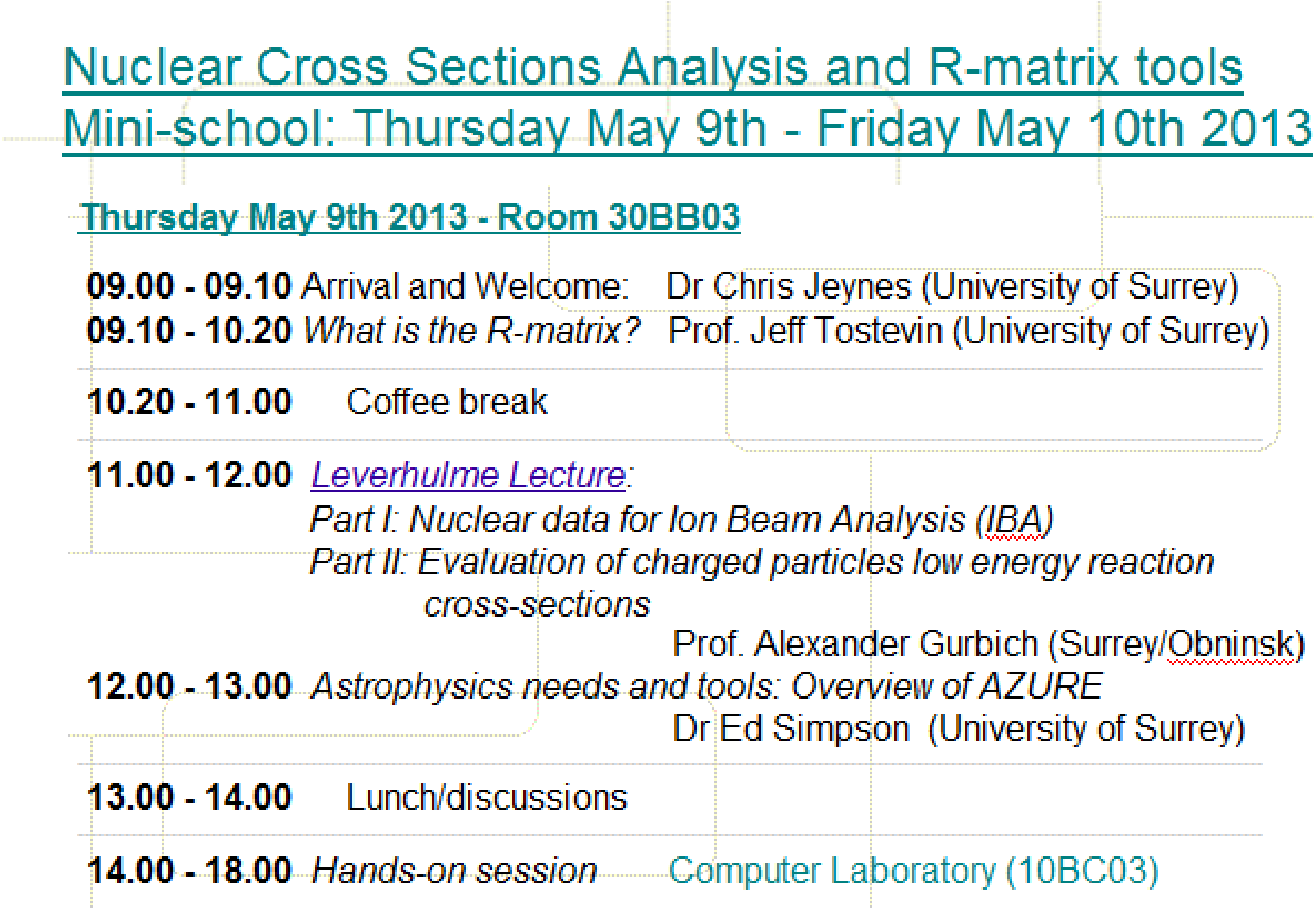


# Nuclear Cross Sections Analysis and R-matrix tools Mini-school: Thursday May 9th - Friday May 10th 2013

## Thursday May 9th 2013 - Room 30BB03

**09.00 - 09.10** Arrival and Welcome: Dr Chris Jeynes (University of Surrey)
**09.10 - 10.20** *What is the R-matrix?* Prof. Jeff Tostevin (University of Surrey)

**10.20 - 11.00** Coffee break

**11.00 - 12.00** *Leverhulme Lecture:*
*Part I: Nuclear data for Ion Beam Analysis (IBA)*
*Part II: Evaluation of charged particles low energy reaction cross-sections*
Prof. Alexander Gurbich (Surrey/Obninsk)
**12.00 - 13.00** *Astrophysics needs and tools: Overview of AZURE*
Dr Ed Simpson (University of Surrey)

**13.00 - 14.00** Lunch/discussions

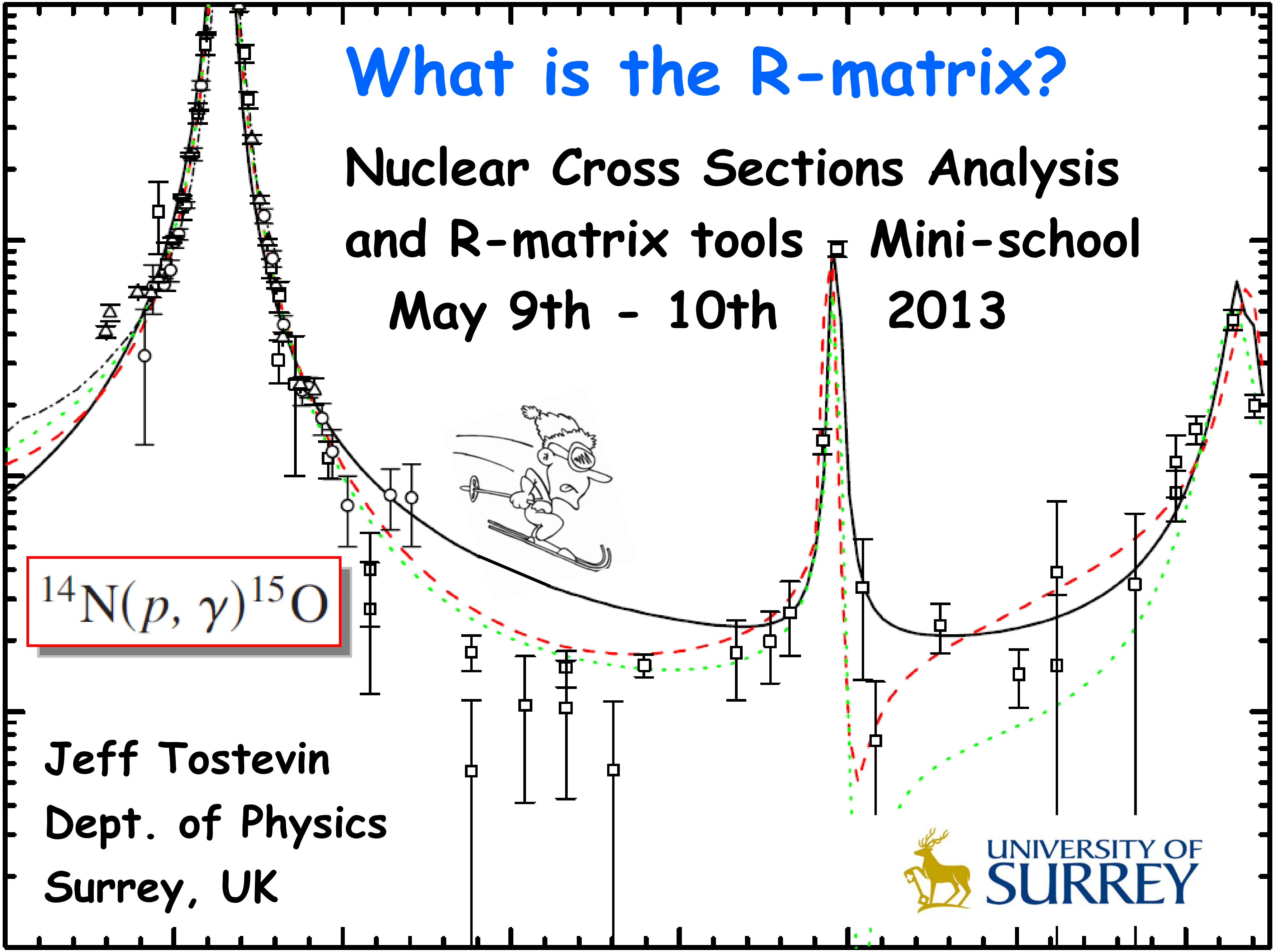
**14.00 - 18.00** *Hands-on session* Computer Laboratory (10BC03)

http://www.nucleartheory.net/NPG/Minischool_R-Matrix/

# What is the R-matrix?

## Nuclear Cross Sections Analysis and R-matrix tools - Mini-school

May 9th - 10th 2013



$^{14}N(p,\gamma)^{15}O$

**Jeff Tostevin**
Dept. of Physics
Surrey, UK

UNIVERSITY OF SURREY

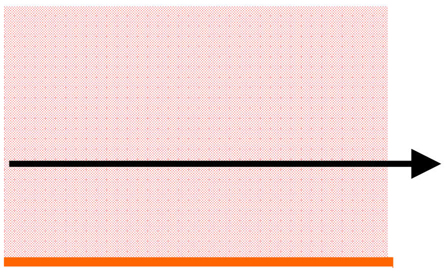
# Low energy collisions and low level densities

Entrance channel

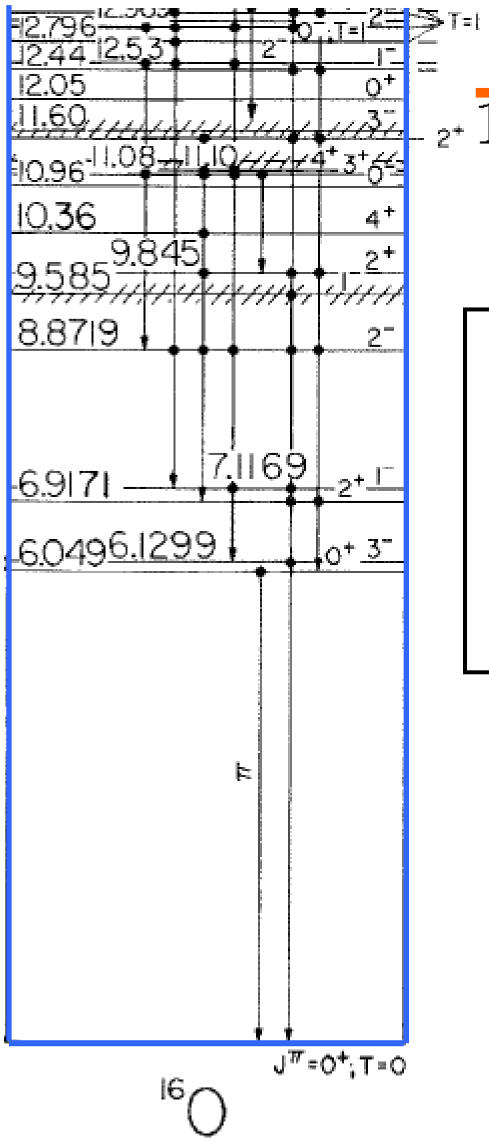
Compound system

$\{J^\pi\}$

$E_{cm}$



$^{12}\mathrm{C}+\alpha \quad 7.162$



$^{15}\mathrm{N}+p \quad 12.128$

A common feature is *resonant* behaviour in measured cross sections/observables

$\alpha: \quad J = L$

$\pi = (-1)^L$

Example for later today

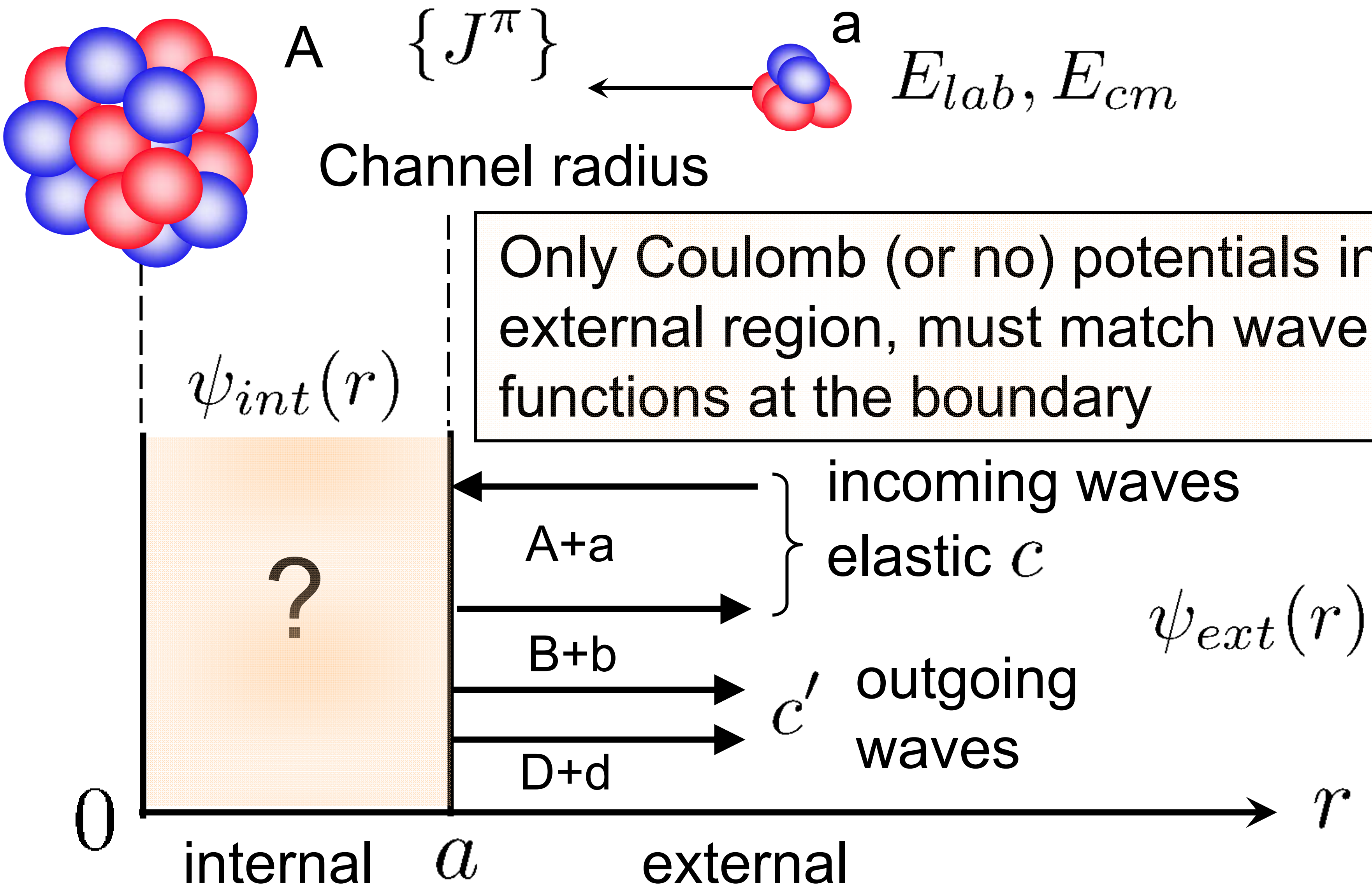
# R-matrix – and approach of this Minischool

In general, the R-matrix method is a formal and quantum mechanical approach to solve the Schrodinger equation for reactions. Problem is, for real nuclear systems, we do not usually know the potentials V(r) accurately enough to write down the correct starting Hamiltonian, H=T+V, to be solved.

However, the structure of the approach, and the form of its solutions, for any assumed V(r), lend themselves to a more phenomenological (parameter fitting) way. Merit is that the fitting parameters (*strengths*, *resonance* positions and *widths*) have a direct *visual* connection with experimental data sets and a well-defined mathematical relationship to physical states of the nuclei involved. So, detailed fitting is often able to describe measured data with high precision.

The code AZURE can perform this fitting task intelligently

# Basic assumptions behind R-matrix-like methods



A $\{J^\pi\}$

a $E_{lab}, E_{cm}$

Channel radius

Only Coulomb (or no) potentials in external region, must match wave functions at the boundary

$\psi_{int}(r)$

?

incoming waves

elastic $c$

A+a

B+b

$c'$ outgoing waves

D+d

$\psi_{ext}(r)$

$0$ $r$

internal $a$ external

# External - phase shifts and the collision matrix U

External solutions (r>a)

$$E_{cm} > 0\,, \quad k = \sqrt{\frac{2\mu E_{cm}}{\hbar^2}}$$

$$\left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} - \frac{2\mu}{\hbar^2}V(r) + k^2\right) u_L(k,r) = 0$$

and beyond the range of the nuclear forces

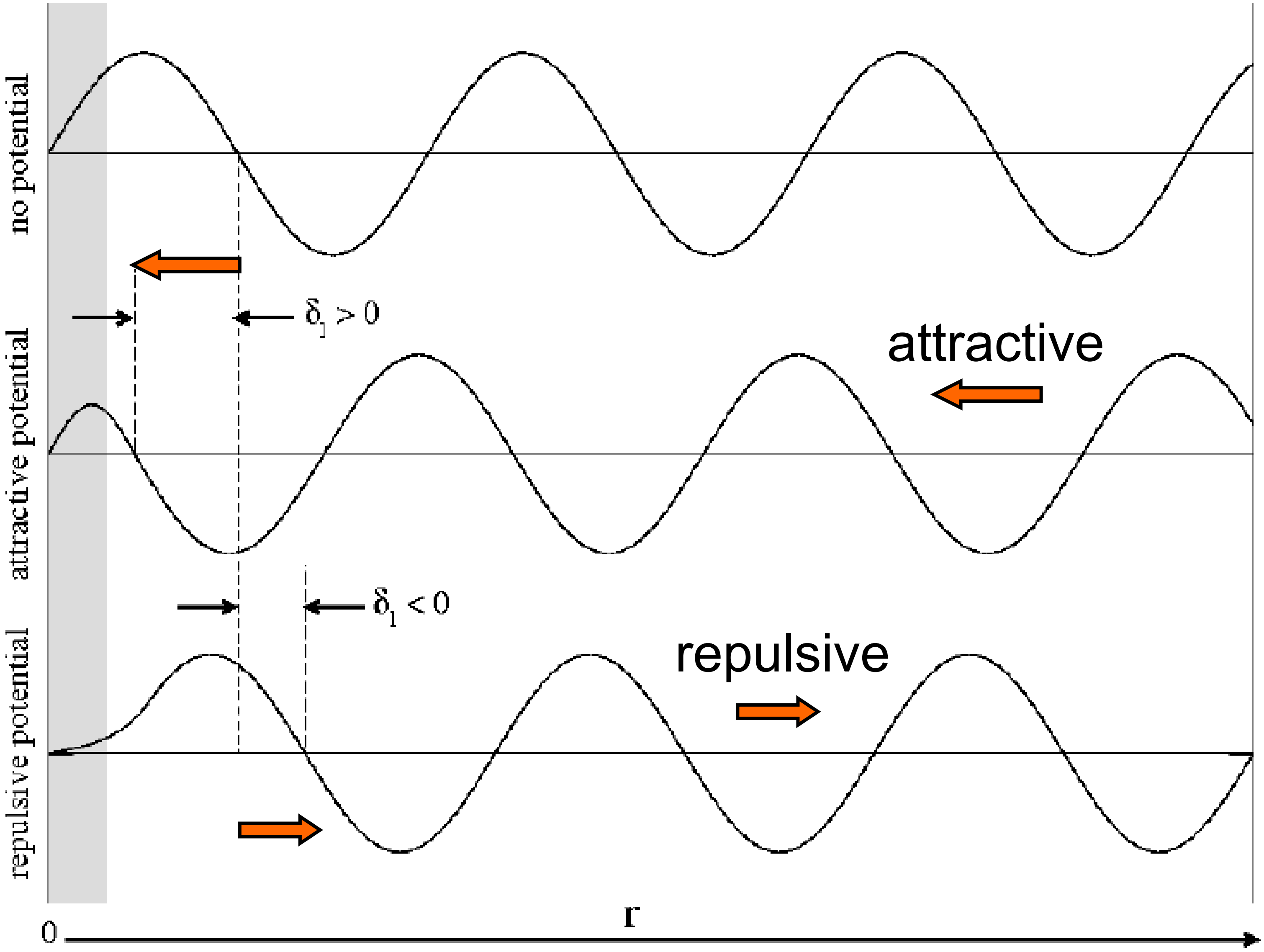
$$\left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} - \frac{2\eta k}{r} + k^2\right) u_L(k,r) = 0, \quad \eta = \frac{\mu Z_A Z_a e^2}{\hbar k}$$

$F_L(\eta, kr),\ G_L(\eta, kr)$ regular and irregular Coulomb functions

$$\begin{aligned} u_L(k,r) &= e^{i\delta_L}\left[\cos\delta_L\, F_L(\eta,kr) + \sin\delta_L\, G_L(\eta,kr)\right] \\ &= (i/2)\left[H_L^-(\eta,kr) - U_L H_L^+(\eta,kr)\right] \end{aligned}$$

$$H_L^{\pm}(\eta,kr) = G_L(\eta,kr) \pm iF_L(\eta,kr) \longrightarrow A_L \exp(\pm ikr)$$

# Phase shifts – a reminder



attractive

repulsive

# Phase shift and partial wave collision matrix U

$$u_L(k,r) = e^{i\delta_L}\underbrace{[\cos\delta_L\, F_L(\eta,kr) + \sin\delta_L\, G_L(\eta,kr)]}$$

If *V(r)* is real, the phase shifts $\delta_L$ are real, and […] also

$$u_L(k,r) = (i/2)[\underline{\underline{H_L^-(\eta,kr)}} - U_L\, \underline{\underline{H_L^+(\eta,kr)}}]$$

Ingoing waves

outgoing waves

$$U_L = e^{2i\delta_L}$$

$|U_L|^2$ survival probability in the scattering

$(1-|U_L|^2)$ absorption probability in the scattering

Given the phase shifts or partial wave U-matrix elements we can compute all scattering observables at this energy – Cross section fitting means fitting these complex U

# Resonance forms of the phase shift /U-matrix (i)

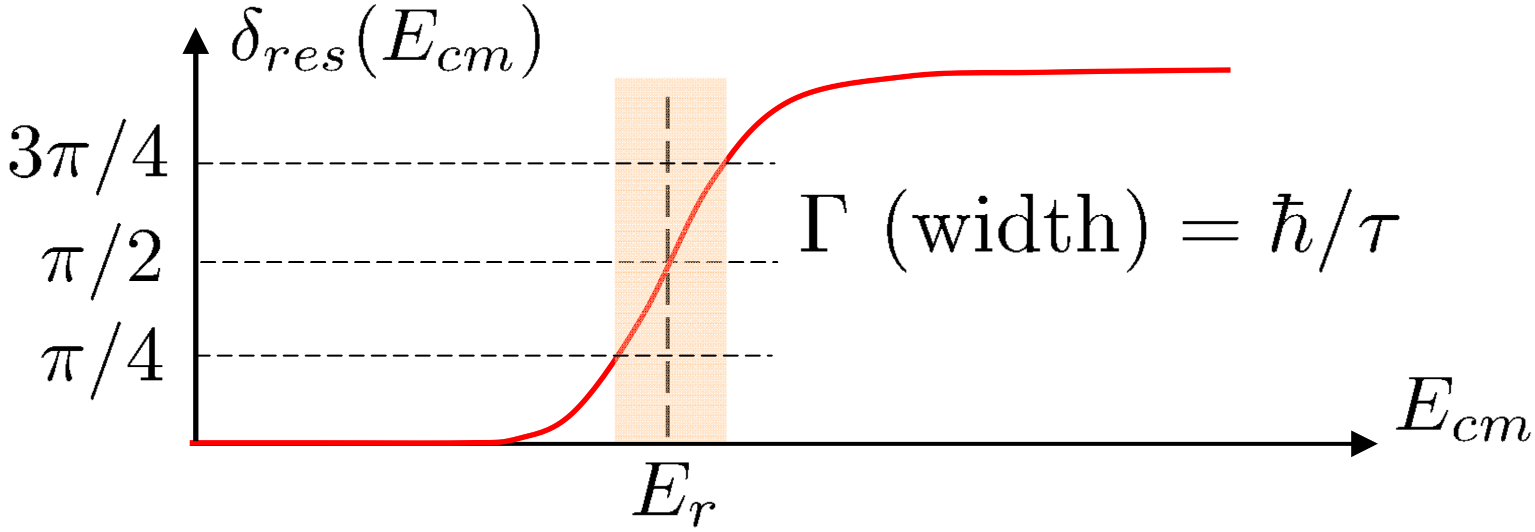
In the vicinity of an isolated (separated) resonance (with L)

$$\delta_L(E_{cm}) = \delta_{res}(E_{cm}) + \delta_{bg}(E_{cm})$$

with rapidly varying $\delta_{res}(E_{cm})$ over a small range of $E_{cm}$

$$\delta_{res}(E_{cm}) = \arctan\left(\frac{\Gamma/2}{E_r - E_{cm}}\right) \quad (\text{modulo } \pi)$$

and a slowly varying background phase $\delta_{bg}(E_{cm})$



# Resonance forms of the phase shift /U-matrix (ii)

If $\delta_{res}(E_{cm})$ was the only phase present, $\delta_{bg} \approx 0$

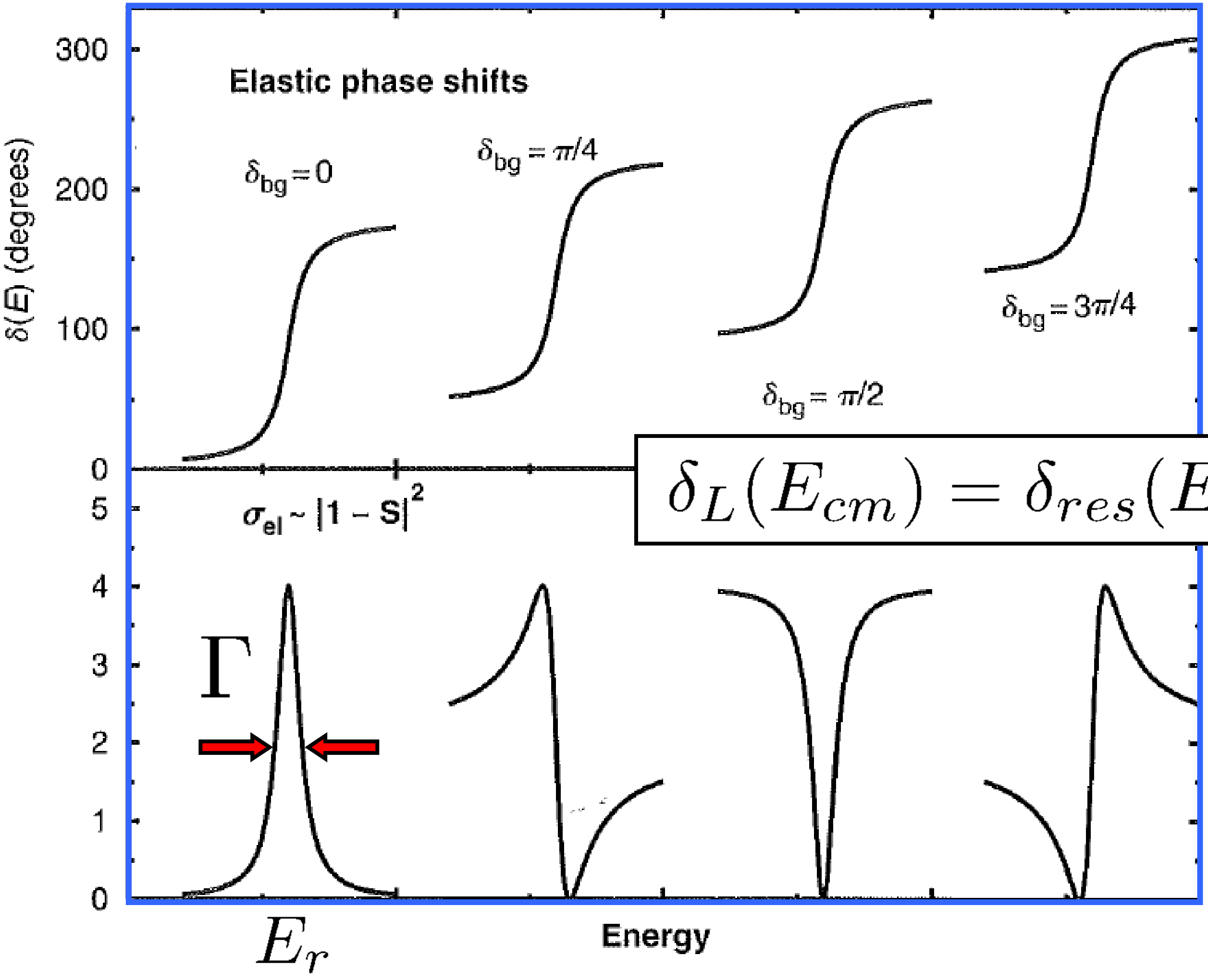
$$\tan \delta_{res}(E_{cm}) = \frac{\Gamma/2}{E_r - E_{cm}}$$

and $$\sin^2 \delta_{res}(E_{cm}) = \frac{(\Gamma/2)^2}{(E_{cm} - E_r)^2 + (\Gamma/2)^2}$$

The (elastic channel) cross section resulting from this partial wave resonance is thus of Breit-Wigner form

$$\boxed{\begin{aligned}\sigma_{res}(E_{cm}) &= \frac{4\pi}{k^2}(2L+1)\sin^2 \delta_{res}(E_{cm}) \\ &= \frac{4\pi}{k^2}(2L+1)\frac{(\Gamma/2)^2}{(E_{cm} - E_r)^2 + (\Gamma/2)^2}\end{aligned}}$$

# Resonance forms of the phase shift /U-matrix (iii)



phase shifts
$\delta_L(E_{cm})$

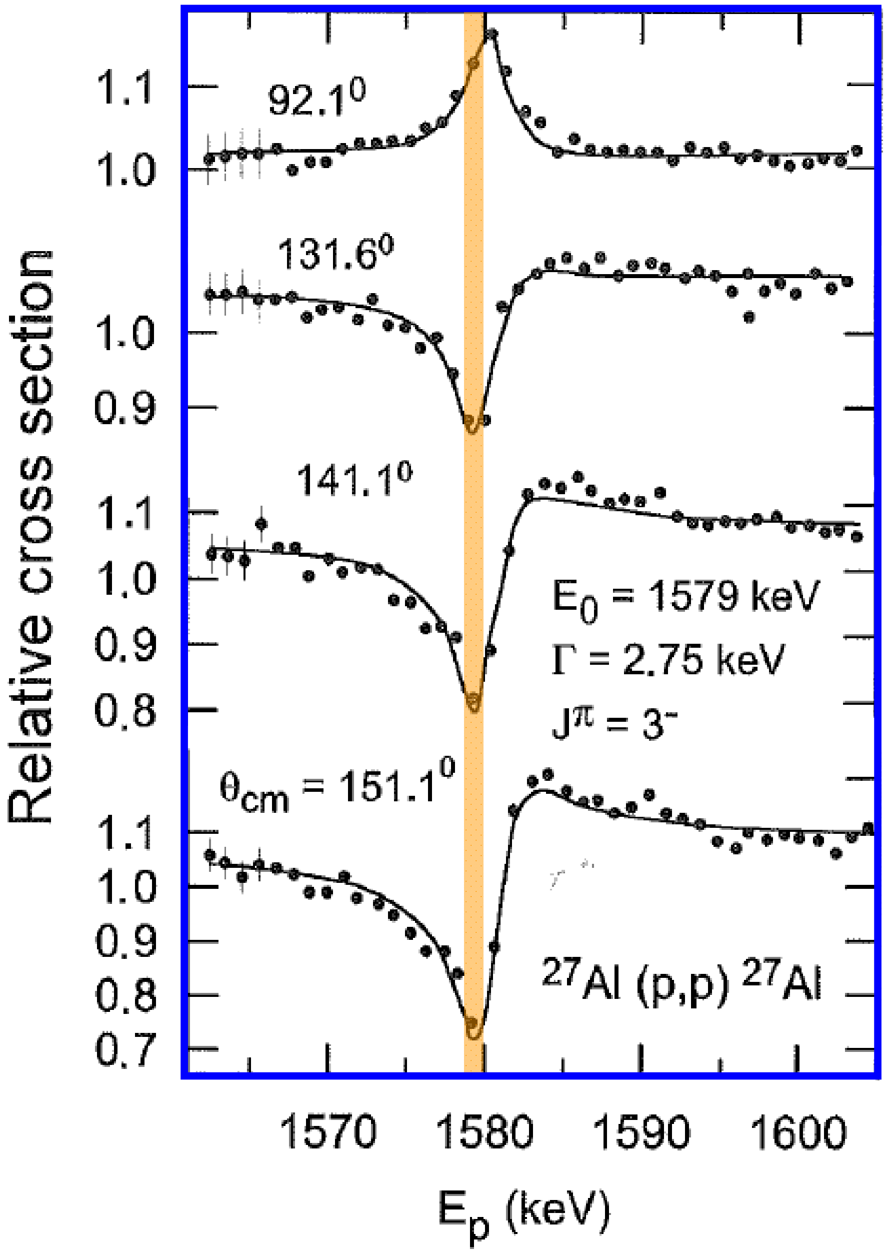
$$\boxed{\delta_L(E_{cm}) = \delta_{res}(E_{cm}) + \delta_{bg}(E_{cm})}$$

cross sections
$\sigma_{res}(E_{cm})$

From: Thompson and Nunes, Nuclear Reactions for Astrophysics, Cambridge University Press, 2009

# proton elastic scattering – resonance behaviour

The appearance of the resonance depends on the proton scattering angle, showing the interference between the localised resonance scattering and (background) potential scattering amplitudes.



From:
Bertulani and Danielewicz, Introduction to Nuclear Reactions, IOP Graduate Student Series, 2004

# Resonance forms of the phase shift /U-matrix (iv)

Additionally,
if

$$\tan\delta_{res}(E_{cm}) = \frac{\Gamma/2}{E_r - E_{cm}}$$

$$\boxed{U_L(E_{cm}) = e^{2i\delta_{bg}}\,\frac{E_{cm} - E_r - i\Gamma/2}{E_{cm} - E_r + i\Gamma/2}}$$

So, cross section fitting means fitting these complex U as functions of the centre-of-mass energy: the $E_r,\ \Gamma,\ \delta_{bg}$

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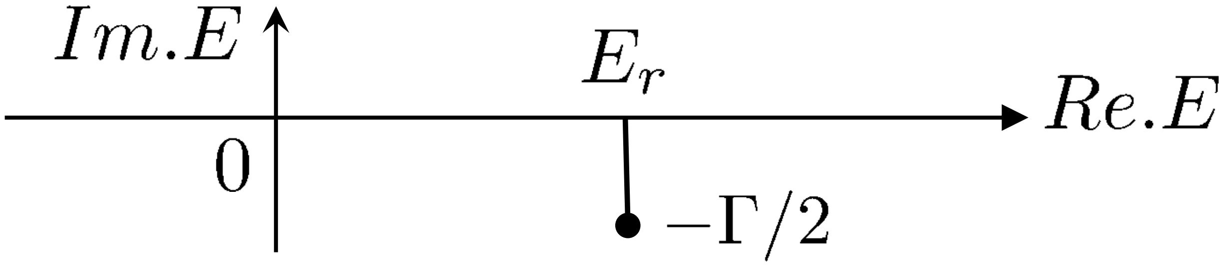
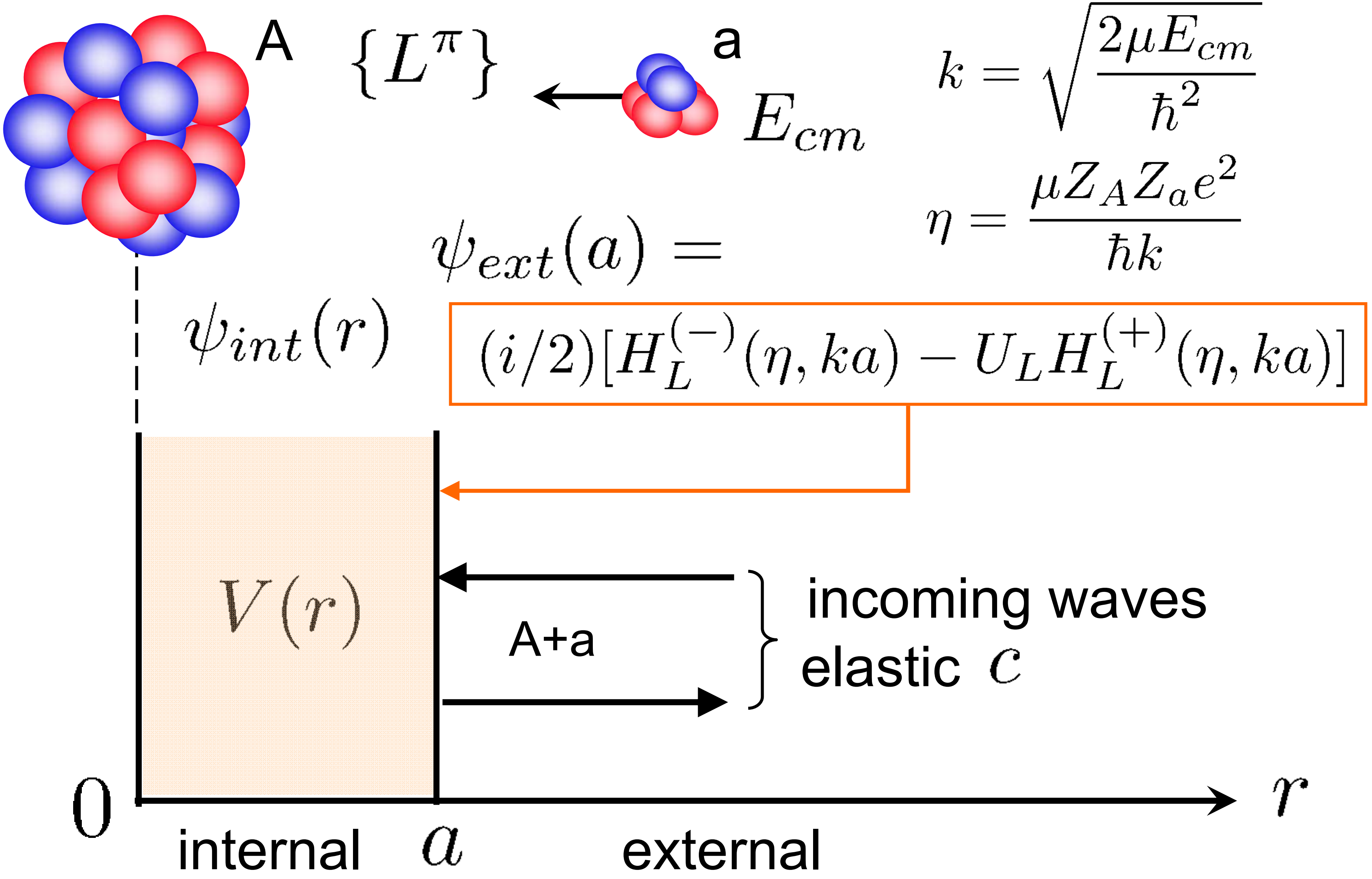
Resonances in the physical system are, mathematically, poles of the complex collision matrix $U_L(E_{cm})$ in the complex energy plane, at $E_{cm} = E_r - i\Gamma/2$



# Formulation using the R-matrix – one channel case



$$k = \sqrt{\frac{2\mu E_{cm}}{\hbar^2}}$$

$$\eta = \frac{\mu Z_A Z_a e^2}{\hbar k}$$

$$\psi_{ext}(a) =$$

$$\boxed{(i/2)[H_L^{(-)}(\eta, ka) - U_L H_L^{(+)}(\eta, ka)]}$$

# Internal region and boundary conditions: $\psi_{int}(r)$

$$H_L\psi_L(r) = [T_L + V(r)]\psi_L(r) = E_{cm}\psi_L(r)$$

$\psi_L(r=0) = 0,\ \psi_L(r=a) = ?$ for matching

Easily shown: **<u>if</u>** we require solutions that, at $r = a$ satisfy

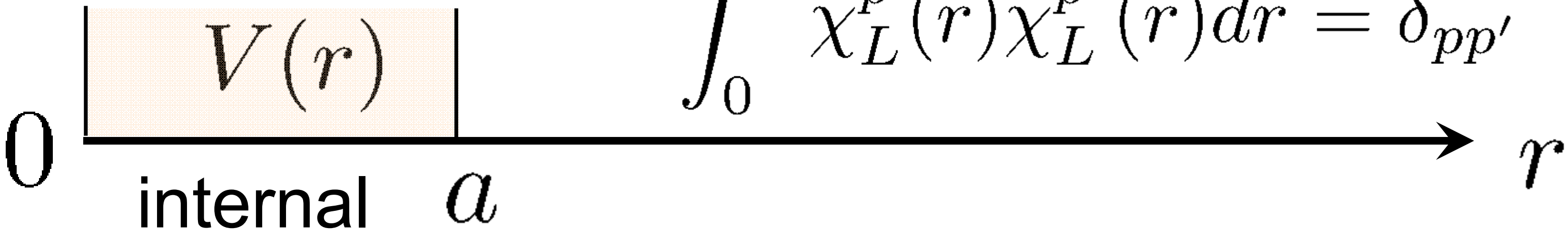
$(r\chi'/\chi)_{r=a} = b$ real, dimensionless constant

then problem is <u>Hermitian</u> on $[0, a]$

complete set,
real eigenvalues,
orthonormal

$$[T_L + V(r)]\chi_L^p(r) = \varepsilon_p\chi_L^p(r)$$

$$\int_0^a \chi_L^p(r)\chi_L^{p'}(r)dr = \delta_{pp'}$$



# Hermitian condition – for convenience

$$\langle \chi_\alpha | \hat{O} | \chi_\beta \rangle = \langle \chi_\beta | \hat{O}^\dagger | \chi_\alpha \rangle^*$$

but our operators O and states $\chi$ are real, so in

$$[T_L + V(r)]\chi_\alpha(r) = E_{cm}\chi_\alpha(r), \quad r \leq a$$

being a Hermitian problem requires that:

$$\int_0^a dr\, \chi_\alpha\, \chi''_\beta = \int_0^a dr\, \chi_\beta\, \chi''_\alpha$$

Integrating by parts, twice, this requires

$\left[\chi_\alpha \chi'_\beta - \chi'_\alpha \chi_\beta\right]_0^a = 0$ and, as the $\chi_\alpha(0) = 0$, that

at $r = a,$ $\boxed{\chi'_\alpha / \chi_\alpha = \chi'_\beta / \chi_\beta}$

# Expand the internal solution using a complete set

$$\psi_L(r=0)=0$$

Can drop the L's in the equations

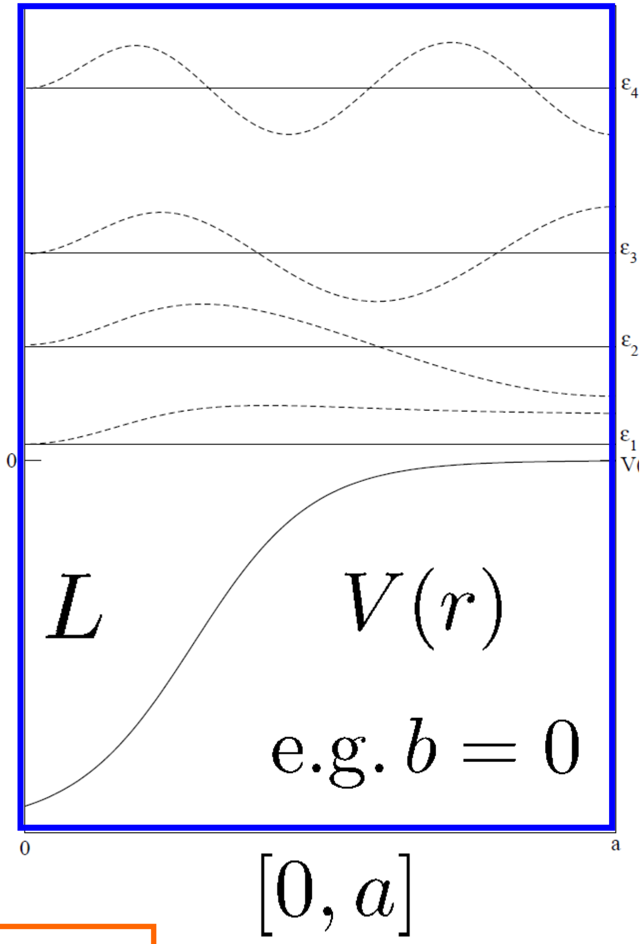
$$\psi_L(r)=\sum_p C_p\chi_p(r),\ \ r\leq a$$

$$C_p=\int_0^a \chi_p(r)\psi_L(r)dr$$

Manipulation of this integral, using

$$\chi_p(r)\psi_L(r)=\frac{\psi_L H_L\chi_p-\chi_p H_L\psi_L}{\varepsilon_p-E_{cm}}$$

$$C_p=\frac{\hbar^2}{2\mu a}\ \frac{\chi_p(a)}{\varepsilon_p-E_{cm}}\left[a\psi_L'(a)-b\psi_L(a)\right]$$



# R-matrix definition – completing the expansion

$$\psi_L(r) = \sum_p C_p \chi_p(r), \ r \leq a \, , \quad C_p = \int_0^a \chi_p(r)\psi_L(r)dr$$

$$C_p = \frac{\hbar^2}{2\mu a} \ \frac{\chi_p(a)}{\varepsilon_p - E_{cm}} \left[a\psi'_L(a) - b\psi_L(a)\right]$$

then, for matching the internal and external solutions at r=a

$$\psi_L(a) = \sum_p \left\{ \frac{\hbar^2}{2\mu a} \ \frac{\chi_p(a)}{\varepsilon_p - E_{cm}} \left[a\psi'_L(a) - b\psi_L(a)\right] \right\} \chi_L^p(a)$$

$$\psi_L(a) = R_L(E_{cm}) \left[a\psi'_L(a) - b\psi_L(a)\right]$$

$$\boxed{R_L(E_{cm}) = \sum_p \frac{\hbar^2}{2\mu a} \ \frac{[\chi^p(a)]^2}{\varepsilon_p - E_{cm}} = \sum_p \frac{\gamma_p^2}{\varepsilon_p - E_{cm}}}$$

# Terminology

$$R_L(E_{cm}) = \sum_p \frac{\gamma_p^2}{\varepsilon_p - E_{cm}}$$

there are poles, and R→ ∞ whenever $E_{cm}$ coincides with an energy eigenvalue $\varepsilon_p$

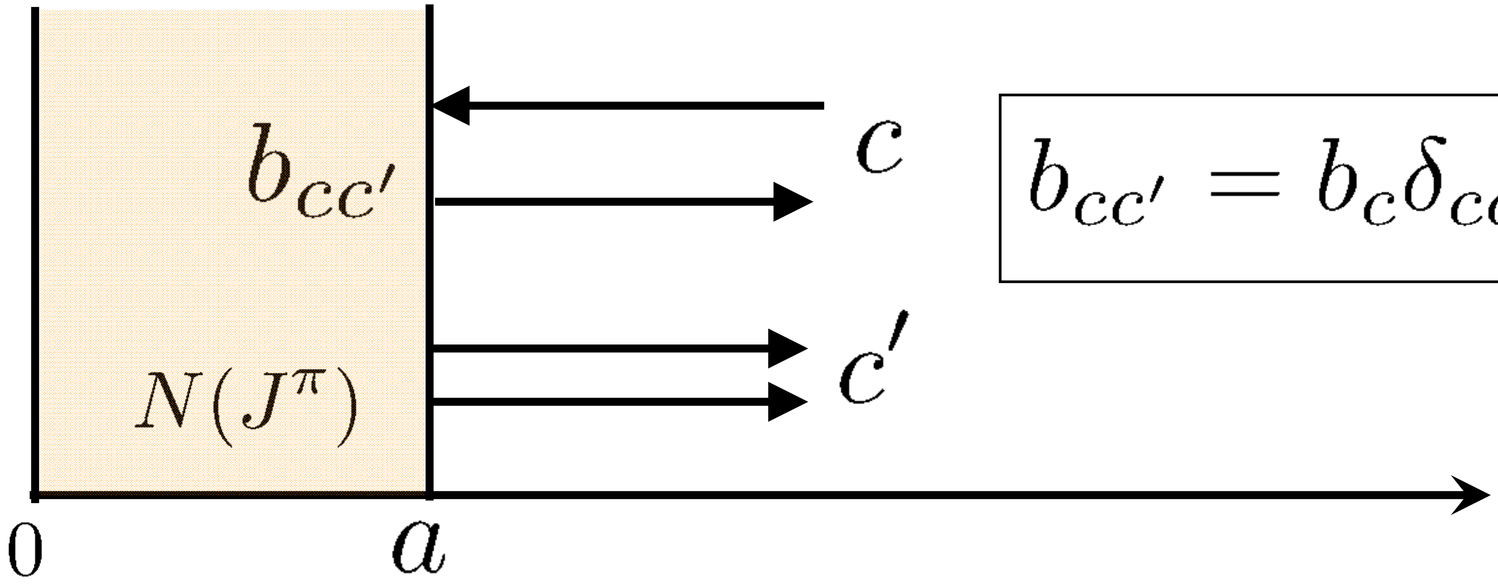
$$\gamma_p^2 = \frac{\hbar^2}{2\mu a} \left[\chi^p(a)\right]^2$$

are called the *reduced widths* – and have units of energy

$\gamma_p$ is the *reduced width amplitude*

Note that the *structure* of these equations does not depend on any particular choice of the potential $V(r)$, although the different numbers, reduced widths, eigen-energies, $\varepsilon_p$, appearing in the R-matrix will depend on the choice of b, a, and the potential. If the sum over all p is performed, the results should not depend on these choices.

# Boundary conditions – finite sets of levels/channels



$$\boxed{b_{cc'} = b_c \delta_{cc'}}$$

Choice of boundary condition $b_c$ for each channel can be made such that, even for a finite number of levels $N(J^\pi)$ and channels N(c), cross sections are independent of choice – done behind the scenes (Barker) and one does not usually need to specify b

F.C. Barker, Aust. J. Phys. 25 341-348 (1972)

# Hard-core phase shift, penetrability and shifts

From the internal region, at r=a must have

$$\psi_L(a) = R_L(E_{cm})\left[a\psi'_L(a) - b\psi_L(a)\right]$$

and externally, that connects to the observables, at r=a

$$\begin{aligned}\psi_L(a) &= (i/2)[H_L^-(\eta, ka) - U_L H_L^+(\eta, ka)] \\ &= (i/2)[H_L^- - U_L H_L^+] \\ \psi'_L(a) &= (i/2)[H_L^{-\prime} - U_L H_L^{+\prime}]\end{aligned}$$

$$\begin{aligned}U_L(E_{cm}) &= \left[\frac{H_L^-}{H_L^+}\right] \times \left[\frac{1 - R_L[a(H_L^{-\prime}/H_L^-) - b]}{1 - R_L[a(H_L^{+\prime}/H_L^+) - b]}\right] \\ &= \exp[2i\delta_L(E_{cm})]\end{aligned}$$

# The hard-core phase shift

The first term on the product form for U

$$U_L(E_{cm}) = \left[\frac{H_L^-}{H_L^+}\right] \times \left[\frac{1 - R_L[a(H_L^{-'}/H_L^-) - b]}{1 - R_L[a(H_L^{+'}/H_L^+) - b]}\right]$$

results from what is called the *Hard-sphere phase shift*, and is seen to be the value $U_L$ if the external wave function were to vanish at r=0, i.e. if

$$\psi_L(a) = (i/2)[H_L^- - \bar{U}_L H_L^+] = 0$$

then $\bar{U}_L = H_L^-/H_L^+ = \exp(2i\delta_L^{HS})$ therefore

$$U_L(E_{cm}) = \exp[2i\delta_L(E_{cm})] = \exp(2i[\delta_L^{HS} + \delta_L^R])$$

and

$$\exp(2i\delta_L^R) = \left[\frac{1 - R_L[a(H_L^{-'}/H_L^-) - b]}{1 - R_L[a(H_L^{+'}/H_L^+) - b]}\right]$$

# Penetrability and shift functions

Remaining in the R-matrix phase shift expression

$$\exp(2i\delta_L^R) = \left[ \frac{1 - R_L[a(H_L^{-'}/H_L^-) - b]}{1 - R_L[a(H_L^{+'}/H_L^+) - b]} \right]$$

are the ratios $aH_L^{\pm'}/H_L^{\pm} = a(G'_L \pm iF'_L)/(G_L \pm iF_L)$

Multiplying out, and noting that $F'_L G - G'_L F_L = k$

$$aH_L^{\pm'}/H_L^{\pm} = S_L \pm iP_L$$

where the shift (S) and penetrability (P) are calculated from the F and G for any L and centre-of-mass energy:

$$\boxed{S_L = a\frac{F'_l F_L + G'_L G_L}{F_L^2 + G_L^2}, \qquad P_L = \frac{ka}{F_L^2 + G_L^2}}$$

# Connection to ‘formal’ resonance parameters (i)

It follows that

$$U_L(E_{cm}) = e^{2i\delta_L^{HS}} \left[ \frac{1 - R_L[S_L^0 - iP_L]}{1 - R_L[S_L^0 + iP_L]} \right], S_L^0 = S_L - b$$

Consider the contribution of a single R-matrix pole, p, i.e. substituting $R_L = \gamma_p^2/(\varepsilon_p - E_{cm})$ and rearranging

$$U_L(E_{cm}) = e^{2i\delta_L^{HS}} \left[ \frac{E_{cm} - (\varepsilon_p - \gamma_p^2 S_L^0) - i\gamma_p^2 P_L}{E_{cm} - (\varepsilon_p - \gamma_p^2 S_L^0) + i\gamma_p^2 P_L} \right]$$

and has the earlier-discussed resonance form

$$U_L(E_{cm}) = e^{2i\delta_{bg}} \frac{E_{cm} - E_r - i\Gamma/2}{E_{cm} - E_r + i\Gamma/2}$$

and that defines <u>formal</u> resonance positions and widths

$$\boxed{\mathbf{E}_r = \varepsilon_p - \gamma_p^2 S_L^0 , \quad \mathbf{\Gamma} = 2\gamma_p^2 P_L}$$

# Connections to 'observed' parameters (i)

Whereas the resonance positions and widths in earlier

$$U_L(E_{cm}) = e^{2i\delta_{bg}} \frac{E_{cm} - E_r - i\Gamma/2}{E_{cm} - E_r + i\Gamma/2}$$

were constants, the formal R-matrix quantities

$$\mathbf{E}_r = \varepsilon_p - \gamma_p^2 S_L^0(E_{cm}), \quad \mathbf{\Gamma}_L = 2\gamma_p^2 P_L(E_{cm})$$

deduced from

$$U_L(E_{cm}) = e^{2i\delta_L^{HS}} \left[ \frac{E_{cm} - (\varepsilon_p - \gamma_p^2 S_L^0) - i\gamma_p^2 P_L}{E_{cm} - (\varepsilon_p - \gamma_p^2 S_L^0) + i\gamma_p^2 P_L} \right]$$

remain $E_{cm}$ dependent near the resonance position. They need to be replaced by constants, 'observed' parameters, in comparisons with and when fitting data.

Can include dominant energy dependence of $S_L$ by Taylor expansion near the resonance position – e.g. iteratively

# Connection to ‘observed’ parameters (ii)

Based on the empirical resonance energy $E_r^{obs}$ and, with

$$\mathbf{E}_r = \varepsilon_p - \gamma_p^2 S_L^0(E_{cm}) = \varepsilon_p - \gamma_p^2 [S_L(E_{cm}) - b]$$

we require

$$\boxed{E_r^{obs} = \varepsilon_p - \gamma_p^2 [S_L(E_r^{obs}) - b]}$$

And, expanding the shift term, to leading order (Thomas)

$$S_L(E_{cm}) = S_L(E_r^{obs}) + [E_{cm} - E_r^{obs}] \left.\frac{dS_L}{dE}\right|_{E_r^{obs}}$$

gives, for $E_{cm} - \mathbf{E}_r = E_{cm} - [\varepsilon_p - \gamma_p^2 S_L^0(E_{cm})]$

$$\boxed{E_{cm} - \mathbf{E}_r \rightarrow [E_{cm} - E_r^{obs}] \, [1 + \gamma_p^2 S_L'(E_r^{obs})]}$$

# Connection to ‘observed’ parameters (iii)

On substituting in

$$U_L(E_{cm}) = e^{2i\delta_L^{HS}} \left[ \frac{E_{cm} - (\varepsilon_p - \gamma_p^2 S_L^0) - i\gamma_p^2 P_L}{E_{cm} - (\varepsilon_p - \gamma_p^2 S_L^0) + i\gamma_p^2 P_L} \right]$$

$$U_L(E_{cm}) = e^{2i\delta_L^{HS}} \left[ \frac{(E_{cm} - \mathbf{E}_r^{obs}) - i\mathbf{\Gamma}_L^{obs}/2}{(E_{cm} - \mathbf{E}_r^{obs}) + i\mathbf{\Gamma}_L^{obs}/2} \right]$$

$$\sin^2 \delta_L^R(E_{cm}) = \frac{(\mathbf{\Gamma}_L^{obs}/2)^2}{(E_{cm} - \mathbf{E}_r^{obs})^2 + (\mathbf{\Gamma}_L^{obs}/2)^2}$$

with <u>constant</u> energy shifts and widths

$$\mathbf{\Gamma}_L^{obs} = \frac{2\gamma_p^2 P_L(E_r^{obs})}{1 + \gamma_p^2 S_L'(E_r^{obs})}, \quad \mathbf{E}_r^{obs} = \varepsilon_p - \gamma_p^2 [S_L(E_r^{obs}) - b]$$

# Summary comments

Have tried to summarise both the basis and structure of the R-matrix formulas and the formal and computational links from R-matrix → predicted observables (cross sections),

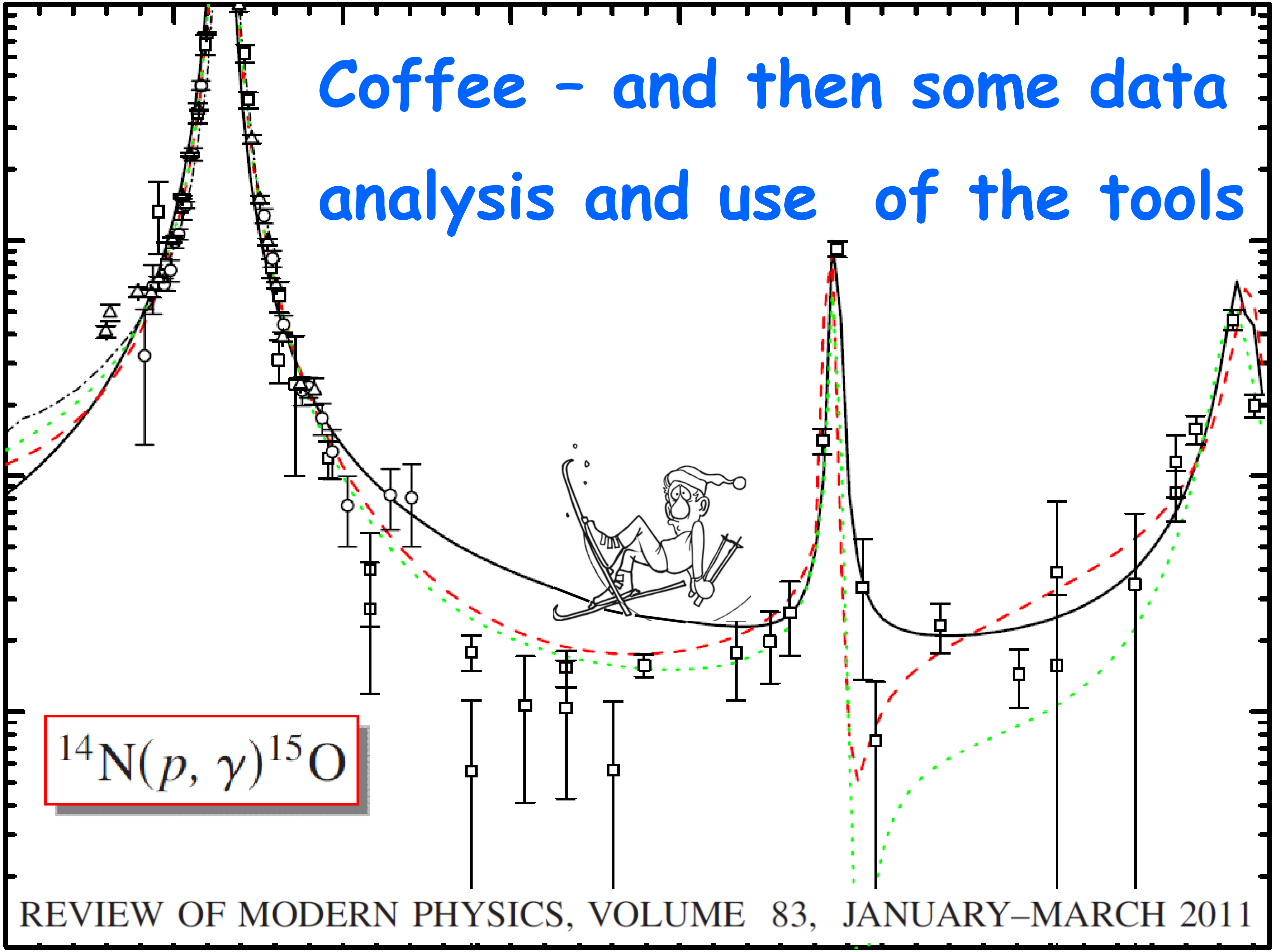
$$(\gamma_p^2, \varepsilon_p) \rightarrow R_L(E_{cm}) \rightarrow U_L(E_{cm}) \rightarrow \text{cross sections}$$

Have also discussed the reverse process and the data → deduced R-matrix parameters linkage, i.e.

$$\text{data} \rightarrow (\mathbf{E}_r^{obs}, \mathbf{\Gamma}_L^{obs}) \rightarrow (\mathbf{E}_r, \mathbf{\Gamma}_L) \rightarrow (\gamma_p^2, \varepsilon_p)$$

When combined and used as a phenomenology, this R-matrix machinery can provide accurate parameterisations of data and the means to inter(extra)polate cross sections (with due caution) between (+beyond) the available data.

Coffee - and then some data analysis and use of the tools



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