and which are two-dimensional matrices. We now see that, apart from the matrix indices Eqn. (71) is the same as Eqn. (25) or Eqn. (35) of the simpler examples.

We can change Eqn. (71) into a more recognizable form – a form, which lends itself more directly, to the R-matrix programs – by observing that:

$$(k_c a_c)^{1/2}\ O_c^{-1}\ \ell_{c'}\ (k_{c'}a_{c'})^{-1/2} = \exp\,[i\,(\Omega_c + \Omega_{c'})\,]\ P_c^{1/2}\ P_{c'}^{-1/2} \quad (72)$$

where Ω_c is the combination of hard-sphere and Coulomb phase shifts given by Eqn. (46) and $L_c \equiv S_c + i\,P_c$. The result for the collision matrix is then:

$$U_{cc'} = \exp\,(i\,\Omega_c + \Omega_{c'})\ P_c^{1/2}\ P_{c'}^{-1/2}\ \Sigma_{c''}\ [1 - RL]^{-1}_{cc''}\ (\delta_{cc''} - R_{c''c'}\ L_{c'}^{*}) \quad (73)$$

This is the few-channel many-level form of the collision matrix to be used in the R-matrix theory and for which Azuma has developed general programs. We call it the "few-channel" form because the cumbersome matrix inversions make this formula easily usable only when we are dealing with only a few channels. In Section 5 we comment further on its use and on the relation of its parameters to nuclear structure.

3.4 Cross Sections in Terms of Collision Matrix Components

These lectures have focused on the relation between the collision matrix and the R-matrix because that is where the nuclear physics occurs. The measurements, of course, pertain to cross sections, not collision matrix components and therefore for the R-matrix programs must incorporate the connection of the observed collision cross sections to the collision matrix. This connection is straightforward but cumbersome and involves no nuclear physics. Many review papers give the connection fully (see, for example, Ref. A of Ref. B) and we only sketch it here somewhat incompletely so that the perspective of the whole problem can be understood. In this sketch we follow Ref. B.

For the cross section formulae one must observe the angular momentum recoupling rules, implied in Eqn. (55) above, and these recouplings lead to all the Clebsch-Gordanerie. Also, one averages over incidents polarizations and sums over final one. The differential

cross section for a reaction pair, α, with channel spin, s, proceeding to reaction pair, α′, with channel spin, s′, is:

$$d\sigma_{\alpha' s';\alpha s} = \frac{(k_\alpha)^{-2}}{(2s+1)} \sum_{L=0}^{\infty} B_L(\alpha' s' : \alpha s) P_L(\cos\theta) d\Omega \tag{74}$$

where

$$\begin{aligned} B_L(\alpha' s';\alpha s) = & \frac{(-)^{s'-s}}{4} \sum_{J_1} \sum_{J_2} \sum_{\ell_1} \sum_{\ell_2} \sum_{\ell_1'} \sum_{\ell_2'} \\ & \times i^{\ell_1 - \ell_2 - L} Z(\ell_1 J_1 \ell_2 J_2; sL) i^{\ell_1' - \ell_2' - L} Z(l_1' J_1 \ell_2' J_2; s' L) \\ & \times R.P.\left[\left(\delta_{\alpha\alpha'} \delta_{\ell_1 \ell_1'} \delta_{ss'} - U_{\alpha' s' \ell_1'; as \ell_1}^{J_1} \right)^* \left(\delta_{\alpha'\alpha} \delta_{s's} \delta_{\ell_2 \ell_2'} - U_{\alpha' s' \ell_2'; \alpha s \ell_2}^{J_2} \right) \right] \end{aligned} \tag{75}$$

The Z coefficients are products of Clebsch-Gordan coefficients. This differential cross section may be integrated over all angles to yield the angle-integrated result:

$$\begin{aligned} \sigma_{\alpha' s';as} &= \frac{4\pi}{(2s+1)k_\alpha^2} B_0(\alpha' s';\alpha s) \\ &= \frac{\pi}{(2s+1)k_\alpha^2} \sum_{J=0}^{\infty} \sum_{\ell=|J-s|}^{J+s} \sum_{\ell'=|J-s'|}^{J+s'} (2J+1) \left| \delta_{\alpha'\alpha} \gamma_{s's} \delta_{\ell'\ell} - U_{\alpha' s' \ell'; as l}^{J} \right|^2 \end{aligned} \tag{76}$$

In turn, this may be summed over all outgoing channels, α′, s′, to yield the total cross section:

$$\begin{aligned} \sigma_T(\alpha\ell) &\equiv \sum_{s,\alpha',s',\ell'} \frac{(2s+1)}{(2l+1)(2i+1)} \sigma_{\alpha' s' \ell'; as \ell} \\ &= \frac{\pi}{(2l+1)(2i+1)k_\alpha^2} \sum_{J=0}^{\infty} (2J+1) 2 R.P.\left[1 - U_{\alpha,s,l;as l}^{J} \right] \end{aligned} \tag{77}$$

The result for the total cross section has employed the fact that the collision matrix is a unitary matrix, a condition that can be written as:

$$\sum_{\alpha',s',\ell'} U_{\alpha' s' \ell'; as \ell}^{J} U_{\alpha' s' \ell'; as \ell}^{J*} = 1 \tag{78}$$

In (77) R.P. stands for "real part". We have also in the total cross section averaged over initial spins and summed over final spins. The factor $[(2I + 1)(2i + 1)]^{-1}$ arises from the initial state average over spins.

The general properties of the collision matrix, such as its unitarity, are very interesting and intimately tied to conservation laws, such as time-reversal invariance, detailed balance, causality, etc. However, this topic is beyond the scope of these lectures. More on this subject can be found in Ref. A.

The matter of the coherence of different partial waves is of some interest. When do waves of different ℓ or J interfere with each other, as in Eqn. (75)? There is a general answer: when we integrate over the angles to which the partial waves, ℓ, pertain the coherence (or interference) disappears. Similarly, if we look at the cross sections for polarized beams or target particles the states of different spin polarization are coherent but this interference disappears when we sum or average over spin polarizations. The cross sections including polarization can be found in my review paper on the Statistical Theory of Nuclear Reactions[13].

4 THE FEW-LEVEL, MULTI-CHANNEL R-MATRIX THEORY

4.1 The Level-Matrix Form of the Collision Matrix

Through what appears to be almost "matrix-magic" the cumbersome problem of inverting a matrix, in Eqn. (73) whose rows and columns refer to channels, can be turned around to, instead, inverting a matrix whose rows and columns refer to levels. In this new form it is easy to handle many channels as long as we restrict the number of levels to something manageable. The result, which we shall prove, yields a form of the collision matrix alternative to Eqn. (73) as follows:

$$U_{cc'} = \exp[\, i\,(\Omega_c + \Omega_{c'})\,]\,\{\delta_{cc'} + i\Sigma_{\lambda\lambda'}\,\Gamma_{\lambda c}^{1/2}\,\Gamma_{\lambda' c'}^{1/2}\,A_{\lambda\lambda'}\} \tag{79}$$

where

$$\Gamma_{\lambda c}^{1/2} = (\,2\,P_c\,)^{1/2}\,\gamma_{\lambda c} \tag{80}$$

and

$$(\,A^{-1})_{\lambda\lambda'} = (E_\lambda - E)\,\delta_{\lambda\lambda'} + \Delta_{\lambda\lambda'} - (i/2)\,\Gamma_{\lambda\lambda'} \tag{81}$$

with

$$\Delta_{\lambda\lambda'} = \Sigma_c\,\gamma_{\lambda c}\,\gamma_{\lambda' c}\,(S_c - b_c) \tag{82}$$

and

$$\Gamma_{\lambda\lambda'} = \Sigma_c\,\gamma_{\lambda c}\,\gamma_{\lambda' c}\,2P_c \tag{83}$$

We comment below on how this level matrix formulation of the R-matrix theory is, generally, at least as useful as the many-level, few-channel formula for application in nuclear astrophysics. It leads very easily to the Breit-Wigner formula. First we prove Eqn. (79).

4.2 Proof of the Level-Matrix Form of the Collision Matrix

The proof of the level-matrix form of the collision matrix was first given by Thomas[14]. It relies on the fact that the R-Matrix, $R_{cc'}$, is a sum over levels of individual terms each of which is a product of one term depending only on c and the other term depending only on c′. To make the proof we assume that:

$$[\,(1 - RL)^{-1}\,(1 - R\,L^*)\,]_{cc'} = \delta_{cc'} + \Sigma_{\lambda\lambda'}\; 2\,i\,P_{c'}\;\gamma_{\lambda c}\;\gamma_{\lambda' c'}\;A_{\lambda\lambda'} \tag{84}$$

and we find $A_{\lambda\lambda'}$ to complete the proof. We begin by multiplying both sides of Eqn. (84) by the matrix (1 – RL) from the left and thus we get:

$$\begin{aligned}(1- RL^*)_{cc'} = \Sigma_{c''}(\delta_{cc''} - R_{cc''}L^*_{c''})\delta_{c''c'} + \Sigma_{c''}[\delta_{cc''} - \Sigma_\lambda\;\gamma_{\lambda c}\;\gamma_{\lambda c''}\;/ \\ (E_\lambda - E)]\;[\Sigma_{\lambda''\lambda'}\,2i\,P_{c'}\gamma_{\lambda'' c''}\gamma_{\lambda' c'}A_{\lambda''\lambda'}]\end{aligned} \tag{85}$$

In Eqn. (85) we have changed the dummy index, λ, of Eqn. (84) into λ''. Writing Eqn. (85) out more fully we get:

$$\begin{aligned}\delta_{cc'} - \Sigma_\lambda\,\gamma_{\lambda c}\,\gamma_{\lambda c'}\,L^*_{c''}\,/\,(E_\lambda - E) = \delta_{cc'} - \Sigma_\lambda\gamma_{\lambda c}\gamma_{\lambda c'}\,L_{c'}\,/\,(E_\lambda - E) + \\ \Sigma_{\lambda\lambda'}\,2i\,P_{c'}\,\gamma_{\lambda c}\,\gamma_{\lambda' c'}A_{\lambda\lambda'} + \Sigma_{\lambda\lambda'\lambda'' c''}\,\gamma_{\lambda c}\gamma_{\lambda c''}\,(E_\lambda - E)^{-1}\,2i\,P_{c'}\,\gamma_{\lambda'' c''}\,\gamma_{\lambda' c'}\,A_{\lambda''\lambda'}\end{aligned} \tag{86}$$

Collecting terms and again relabelling some of the dummy indices, which are summed, yields:

$$0 = \Sigma_{\lambda\lambda'}\,2i\,P_{c'}\,\gamma_{\lambda c}\gamma_{\lambda' c'}\,(E_\lambda - E)^{-1}\left[\,\delta_{\lambda\lambda'} - (E_\lambda - E)\,A_{\lambda\lambda'} + \Sigma_{\lambda''}\xi_{\lambda\lambda''}A_{\lambda''\lambda'}\,\right] \tag{87}$$

with

$$\xi_{\lambda\lambda''} = \Sigma_{c''}\,\lambda_{\lambda c''}\,\gamma_{\lambda'' c''}\,L_{c''} = -\,\Delta_{\lambda\lambda'} + (i/2)\Gamma_{\lambda\lambda'} \tag{88}$$

Since Eqn. (87) must hold for arbitrary values of $\gamma_{\lambda c}$ and $\gamma_{\lambda' c'}$ we can set the square bracket equal to zero and therefore we have, finally,

$$(A^{-1})_{\lambda\lambda'} = (E_\lambda - E)\,\delta_{\lambda\lambda'} + \Delta_{\lambda\lambda'} - (i/2)\Gamma_{\lambda\lambda'} \tag{89}$$

Having found that the A matrix assumed in Eqn. (84) exists, we have proven the level-matrix formula Eqn. (79).

4.3 Working with the Level-Matrix Formula

We examine the level-matrix by looking at its full matrix glory:

$$(A^{-1}) \;=\; \begin{pmatrix} E_1 + \Delta_1 - E - \frac{i}{2}\Gamma_1 & \Delta_{12} - \frac{i}{2}\Gamma_{12} & \Delta_{13} - \frac{i}{2}\Gamma_{13} & \square & \square \\ \Delta_{12} - \frac{i}{2}\Gamma_{12} & E_2 + \Delta_2 - E - \frac{i}{2}\Gamma_2 & \Delta_{23} - \frac{i}{2}\Gamma_{23} & \square & \square \\ \Delta_{13} - \frac{i}{2}\Gamma_{13} & \Delta_{23} - \frac{i}{2}\Gamma_{23} & E_3 + \Delta_3 - E - \frac{i}{2}\Gamma_3 & \square & \square \\ \square & \square & \square & \square & \square \\ \square & \square & \square & & \end{pmatrix} \tag{90}$$

It is a symmetric matrix with a denumerably infinite number of rows and columns. Of course, in the few-level approximation we drop all but the relevant few levels. With such an approximation the collision matrix in its level-matrix form, Eqn. (79), is the best formula for many low energy astrophysical reaction cross sections. Probably, even, it applies in the majority of such cases. It is one of the two formulas of U in Azuma's programs.

We note that the off-diagonal elements of the level matrix, A^{-1}, contain "mixed" widths and shifts, that is, terms like the total shift or total width (they are summed over all channels) which are sums of terms of arbitrary sign because they contain products of reduced width amplitudes (not reduced widths) which do not refer to the same level and which can then have arbitrary sign.

If we ignored the off-diagonal elements of the level matrix then the collision matrix would be simply a sum of Breit-Wigner amplitudes. In other words, we would have something very much like the Kapur-Peierls formalism. Life would be simple. Do the off-diagonal elements matter? The answer is that in a number of cases, such as most astrophysical reaction in light nuclei, they do matter. There are other cases, such as neutron capture in heavier nuclei where they do not matter much.

For instructive reasons let's look briefly at low energy (s-wave) neutron cross sections in heavier nuclei such as those for neutron capture on a rapid timescale. Here the shift function vanishes and so we have no shift terms in Eqn. (90). The total width for neutron resonances pertains to the neutron width itself and to the capture width. In many cases the capture width dominates: in a few it does not. If the capture width dominates then Eqn. (90) reduces to the diagonal terms and we really have a sum over Breit-Wigner amplitudes. The reason that the off-diagonal elements are unimportant in this case is first, that the neutron widths are small and, secondly, that the capture widths refer to a sum over literally thousands or even millions of individual radiative transitions (except when we are really near to the neutron drip lines, the neutron brings in about 7 MeV into the compound nucleus and the resonances so far above the ground state can decay to many of the levels below). The "mixed" widths, involving many products of reduced-width amplitudes of random sign, vanish. Because there is such a plethora of radiative capture partial widths the total capture width does not fluctuate much and is roughly equal to about 0.030 eV for most heavy nuclei, give or take a factor of about two. The total width is much smaller than the level spacing and we have well separated resonances as one found in even the earliest neutron cross-section data seventy years ago. It was garden variety cross sections of this kind which immediately led to Bohr's picture of the compound nucleus and, indeed, to the reaction theory frameworks which we are discussing. In this case of dominance of the capture width the peak resonance cross section is $(4\pi/k^2)(\Gamma_{\lambda n}/\Gamma_{\lambda\gamma})$ and therefore fluctuates greatly because the neutron widths fluctuate (see Section 5). The cross section area (total width times peak cross section) is directly proportional to the neutron width.

In the fewer cases where the neutron width dominates the capture width (for example, for Th^{232}, Mn^{55} or U^{238}) we have a somewhat simpler situation, illustrated on Fig. 5, where the individual resonances all have the same peak cross section, $(4\pi/k^2)$. In the case of Xe^{135}, the famous fission product which was recognized as a reactor "poison", such a

cross section happens to fall right at thermal neutron energy (0.025 eV) and the cross section is then 30 million barns, which is 30 million times greater than the normal geometric cross section! Even in this case where the neutron width is larger, the off-diagonal elements of the level matrix do not appear to matter much.

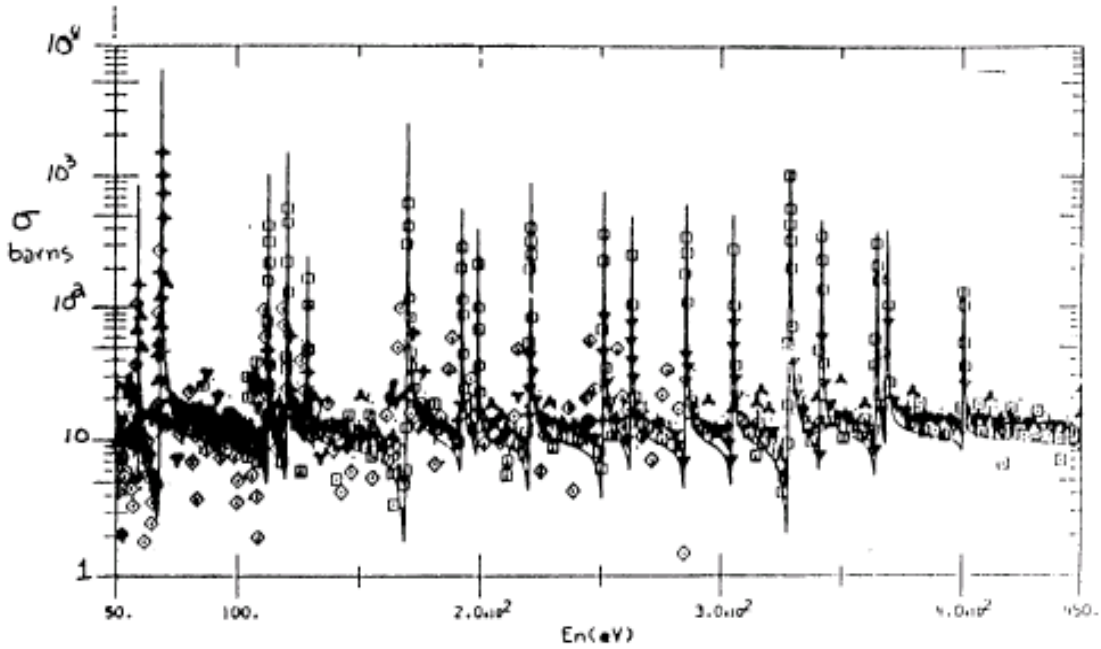

Fig. 5. The total neutron cross section for Th^{232}, shown from a neutron energy of 50 eV up to 450 eV.

The seeming irrelevance of the off-diagonal elements of the level matrix does not apply to situations where we have some broad resonances, which overlap other resonances. This is commonly the case for astrophysical reactions in light nuclei. Here one should use the proper level-matrix, which Azuma has programmed. It would be interesting to explore some of these cases, for example, C^{12} + α scattering, to examine how the fit might be affected if one ignores these off-diagonal elements. This would be a good testing ground for the applicability of the R-matrix framework. There is an even better one.

If some ambitious theorist were to ask me where could he/she find the best test for R-matrix applicability I would point to the fission cross sections of the fissile isotopes, U^{235}, U^{233} and Pu^{239}. (The astrophysics readers of these notes can ignore the story told in this paragraph.) These cross sections have strongly overlapping levels – unlike most low-energy neutron cross sections – because of the decay into fission channels for which the widths are much larger than the neutron widths. In the 1940's and 1950's these were the most important cross section data (until the mid-1950's the US falsified the data to confuse the enemy!). It was difficult to fit these data with the R-matrix formulae or, indeed, with those of any other framework, because no one really knew what was meant by a fission channel. A fission channel was certainly not the various final fission products because these were known to be formed only in the final stages of the break-up of the liquid drop. But the modes of drop break-up were not known and only the total fission cross-section was measured, not the partial cross section to any perceived fission channel.

Even now, when we know much more about the process of fission, with its second and third wells, the specification of a fission channel is not entirely clear nor its relation to what is measured. Soon after Thomas invented the level-matrix formulation the present author[15] was able to show that it lent itself admirably to the description of these fission cross sections. If we look at Eqn. (90) again we see that the diagonal elements require only the total width for fission. The "mixed" widths in the off-diagonal terms also sum over all channels. We can regard these "mixed" widths as scalar products, in channel space, of vectors in channel space whose length is the square root of the total fission width. Therefore each such "mixed" width requires only a single new parameter, the cosine of the angle between these vectors. No specification of the nature of fission channels is required. Further, the average value of the cosines from the various off-diagonal elements tells us how many fission channels there must be without specifying them (as the number of dimensions grows the average value of the cosine of the angle between two arbitrary vectors falls off). This treatment was very successful in 1958 but at that time only very slow computers were available (one could watch the lights of the computer in action for many minutes as it diagonalized the 3x3 level matrices!). It was not possible to make any proper least squares fit. I don't believe that anyone has returned to the analysis of these fission cross sections or used them as a vehicle to test the applicability of the R-matrix formulation. It is my choice for the best such vehicle.

5 THE R-MATRIX AND NUCLEAR SPECTROSCOPY

No treatment of data for the cross sections of nuclear astrophysics should be made without careful consideration of the relationship of the data to nuclear spectroscopy. As we shall see, the R-matrix goes hand-in-hand with nuclear spectroscopy. This section deal with topics pertaining to the applicability of the R-matrix theory and it will then, necessarily, take us into discussing nuclear spectroscopy.

This is only the briefest of glimpses into the nuclear spectroscopy relevant for astrophysics. Unfortunately the whole subject of nuclear spectroscopy has fallen into neglect in recent years and deserves better attention. During the 1960's, when the initial ideas about nucleosynthesis were being explored, nuclear spectroscopy was in full flourish and, in fact, was one of the main vehicles then for the application of quantum mechanics. During that time a great deal was learned about the energy levels of atomic nuclei. Perhaps these notes will help to direct some of the students in nuclear astrophysics back to the important ideas associated with the development of nuclear structure and will thus aid them in making better descriptions of the cross section data. For heuristic reasons, only the simplest and oldest ideas of nuclear spectroscopy will be used. There are now much more powerful methods available to calculate spectroscopic factors and spectral functions, including the effects of core polarization and collective motion.

5.1 Spectroscopic Factors and Single-Particle States

The level widths of the R-matrix theory can be written (cf. (48)):

$$\Gamma_{\lambda c} = 2P_c\gamma_{\lambda c}^{\ 2} = S_{\lambda c}\Gamma_c \tag{91}$$

where $S_{\lambda c}$ is called the spectroscopic factor and $\Gamma_{\lambda c}$ is a single-particle width pertaining to the channel c. In words, the spectroscopic factor, which has a maximum value of unity, gives the fractional component, contained in the compound state, of a single-particle internal state belonging to the channel c. We examine this relationship more closely.

It is the messy two-body nucleon-nucleon interactions, which complicate things and make spectroscopic factors necessary. Let's begin by assuming that a benevolent deity (theological allusions are particularly appropriate here at Notre Dame University) decreed that an incoming nucleon does not interact with all of the nucleons of the target but, instead, interacts with the target only through a mean field – the average of the nucleon-nucleon force and also the potential of the nuclear shell model. In that case we have the kind of potential scattering treated in Section 2. The target nucleons are not excited by the beam. All of the spectroscopic factors Eqn. (91) are unity. For each partial wave (it is trivial to add spin to the discussion of Section 2 so that the single-particle states may correspond to the actual states of the j-j coupling shell model) we see only widely spaced single particle states, typically several tens of MeV apart for all nuclei. In shell model calculations one often uses an infinite harmonic oscillator to show all of the levels, for example, $1s_{1/2}$, $2s_{1/2}$, etc., $1p_{1/2}$, $1p_{3/2}$, $2p_{1/2}$, etc., $1d_{5/2}$, etc., etc., in an obvious notation for

all of the partial waves which gives the principal quantum number (equal to the number of nodes of the corresponding radial wave function) as well as the orbital angular momentum, ℓ, and the value of j. In a comparable realistic nuclear potential – such as a Saxon-Woods potential of finite depth – we must, of course, add the "natural" boundary condition to establish the corresponding resonant states whose spacing is the same as for the infinite harmonic oscillator. The wave functions and their energies are also very similar to those of the infinite harmonic oscillator used in the shell model.

But then we look at the resonances of protons or neutrons, as in Fig. 5, and see that at moderate excitation energy above the ground state the spacing between levels is not 10 MeV but rather only a few keV or even a few eV; there are thousands or even millions of more resonances than this single-particle picture provides. What happened? The trouble is that the devil interfered with this simple view of the deity: the single-particle states are mixed, by the nucleon-nucleon interactions, into the vast sea of states involving excitation of the target nucleus. This is the compound nucleus, a descent into nuclear quantum chaos. In the early days of the nuclear shell model it was thought that perhaps the shell model applied only to the nuclear ground states and that at higher excitation energies one fell immediately into such chaos. Further work showed that the descent was more gradual. We illustrate this with a simple example, which should be very helpful in giving us some of the guidance principles from nuclear structure for the analysis of the kinds of resonant reactions pertinent to astrophysical reaction rates in light nuclei.

Consider the shell model view of the structure of the nucleus Ne^{20}. In the simplest approximation for its structure we assume that there is a closed shell O^{16} core and four extra nucleons in the next open shell: the $2s_{1/2}$, $1d_{5/2}$, $1d_{3/2}$, configuration. That is, higher configurations or excitation of the O^{16} core are ignored. Therefore one might expect that the levels arising from this configuration should occur in the first 10 MeV or so above the ground state and that the large number of levels from other configurations, which we are neglecting, are relevant only at higher energies. Even so, there are very many levels in this configuration, only one or two of which might correspond to single-particle nucleon states (here, clearly, s or d states) with a Ne^{19} or F^{19} target in its ground state. The number of different levels – all of positive parity – is easy to calculate, putting two neutrons and two protons into the twelve magnetic sub-states of the configuration. We find 640 energy levels of Ne^{20} (if we had chosen Mg^{24}, instead, with eight particles in the same configuration we would have found almost a hundred times as many states!) distributed in spin as follows: 4 (8+), 12(7+), 36(6+), 64(5+), 109(4+), 129(3+), 143(2+), 97(1+) and 46(0+). Even with such riches the shell model soon learned how to cope and thus keep the devil of nuclear quantum chaos at bay.

If we neglect the nucleon-nucleon interactions, in Ne^{20}, of the four extra nucleons beyond the closed O^{16} core, then, initially, all of the 640 energy levels are degenerate in energy. This degeneracy is removed when we turn on the interactions. Diagonalizing the interaction Hamiltonian then yields the shell model ground state of Ne^{20}, as well as the shell model description of all 640 states of the chosen configuration. For each of these states we have a prediction of all of their properties: level energy, spin, parity, electromagnetic transition probabilities, etc. What is most important for the present discussion is that we also have a prediction for all of the spectroscopic factors, $S_{\lambda c}$, in quantities such as the partial width Eqn. (91). These spectroscopic factors are the square

of the overlap integral between any particular excited state, as yielded by the shell model, and a single-particle state for the channel under consideration. For the Ne^{20} problem, if we are thinking of a neutron channel then the single-particle state is either a $2s_{1/2}$ or $1d_{5/2}$ or a $1d_{3/2}$ neutron coupled to a Ne^{19} ground state wave function. Alternatively we could choose a channel wave function corresponding to an alpha particle single-particle state coupled to an O^{16} ground state. Assuming that the states are all properly normalized the spectroscopic factors have a maximum value of unity but will generally be smaller. They do represent the fraction of the channel wave function contained in the excited compound state. We make this connection more formally in the next section.

Such shell model calculations of nuclear structure are relevant even though they must be guided by good physics. First of all, there appears to be some arbitrariness in the choice of the nucleon-nucleon interactions between the four neutrons and protons of the configuration, the so-called residual interaction. One certainly does not work from first principles (QCD) for the interactions. QCD gives some guidance about the two-body phenomenological force between free nucleons. When this force takes place within a nucleus it is modified by the Pauli principle into an appropriate shell-model residual interaction. Fifty years of experience with the nuclear shell model[16] has led to reasonably good understanding of such residual interactions and also descriptions of excited states, which fit a vast body of data reasonably well. Second, higher configurations or core excitation cannot always be ignored without impunity. For example, for Ne^{20}, the chosen configuration yields only positive parity states. Yet the fourth, fifth and sixth states of this nucleus all have negative parity. The states must arise from higher configurations for which the diagonalization process produces intruders into the energy regime of states of the configuration, which we chose. Significantly higher configurations are required to describe the alpha-particle cluster states known to occur at moderate energies in nuclei such as Ne^{20}. Yet the simple picture dealing with only the lowest configuration has had great success for many of the observed excited states. Third, some bravery is required in tackling the diagonalization of, say, 143 2+ states in Ne^{20}, which is necessary for a full shell-model treatment of these states which arise from only the lowest configuration!

The route to an understanding with the shell model of nuclear energy levels is full of brilliant insights. Each nucleus has its own story. For example, for the Ne^{20} problem, which we have chosen as an illustration the first three states, 0+, 2+ and 4+, have a spacing suggestive of the kinds of rotational bands, which were commonly found at low energies in heavy nuclei. In the first decade of the shell model – the 1950's – there appeared to be an almost irreconcilable difference in the collective rotational picture applicable to heavy nuclei and the single-particle shell model picture which pertained to light nuclei. This difference was bridged in that decade by studies with a number of nuclei in the 2s-1d shell, including Ne^{20}, which focused on pieces of the residual interaction and on special classification, using spatial symmetry, of the states of the configuration. Some outstanding work on Ne^{20} by Elliott[17], in 1957, led to the SU_3 model, which had this application in nuclear physics before this symmetry group became important for the quark model in particle physics.

This example leads us to write down a number of useful guidance principles, for resonance reactions (particularly in light nuclei). These principles arise from consideration of nuclear structure. They are:

1) The R-Matrix has parameters, E_λ and $\gamma_{\lambda c}^2$, which can be directly related to the energy levels and spectroscopic factors of shell model studies.

2) The single-particle width, Γ_c, is that which we encountered in Section 2. Thus we can write this width as:

$$\Gamma_c = 2P_c f\left(\hbar^2 / ma_c^2\right) \tag{92}$$

where $(\hbar^2 / ma_c^2)$ is the square-well reduced width, depending on the square-well radius, P_c is the normal penetration factor Eqn. (44), and f is the reflection factor Eqn. (52), which corrects the square-well results for the artificially high reflection of the square-well. We can think of f as being associated with either the penetration factor or the square-well reduced width.

3) The single-particle width Eqn. (92), leads at once to a familiar upper limit, often called the sum-rule limit, of any empirical reduced width extracted from a reaction analysis: this sum-rule limit is:

$$\gamma_{\lambda c}^2 \le \left(\hbar^2 / ma_c^2\right) \tag{93}$$

In the Ne^{20} example which we illustrated above the lowest 2s-1d configuration has two single particle states, the 2s and the 1d, and no others. The 1d single-particle state is split by the spin-orbit interaction and so its reduced width is also split. The reactions reaching the compound nucleus levels of Ne^{20} in the energy regime of the 2s-1d configurations might contain individual states whose nucleon reduced widths approached the sum-rule limit. Further, the sum of all observed reduced widths for each partial wave, in the same energy regime, should not exceed the sum-rule limit. There is some flexibility in the sum-rule limit, partly because of the reflection factor which may be associated with it and partly, in the analysis, one might have chosen an unrealistically large matching radius which reduces the penetration factor and then increases the reduced width proportionally. There is no need to associate a factor of 3/2 with the limit Eqn. (93), as was sometimes done in the early (pre-shell-model) papers of the R-matrix theory.

4) The extracted reduced widths should be compared to shell-model – or other nuclear model – predictions for spectroscopic factors whenever possible. Again, because of reflection factors and the choice of matching radius, any individual spectroscopic factor extracted from data might be somewhat ambiguous in such a comparison but the ratios of reduced widths for different resonances should be a better measure of the predictions of the model or, turning this around, a better measure of whether or not the parameters deduced from the fit are physically reasonable.

5) The single-particle states (and their "strength" as given in the sum rule limit) is spread by the residual interaction but only into a region of several MeV about the original energy of the shell model state (in the next section we explore the "strength function" more fully) so that we expect resonances far from the single-particle states to have little strength, that is, they will have small reduced widths. For example, for the Ne^{20} compound system discussed above we would expect the reduced widths for p-wave or f-wave nucleons to be small while those of s-waves and d-waves might be large.

In general, in embarking on a data analysis of resonance cross sections with the R-matrix theory one should begin by asking what does our knowledge of the nuclear structure of the compound system tell us. We should ask: how far away are we from known single-particle states? Such a question is particularly important when we choose to restrict our attention to a few states in the energy interval of interest but allow a distant level or two to be added to the fitting procedure. Such a treatment of distant levels as modifying the local fit is often to be recommended. But we need not allow all properties of the distant state to be entirely determined by the fit. For example, for any analysis involving Ne^{20} the positions of the s-wave and d-wave and f-wave and p-wave nucleon states are reasonably well known. If we want to add a distant level to the analysis for states involving f-waves we should explore where the dominant $f_{7/2}$ state is located and choose the energy of the distant state to be that location – and expect that the analysis will require a reduced width close to the single-particle limit, if it turns out that a distant level is important at all. This applies even to bound single-particle states, as would be the case for 1p states for Ne^{20}.

A very different case is encountered in the $C^{12} + \alpha$ data discussed by Azuma at this school and pertaining to the new Notre Dame data for this process. I believe that if one wishes to add a distant resonance in this analysis while considering in detail the relevant local resonances one should give cognizance to the known alpha particle states in the compound system, O^{16}, particularly to the broad alpha particle states several MeV above the alpha particle threshold. One can use the known energy of these levels and expect that the widths should be close to the single-particle value for alpha emission (note that the alpha sum rule limit corresponding to Eqn. (93) is smaller than that for nucleons because of the larger reduced mass of the alpha particle). It is instructive to remember that the atomic nucleus is richer than that implied by the shell model for nucleons. For some nuclei, such as Be^8, C^{12}, O^{16}, Ne^{20}, Mg^{24}, etc., an alpha particle cluster model applies and one finds, among the usual shell model states of these nuclei, intruder states (they are called "intruder" because in the shell model, which is all encompassing, one needs much higher configurations to describe such alpha-cluster states which then intrude the energy regime of the normal shell model states from the higher energy of these configurations). For O^{16} these alpha particle cluster states might pertain either to tetrahedral clusters or to a linear chain of alpha particles.

Although much is known about nuclear structure for a considerable distance above the ground state, eventually the individual nuclear energy levels get to be so numerous and so complicated that we have true nuclear quantum chaos. In the next subsection we discuss more systematically how the single-particle strength is distributed even at these higher energies.

5.2 The Distribution of Single-Particle Strength

If we look at low-energy neutron resonances in heavy nuclei, as in Fig.5, there are thousands of levels of each spin and parity per MeV. Correspondingly the neutron-reduced widths of individual levels, given in Fig. 6, get to be very much below the sum-rule limit. We then have a regime in which it seems hopeless that any nuclear model could ever predict the properties of individual states. This is nuclear quantum chaos. The individual reduced-width amplitudes are equally likely to be positive or negative and, assuming them to be thus random, the reduced widths themselves have a Gaussian (called

Porter-Thomas) distribution about their mean value. The spacing of levels of the same spin and parity is not quite random – as one might expect from the random matrix elements involved – but rather still obey some powerful mathematical theorems first enunciated by Neumann and Wigner[18]. These theorems pertain to the so-called "no-crossing" phenomenon for the eigenvalues of a random matrix. Because of them the probability of zero spacing between levels is zero – there is level repulsion. The Wigner level spacing law for this purpose is a touchstone for a cult devoted to nuclear quantum chaos. This cult meets frequently although its direct relevance to physics does not appear to be very profound. Chaos exists and does need to be generally understood but apart from this it does not appear to contribute greatly to our understanding of the physics of the nucleus.

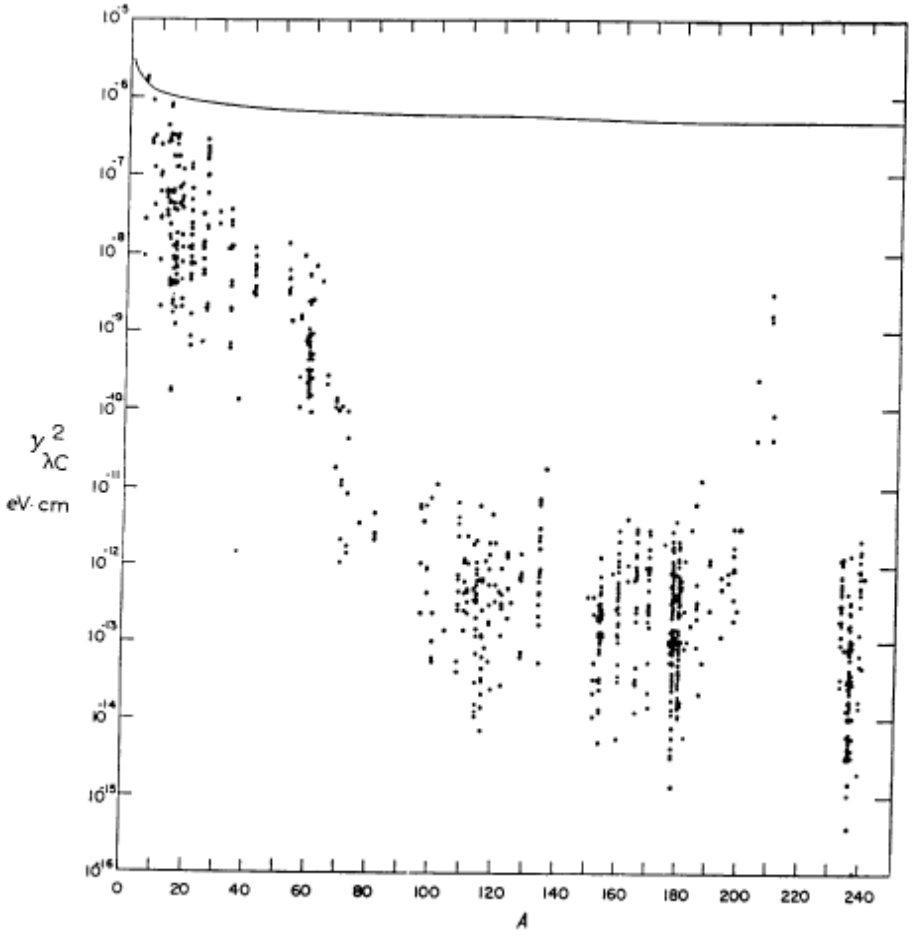

Fig. 6. The early data (<1958; taken from Ref. C) for reduced widths for nucleon emission as a function of atomic weight. The units of the reduced width are those which were the fashion of the time (differing from those of the present article by a factor of *a*, where *a* is the nuclear radius. Similarly the sum rule limit is (h^2/ m*a*). The plot contains 730 individual reduced widths obtained from resonance analysis. The small value of the reduced widths for large A is clearly evident as is the wide distribution (Porter-Thomas) of the reduced widths about their mean value. It is from the average of such data, and from the mean level spacing, that one obtains the strength functions of Fig. 7 and Fig. 8.

It is the average reduced width divided by the average level spacing – called the nuclear strength function – which survives, even in the regime of nuclear quantum chaos. The resulting single-particle resonances of average cross sections (averaged over closely-spaced resonances) is described phenomenologically by the optical model. We describe now the basis of the optical model in R-matrix theory and in so doing we also elucidate the single-particle resonances discussed in the previous subsection pertaining to nuclear spectroscopy.

Consider again the resonant states of the compound nucleus as defined by Eqn. (59) and Eqn. (60). We used those resonant states, X_λ, to decompose the full wave function of the full Hamiltonian in Eqn. (61). Here we now define a single-particle Hamiltonian whose wave functions can be used to decompose the resonant states, X_λ. This single-particle Hamiltonian is obtained from the full Hamiltonian of Eqn. (59) by splitting it into two parts:

$$H=\Sigma_{i=1}^{A} T_i+\Sigma_{i=1}^{A}\Sigma_{j=i+1}^{A} v_{ij} = H_0 + H_R \tag{94}$$

where H_0 is the single-particle Hamiltonian and H_R is the residual interaction. In Eqn. (94) the full Hamiltonian is a sum of kinetic energy terms and two-body interactions between all of the nucleons. Ignoring anti-symmetry, we make the split of the Hamiltonian in the following way:

$$H_0 =\Sigma_{i=1}^{A} T_i+\Sigma_{i=1}^{A-1}\Sigma_{j=i+1}^{A-1} v_{ij} + V_A \tag{95}$$

$$H_R =\Sigma_{j=1}^{A-1} v_{Aj} - V_A \tag{96}$$

where V_A is a real single-particle potential of the kind envisaged in Section 2. Thus H_0 contains the full Hamiltonian for all of the A-1 target nucleons but only a potential well for the nucleon A. The internal states generated by the Hamiltonian H_0 can be written as products of the target nucleus wave function, plus the spin and angular parts of the wave function for nucleon A, times the radial wave function, u, for the nucleon A. If we add a boundary condition (cf. Eqn. (31)) at the matching radius for the nucleon A, such as:

$$\left[\left(r_A\, du/d r_A\right)/u\right]\Big|_{r=a} = b \tag{97}$$

where b is a real number (best chosen as the "natural" boundary condition number Eqn. (51)) then the wave functions u are single-particle wave functions, u_p, for which the subscript gives the principle quantum number and the angular momentum of the state. We can then write the internal wave functions, which are eigenfunctions of H_0, as:

$$H_0\, \psi_c\, U_p = E_{cp}\, \psi_c\, u_p \tag{98}$$

for which the energy, E_{cp} , is the sum of the single-particle energy and the energy of the target nucleus. In the context of the full nuclear problem it is such states, which one can refer to as single-particle states especially when the target nucleus is in its ground state. They allow the target to be in any state of excitation.

These true single-particle states are not, in general, the resonant states, X_λ, but they form a complete set of states in terms of which the actual resonances can be expanded:

$$X_\lambda = \Sigma_{c,p} C_{\lambda;cp} \psi_c u_p \tag{99}$$

where c runs over all of the channels for nucleon emission. Since all of the states are properly normalized we have a real orthogonal transformation for which:

$$\Sigma_\lambda C_{\lambda;cp} C_{\lambda;c'p'} = \delta_{cc'} \delta_{pp'} \tag{100}$$

and

$$\Sigma_{c,p} C_{\lambda;cp} C_{\lambda';cp} = \delta_{\lambda\lambda'} \tag{101}$$

In the transformation Eqn. (99), the expansion coefficients, $C_{\lambda;cp}$, are precisely the square roots of the spectroscopic factors, $S_{\lambda c}$, in Eqn. (91). Then Eqn. (100) clearly shows us that the sum of all of the spectroscopic factors for all resonances is unity. The single-particle reduced width is spread among the resonances but retains its sum-rule value. In fact Eqn. (100) is the sum-rule, which provides the name for the sum-rule limit.

This is also the language of the R-matrix. The R-matrix reduced widths are:

$$\gamma_{\lambda c}^2 = \left(\hbar^2 / 2ma_c\right)\left[\Sigma_p u_p(a_c) C_{\kappa;cp}\right]^2 \tag{102}$$

If the vestiges of the shell model remain, even in the energy regime of nuclear quantum chaos, then a single value of the principal quantum number, p, will dominate the sum of Eqn. (102). Therefore we can drop the sum and write:

$$\gamma_{\lambda c}^2 = \left(\hbar^2 / 2ma_c\right) u_p^2(a_c) C_{\lambda;cp}^2 \tag{103}$$

If the potential, V_A, is a square-well then this reduces to:

$$\gamma_{\lambda c}^2 = \left(\hbar^2 / ma_c^2\right) C_{\lambda;cp}^2 \tag{104}$$

which clearly displays the single-particle reduced width and the spectroscopic factor. Of course if the average potential is not a square-well we might want to add the reflection factor to Eqn. (104) as we did in Eqn. (92).

When we deal with regime of nuclear quantum chaos we are interested in the strength function, s(E), which is:

$$s(E) = \langle C_{\lambda;cp}^2 \rangle / D = (W/\pi)\Sigma_p \left[\left(E_p - E\right)^2 + W^2\right]^{-1} \tag{105}$$

where D is the average spacing of the resonances and W is a "spreading width" which gives a measure of the energy interval into which the single-particle strength is spread among the compound states. The angular brackets around the spectroscopic factor

indicate that it is averaged over the resonances. Typically the spreading width is several MeV (or more if we are dealing, instead with cluster states, etc.). In the nuclear quantum chaos regime, such as that for neutron resonances in heavy nuclei, one can average the cross sections over resonances to extract the strength function. The data for the s-wave neutron strength function is shown in Fig. 7 and Fig. 8. The data clearly display the 3s and 4s neutron single-particle resonances, but the peaks of the strength function are split by deformations and other physics. The average cross sections of resonance reactions, such as those of Fig. 5 are also reasonably described by the nuclear optical model.

In the nuclear optical model it is assumed that the cross sections averaged over resonances can be described by a potential well, which contains both a real and an imaginary part.

$$V_A = V_0 + iW \tag{106}$$

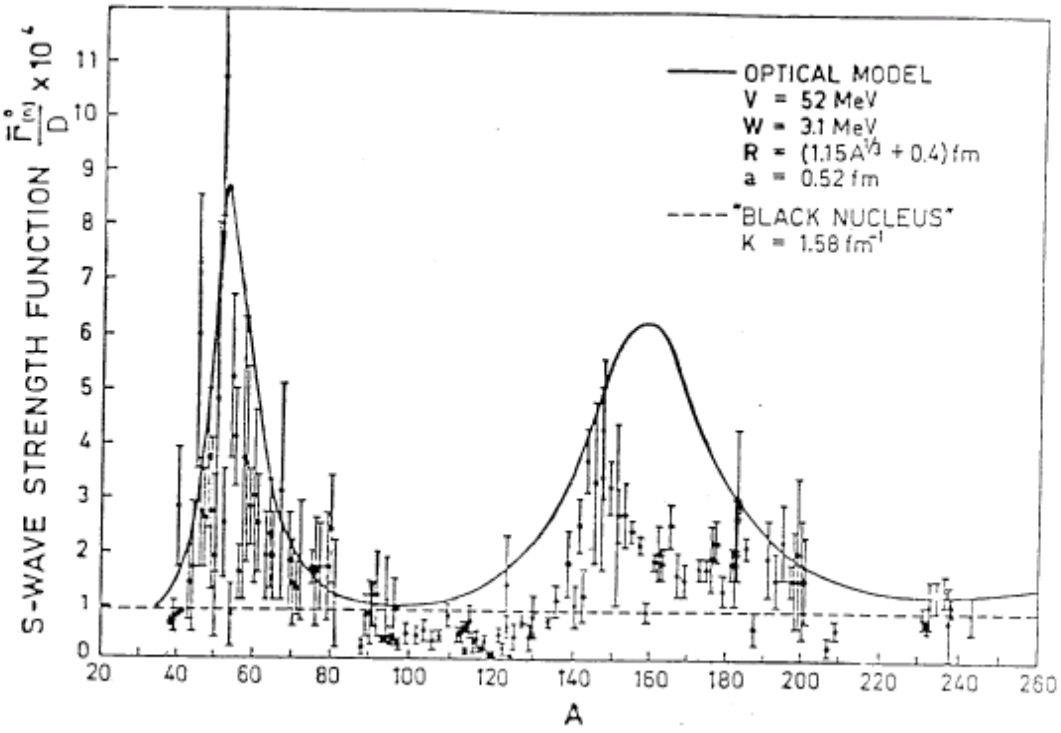

Fig. 7. The early neutron strength function data (<1958) for s-wave neutrons as a function of the atomic weight, A. Also shown are the optical model prediction for the strength function and the "black nucleus" prediction.

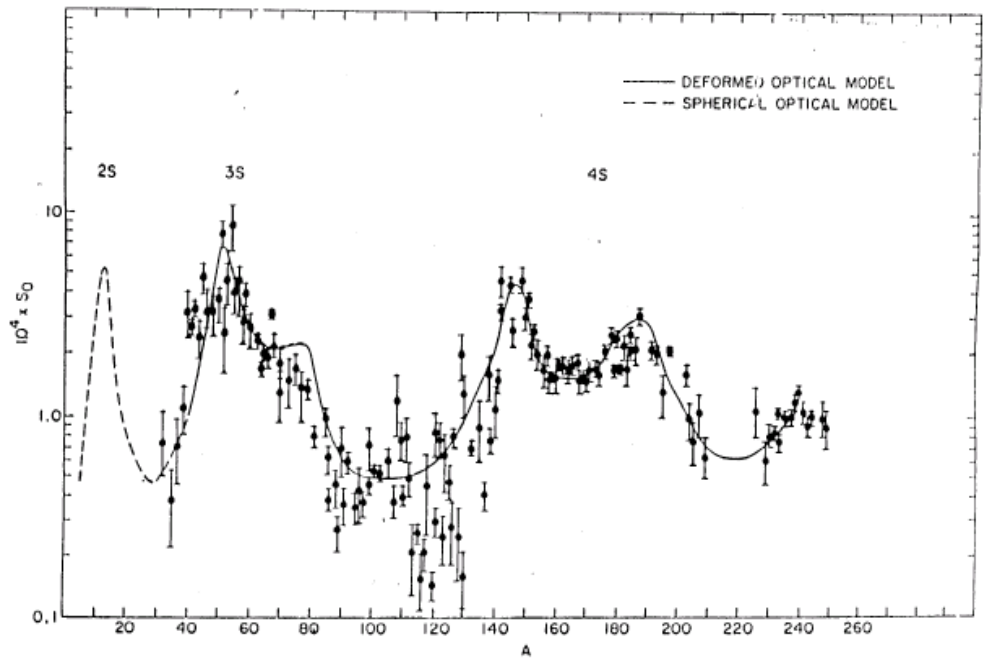

Fig. 8. A more recent plot of the data for the s-wave neutron strength function and the predictions of a spherical and deformed optical potential.

A description of the cross sections of the optical model and of the average over resonances of the R-matrix cross sections (the Statistical Theory of Nuclear Reactions[13]) is beyond the scope of these lectures. We point out, however, that a minor miracle occurs in the comparison of the optical model results with those of the statistical theory. The result for the optical model is identical to those for the statistical theory if we use the same W in both. That is, the spreading width of the strength function is the same as the imaginary part of the optical potential. Then fits to many cross sections (especially, in the early 1950's, Wisconsin data on neutron cross sections) using the optical model yielded the imaginary part of the optical potential (about 1 MeV for low energy neutrons) and therefore much information about spreading widths.

The results from the optical model were essential in establishing the validity of the nuclear shell model. The small value of the imaginary part of the potential meant that a nucleon was able to travel a distance greater than the nuclear radius before the residual interaction destroyed the single-particle motion. At the time it became a crucial problem to understand the origin of the small spreading width directly from knowledge of the nucleon-nucleon interaction. This understanding was not achieved easily. The residual interaction is so strong and short range that early estimates suggested that the spreading width was likely many tens of MeV and therefore the nucleus should be essentially black for nucleons. In fact, it was such early estimates which led the leading physicists, such as Wigner, to abandon any hopes for the shell model in the 1930's. It wasn't until the evidence from ground-state properties overwhelmingly pointed to the validity of the shell model, in about 1950, that the problem of the calculation of the spreading width from the residual interaction was revisited and it was found that the Pauli Principle was

responsible for reducing the predicted spreading width from about 50 MeV to only several MeV as required for the success of the shell model. This was a very important problem at the time.

Let me close these lectures with a personal anecdote about this important problem. At MIT, Weisskopf asked his graduate student, Murray Gell-Mann, to tackle this problem in 1952. This formed Gell-Mann's PhD thesis a year later but the attempt was not very successful. As Gell-Mann's biographer[19] says: "later Wigner did it better". This was, in fact, an important part of my own PhD thesis at Princeton in 1955. Wigner had me use a method he had developed earlier for electron correlations in metals to estimate the spreading width. I did so, and in my thesis the result found was a disappointing 50 MeV. Using a different method Tony Lane also found this large value for the spreading width in 1955. We decided that both of us would publish separate abstracts – at a Mexico City meeting of the APS that summer – giving this disappointing result. I obtained my PhD thesis but fortunately, a few months later, before writing a paper[20] on the result, I found out that all of us had treated the effects of the Pauli Principle incorrectly and that when the correct calculation was made one obtained several MeV, as wanted, for the spreading width. By that time I was a postdoctoral fellow working with Rudolf Peierls in Birmingham. Wigner was pleased that nature had turned out to be friendly to the shell model.

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