The Early Days of R-Matrix Theory
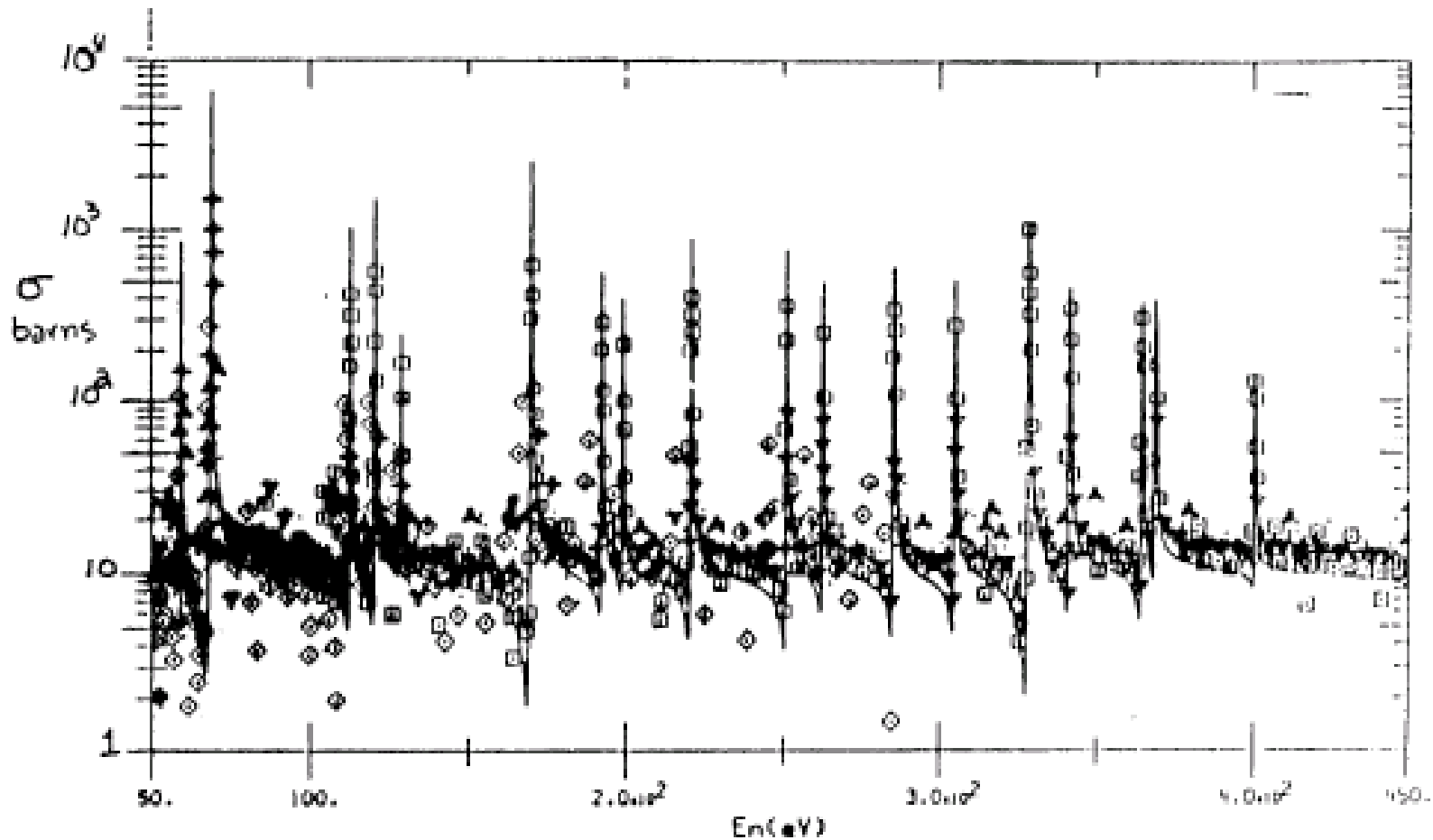
Erich Vogt, TRIUMF

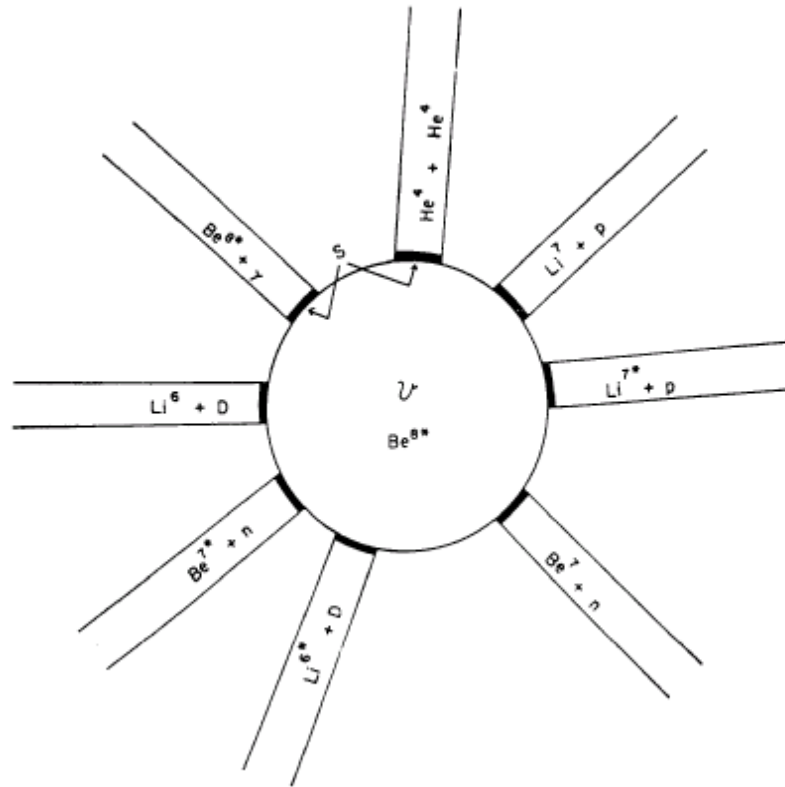Santa Fe Workshop, April 21-23,2008

The Beginning of Nuclear Physics

- [Milestones](The impetus for reaction theory frameworks)
  - 1. Discovery of the neutron (Chadwick, 1932)
  - 2. Short range and great strength of nuclear forces (Wigner,1933)
  - 3. Slow neutron resonances (Fermi, 1935)
  - 4. The Compound Nucleus (Bohr, 1935)
  - 5. The Breit-Wigner Formula (1936)

Slow neutron resonances in Th^{232}

The Compound Nucleus Be^8

The Breit-Wigner Formula

(Based on the analogy of the dispersion of light)

$$\sigma_{cc'} = (\pi / k^2) \, | \, \Gamma_{\lambda c}^{1/2} \Gamma_{\lambda c'}^{1/2} \, / \, \{(E_\lambda - E) - (\iota/2)\Gamma_\lambda\} \, |^2$$

$$\Gamma_{\lambda c} = 2 \, P_c \, \gamma_{\lambda c}^2 \, .$$

$$\Gamma_\lambda = \Sigma_c \, \Gamma_{\lambda c} \, .$$

Cross sections and the Collision Matrix

- In the many-channel space external to the Compound Nucleus, nuclear reaction measurements are given in terms of cross sections, $\sigma_{cc'}$, but the physics is described in terms of the collision matrix, $U_{cc'}$.

- The connection between the cross sections and the collision matrix is important but the discussion of the physics of resonance reactions focuses on the collision matrix and, in turn, on the matrices (such as the R-Matrix) used to provide frameworks for the description of resonances which occur inside the Compound Nucleus.

s-wave neutron resonances in a square well potential

- Neutron resonances in a square well potential (depth = 51 MeV, radius =
- 6.715 fm, corresponding ~ to A = 155)

- There is a "resonance" inside the well when the derivative of the wave function at the radius is zero

- Thus the "natural" boundary
- condition number is b = 0.

- The energies and wave functions of the six lowest "resonances" are shown.
- Here, at zero energy, only the 4th resonance matters

$\lambda = 6$ $E_\lambda = 78.12$ MeV

5   34.48

4   -0.43

3   -26.61

2   -44.06

1   -52.79

R_1
r
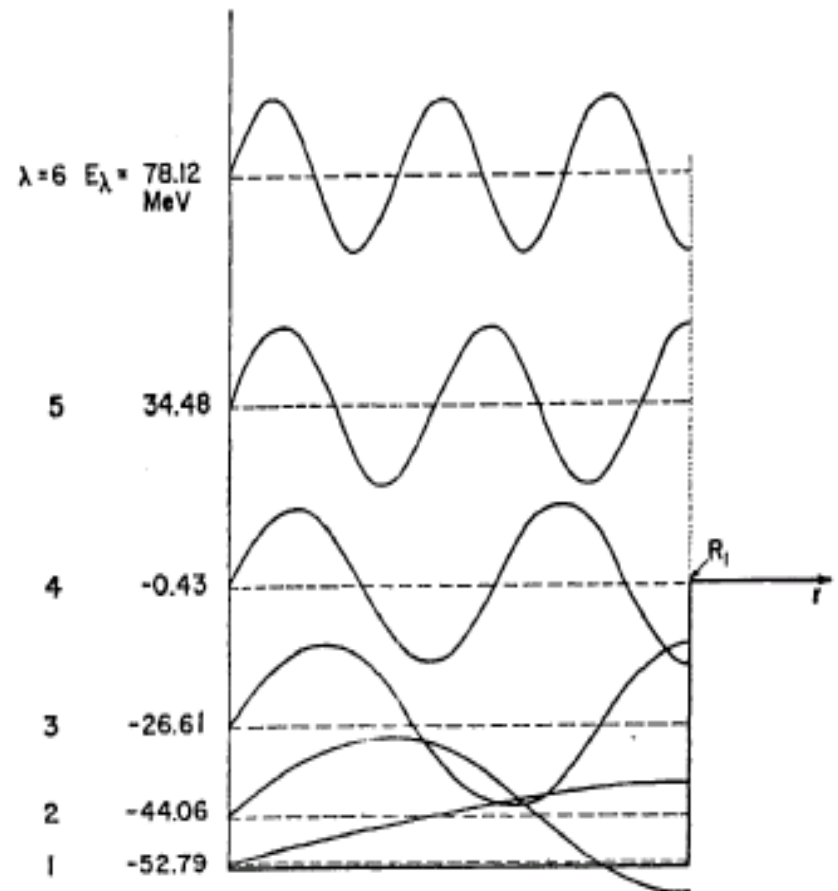
The resonances for s-wave neutrons in the square well

In this one-dimensional problem all the matrices are simply functions. From the region external to the square well we get the cross section in terms of the collision function, U, or the phase shift, δ.

- $$\sigma = (\pi / k^2) \sin^2 \delta = (\pi / k^2) | 1 - U |^2.$$

- With

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

- If we choose to characterize the square well by its resonances, defined by its radius, a, and by the boundary condition, $b = a (dX_\lambda / dr)_{at\ r=a} / X_\lambda$, then we get the resonances which we have just seen

The R-function and the Resonances of the square well

- If we expand the actual internal wave function in terms of the resonances we have defined we find that at the square well radius, a, the inverse of the wave function's logarithmic derivative is given by:

- $$R = \phi(a) / \phi'(a) = \Sigma \, \gamma_\lambda^2 / (E_\lambda - E)$$

- .where $\gamma_\lambda^2 = (h/2\pi)^2 /2ma^2$ is called the reduced width. R is, in effect, the Fourier Series expansion of the internal part of the phase shift, that is, of
- (1/Ka) tan Ka.

- Using this to equate the external and internal logarithmic derivatives at the nuclear radius we get the collision function:

- $$U = O^{-1} (1 - RL)^{-1} (1 - RL^*)O^* = e^{-2ika} (U \, 1\text{-}ikaR)^{-1} (1+ikaR)$$

- Where O is an outgoing wave (e^{ika}) evaluated at the well radius and L is the logarthmic derivative of O

Exhibiting a square well resonance

Having expanded the internal part of the square well wave function by a Fourier Series of the resonances it is now easy to exhibit a single resonance by approximating the R-function with only one term (that for the fourth resonance of the Fourier Series). With this approximation we have $R = [(h/2\pi)^2 /ma^2] / (E_4 - E)$ and then we get:
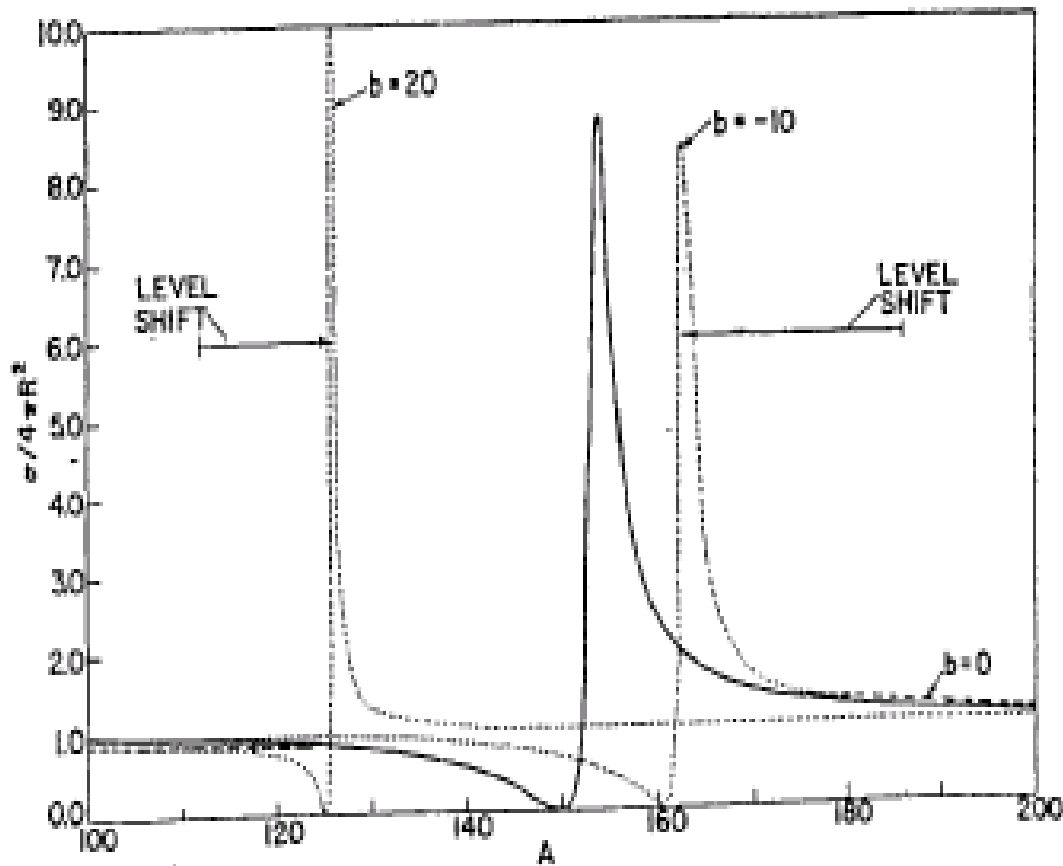
$$\sigma = (\pi/k^2) \mid 2 \sin ka\ e^{ika} - \Gamma_\lambda / (E_4 - E - i\ \Gamma_\lambda / 2 \mid^2.$$

with $\Gamma_\lambda = 2P\ \gamma_\lambda^2 = 2ka\ (h/2\pi)^2 / ma^2.$

Here we have the familiar Breit-Wigner formula for s-wave neutrons and a square well. On the next slide we show this resonance for fixed neutron energy (50 keV) as a function of well radius, a, or atomic number A

s-wave neutron resonance in a square well

(shown for various boundary conditions for the resonances)

Generalizing the one-dimensional square well case to the many-dimensional Compound Nucleus

- Keeping the idea of connecting the cross section to the collision function (or matrix) in the external region and, in turn, connecting the collision matrix to the R-Matrix in the internal region of the Compound Nucleus, we now add all of the geometrical complications arising from having many channels (defined by spin, orbital angular momentum and the various reaction pairs) as well as the complications from the external Coulomb field, we achieve connections between σ and U and between U and R which are very similar to those of the square-well case.

- This is what Wigner and others did to achieve the
- R-Matrix framework.

Analogues of the Compound Nucleus
An electric circuit junction and a wave guide.

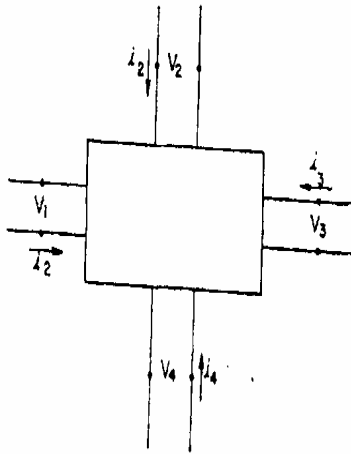(from E.P. Wigner, American Journal of Physics, Vol. 17 page 99, 1949)

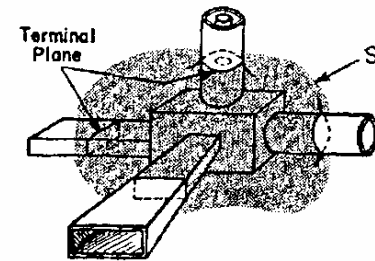FIG. 2. A junction of interdependent electric circuits.

FIG. 1. A transmission line (wave guide) junction.

The cross sections and the collision matrix

- The general differential cross section is connected to the collision matrix components by the products of many Clebsch-Gordan coefficients

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

$$B_L(\alpha's';\alpha s) = \frac{(-)^{s'-s}}{4} \sum_{J_1} \sum_{J_2} \sum_{l_1} \sum_{l_2} \sum_{l_1'} \sum_{l_2'}$$

$$\times i^{l_1 - l_2 - L} Z(1_1 J_1 1_2 J_{2'} sL) i^{l_1' - l_2' - L} Z(l_1' J_1 1_2' J_{2'} s'L)$$

$$\times R.P. \left[\left(\delta_{\alpha\alpha'} \delta_{1_1 1_1'} \delta_{ss'} - U_{\alpha's'1_1'}; as l_1{}^{J_1} \right)^* \left(\delta_{\alpha'\alpha} \delta_{s's} \delta_{1_2 1_2'} - U_{\alpha's'1_2'}; \alpha s l_2{}^{J_2} \right) \right]$$

The Collision matrix in terms of the R-Matrix
(for the few-channel, many-level framework)

- We use the external Coulomb wave functions, F_l and G_l, and their derivatives, evaluated at the channel radius, and the boundary conditions, b_l, for each channel to define:

- the logarithmic derivative: $L_l = (O'_l / O_l) - b_l = (S_l - b_l) + P_l$.

- the penetration factor: $P = (kr) / (F_l^2 + G_l^2)$

- the shift factor: $S_l = (F_l' F_l + G_l' G) / (F_l^2 + G_l^2)$

- the phase shift: $O_l^{-1} I_l = \exp(2i \Omega_l)$ with $\Omega_l = \omega_l - \tan(F_l / G_l)$

- where ω_l is the Coulomb phase-shift and $\tan(F_l / G_l)$ the hard-sphere phase-shift

- with these terms we get the collision matrix in terms of the R-Matrix:

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

The Few-Level, Multi-Channel R-Matrix Framework

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

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

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

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

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

The Inverse of the Level Matrix

(Diagonal terms which are Breit-Wigner Amplitudes and off-diagonal terms which are "cross talk" between levels)

$$
(A^{-1}) = \begin{pmatrix}
E_1 + \Delta_1 - E - \dfrac{i}{2}\Gamma_1 & \Delta_{12} - \dfrac{i}{2}\Gamma_{12} & \Delta_{13} - \dfrac{i}{2}\Gamma_{13} & \cdot & \cdot \\[2ex]
\Delta_{12} - \dfrac{i}{2}\Gamma_{12} & E_2 + \Delta_2 - E - \dfrac{i}{2}\Gamma_2 & \Delta_{23} - \dfrac{i}{2}\Gamma_{23} & \cdot & \cdot \\[2ex]
\Delta_{13} - \dfrac{i}{2}\Gamma_{13} & \Delta_{23} - \dfrac{i}{2}\Gamma_{23} & E_3 + \Delta_3 - E - \dfrac{i}{2}\Gamma_3 & \cdot & \cdot \\[2ex]
\cdot & \cdot & \cdot & & \\[1ex]
\cdot & \cdot & \cdot & & \cdot \quad \cdot
\end{pmatrix}
$$

The "Cross-Talk" terms of the Level Matrix

- Removing the level-shift terms by proper choice of the boundary condition numbers, the off-diagonal or "cross-talk" terms of the reciprocal of the level matrix are:

$$- (i/2) \; \Sigma_c \; \Gamma_{\lambda c}^{1/2} \; \Gamma_{\lambda' c}^{1/2}.$$

- ☐ This is a scalar product in channel space and can therefore be written as:

$$- (i/2) \; \Gamma_{\lambda}^{1/2} \; \Gamma_{\lambda'}^{1/2} \; \cos (\theta_{\lambda\lambda'})$$

- Where $\Gamma_{\lambda}^{1/2}$ and $\Gamma_{\lambda'}^{1/2}$ are the square roots of total level widths already occurring as parameters in the diagonal terms. Therefore, regardless of the number of channels or levels, a single new parameter, $\cos (\theta_{\lambda\lambda'})$, is needed for each of the cross-talk terms and this parameter has values between -1 and +1. Sometimes this parameter is necessary and useful.

The U^{235} cross sections fitted with the level matrix formula (1958)

(Broad levels clearly requiring the "cross-talk" terms)
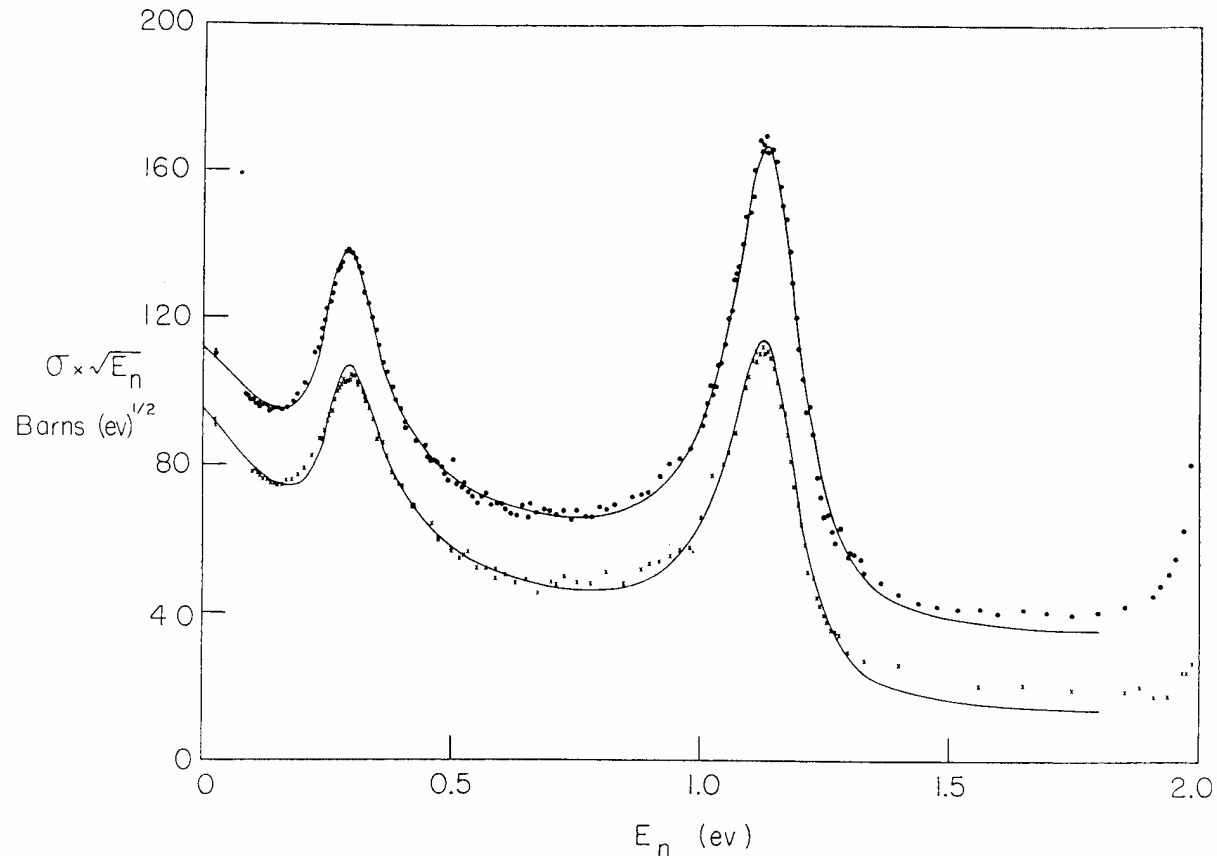
Comparison of Various Reaction Theory Frameworks

- Next we compare various frameworks for the description of resonance reactions

- Kapur and Peierls (1938)

- R-Matrix theory (Wigner et al, 1938-1958)

- K-Matrix theories (1960 -   )

The Kapur-Peierls Framework

First in the field: P.L. Kapur and R.E. Peierls, Proc. Roy. Soc. (London),**A166**, 277 (1938)

- Basis: the boundary condition numbers in each channel are chosen to be those of an outgoing wave. Intuitively a very good idea.

- Great advantage: with this choice of boundary conditions each L_c vanishes identically and therefore the matrix inversion disappears because $1 - LR = 1$. L* however does not vanish and the collision matrix becomes the square of the sum of Breit-Wigner amplitudes

- Disadvantages:

- 1) The boundary conditions are strongly energy dependent: $b_c = S_c + i P_c$. This is a crushing problem.

- 2) The boundary condition is complex. Therefore we don't have a Hermitian set of states and there are questions about completeness and many other things.

R-Matrix frameworks

- ## References for the development:

- The work by Wigner and his students was begun before WWII but was interrupted by the war. Some of the milestones were:

- 1. L.Eisenbud and E.P. Wigner, Proc. Natl. Acad. Sci. U.S.,**27,** 281 (1941).

- 2. E.P. Wigner, Phys. Rev. **70**, 15 (1946) & **70**, 606 (1946)

- 3. E.P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947).

- 4. T. Teichmann and E.P. Wigner, Phys. Rev. **87**, 123.

- 5. R.G. Thomas, Phys. Rev. **97**, 234 (1955)

- 6. C. Bloch, Nuclear Phys. **4**, 503 (1957).

- 7. A.M. Lane and R.G. Thomas, Revs. Modern Phys. **30**, 257 (1958)

- 8 EWV review papers in 1959, 1962 & 1968.

- 9. EWV Lecture notes at JINA (2005)

Advantages &Disadvantages of R-Matrix Theory

- ## Disadvantages:

- 1. For each approximation formula it is necessary to have matrix inversion.

- 2. The parameters, the channel radii, a_c, and the boundary condition numbers, b_c, appear arbitrary.

- 3. The difficulty of accommodating direct reactions

- ## Advantages:

- 1. The channel radii and boundary conditions have "natural" definitions which make the framework physically appealing.

- 2. The reduced widths have a very appealing connection to nuclear spectroscopy and the nuclear mean field. All aspects of the framework are intuitively appealing.

The Choice of Channel Radii and Boundary Conditions

- In the early days of R-Matrix theory there was much confusion about the apparent arbitrariness of the choice of channel radii and boundary condition numbers.

- With the advent of the optical model and the nuclear mean field (Saxon-Woods potential wells), in the 1950's, "natural" choices of these parameters emerged.

- "NATURAL" CHOICES:

- The "natural" choice of boundary condition number for each channel is to set it equal to the shift function at some point in the energy interval of the measurement. This works because the shift function generally varies slowly with energy.

- The "natural" choice of channel radii, for a Saxon-Woods mean field, is to choose it slightly larger (by about a fermi) than the mid-point radius.

Boundary Condition Numbers

- Even though the "natural" choice of boundary condition numbers makes the level shift quite small in most cases, one should not omit the shift functions from the fit to data, particularly for broad levels. (In effect, the energy dependence of the level shift renormalizes the level widths)

- There is only one case - bound s-wave neutron levels - where the shift function varies unreasonably rapidly with energy. Such levels, of course, correspond to "halo" states which require special treatment. Here the rapid energy variation of the shift function is a warning sign to be careful about the resonance analysis

- In general, the constancy of the shift function makes the R-matrix framework valid and useful for fitting resonance reactions and makes the fits relatively insensitive to the choice of boundary condition numbers.

Channel Radii

- The "natural" choice of the channel radius, for a Saxon-Woods mean field, is to make it slightly larger (by about a fm) than the mid-point radius: this makes the connection to nuclear spectroscopy simpler.

- A different choice of the channel radius impacts the value of the single-particle width in the one-level approximation, although in almost all cases the fit to data is remarkably insensitive to the choice of channel radii. Choosing a channel radius very different from the mid-point radius is physically unappealing.

Spectroscopic Factors

- For the approximations within the R-Matrix framework the partial level widths have the following very appealing form:

- $$\Gamma_{\lambda c} = 2\, P_c\, \gamma_{\lambda c}{}^2 = S_{\lambda c}\, \Gamma_c .$$

- Here Γ_c is the single-particle width of the mean field: for a square well it is $(h / 2\pi)^2 / ma^2$, but for a diffuse-edge well it increases by a reflection factor, with the surface thickness.

- $S_{\lambda c}$ is the spectroscopic factor - with a maximum value of unity - which gives the fraction of the compound state, λ, corresponding to the component single-particle state.

- Useful tip: when fitting data, especially alpha particle scattering, one should include nearby states with huge spectroscopic factors.

Direct Reactions

- The R-Matrix framework is, of course, complete and should be able to describe everything, including both resonance reactions and direct reactions. However, when we make approximations we can throw away some of the physics. As Claude Bloch first showed, when we throw away the very distant levels we throw away the direct reactions.

- The direct reactions can simply be added in to any description of resonances with R-Matrix approximations

- Similarly, the hard-sphere phase shifts can be replaced by phase shifts of the corresponding mean field

K-Matrix Frameworks

- In the early 1960's Rosenfeld became unreasonably excited about the parameters of R-Matrix theory - the channel radii and boundary conditions - which he regarded as unreasonably artificial: on the contrary, they are one of the strengths of R-Matrix theory.

- Following the fashion of the time   - which for particle physics focused on the analytic properties of the S-Matrix – he and Humblet devised the K-Matrix framework.

- In particle physics this approach has long been abandoned and deserves to be abandoned for resonance reactions: it involves all kinds of physically unattractive states. The compound nucleus really is a resonator deserving of an R-Matrix framework.

CONCLUSIONS

- The R-Matrix framework has turned out to be very resilient because it is so strongly rooted in the physics of the nucleus:

- The nucleus is really a "resonant" cavity and the parameters of the R-Matrix theory describe the properties of the Compound Nucleus.