Potential models, bound and continuum states

Mini-school on Nuclear Reaction Theories for Nuclear Astrophysics Surrey, 7th January 2009

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This session (learning) aims:

Solutions of the Schrodinger equation for states of <u>two</u> bodies, with specific quantum numbers, over a wide range of energies – the need for bound, resonant, continuum and continuum bin states for reactions.

Reminder of the form of these two-body solutions at large separations and their relationships to absorption, reaction and scattering studies.

Constraints on two-body potentials and their parameters. Parameter conventions. The need to cross reference to known nuclear structure, resonances, nuclear sizes and experiment (whenever possible) in constraining all parameter choices.

This session (learning) outcomes:

To (re)gain familiarity with solutions of the Schrodinger equation over a range of energies: properties of bound, resonant, continuum and bin states. These enter reaction models and codes (such as FRESCO). To appreciate the need to understand <u>sensitivities</u> to input parameters that enter into final calculations.

To recall the role of the S-matrix in determining scattering and absorptive properties of a two-body interaction.

To question the use of 'standard' potential parameter sets and understand the need to explore the quality of these by reference to experimental data and to systematics from theoretical models – e.g. from the shell model and Hartree-Fock. To see examples in each energy regime.

There is a <u>lot</u> of literature to refer to:

<u>Direct nuclear reaction theories</u> (Wiley, Interscience monographs and texts in physics and astronomy, v. 25) <u>Norman Austern</u>

<u>Direct Nuclear Reactions</u> (Oxford University Press, International Series of Monographs on Physics, 856 pages) <u>G R Satchler</u>

Introduction to the Quantum Theory of Scattering (Academic, Pure and Applied Physics, Vol 26, 398 pages) LS Rodberg, RM Thaler

<u>Direct Nuclear Reactions</u> (World Scientific Publishing, 396 pages) <u>Norman K.</u> <u>Glendenning</u>

<u>Introduction to Nuclear Reactions</u> (Taylor & Francis, Graduate Student Series in Physics, 515 pages) <u>C A Bertulani</u>, <u>P Danielewicz</u>

<u>Theoretical Nuclear Physics: Nuclear Reactions</u> (Wiley Classics Library, 1938 pages) <u>Herman Feshbach</u>

Introduction to Nuclear Reactions (Oxford University Press, 332 pages) GR Satchler

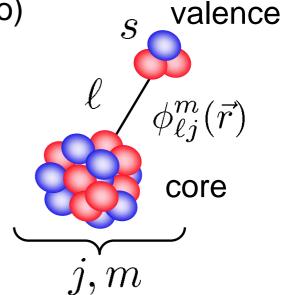
<u>Nuclear Reactions for Astrophysics</u> (Cambridge University Press, almost in press) <u>Ian Thompson and Filomena Nunes</u>

Introduction to "The tools of the trade..."

Solution of Schrodinger's equation for (two) bodies interacting via a potential energy function of the form*

$$U(r) = V_C(r) + V_{so}(r) \vec{\ell} \cdot \vec{s}$$
 Coulomb Nuclear

Need descriptions of wave functions of:

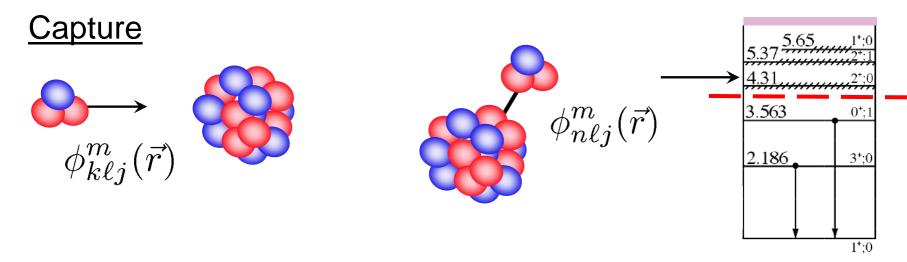


- (1) <u>Bound states</u> of nucleons or clusters (valence particles) to a core (that is assumed for now to have spin zero).
- (2) <u>Unbound</u> scattering or resonant states at low energy
- (3) <u>Distorted</u> waves of such bodies in complex potentials

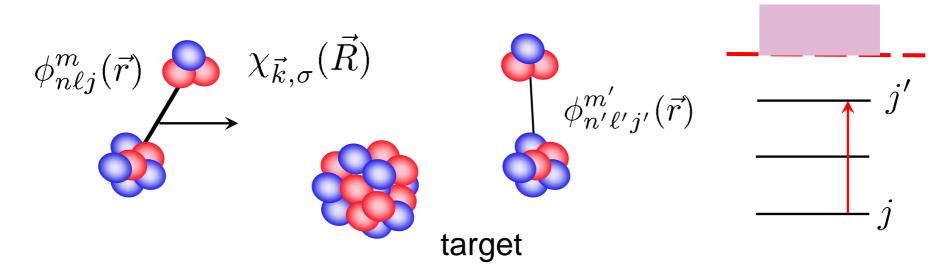
$$U(r) = V_C(r) + V(r) + iW(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

^{*}Additional, e.g. tensor terms, when s=1 or greater neglected

Direct reactions – types and characteristics

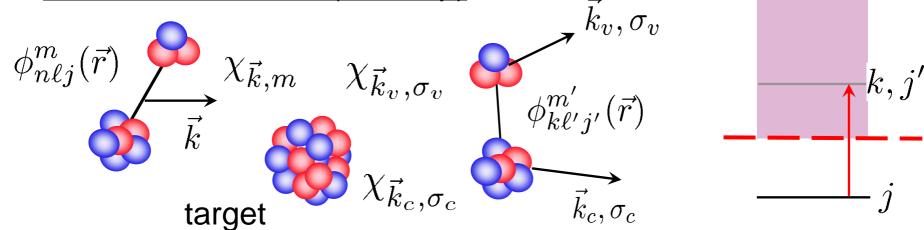


Inelastic excitations (bound to bound states) DWBA

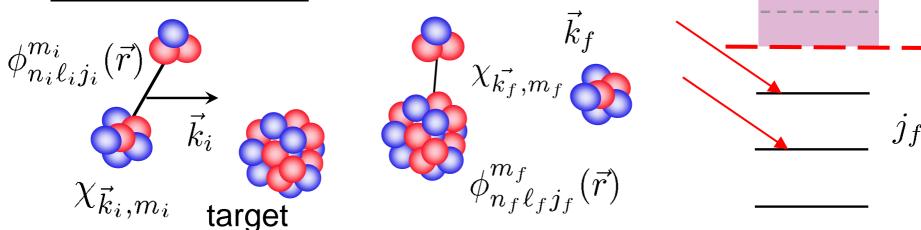


Direct reactions – types and characteristics

Inelastic excitations (breakup)



Transfer reactions



Direct reactions – requirements (1)

Description of wave functions of **bound** systems (both nucleons or clusters) – (a) can take from structure theory, if available or, (b) more usually, use a real potential model to bind system with the required experimental separation energy.

Refer to core and valence particles

$$U(r) = V_C(r) + V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

$$\phi_{n\ell j}^{m}(\vec{r}) = \sum_{\lambda \sigma} (\ell \lambda s \sigma | j m) \frac{u_{n\ell j}(r)}{r} Y_{\ell}^{\lambda}(\hat{r}) \chi_{s}^{\sigma}, \quad \int_{0}^{\infty} [u_{n\ell j}(r)]^{2} dr = 1$$

Usually just one or a few such states are needed.

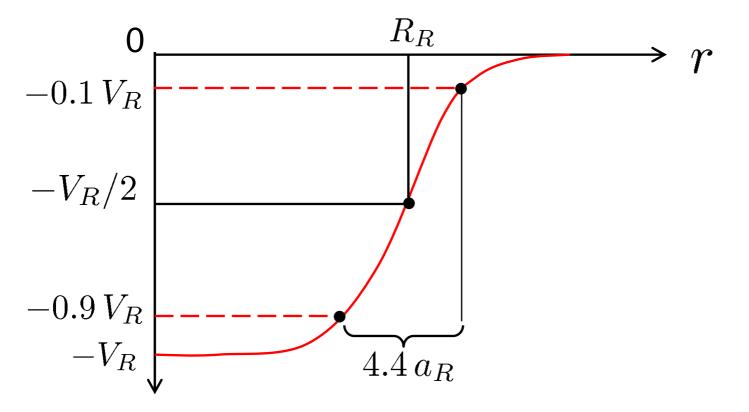
Separation energies/Q-values: many sites, e.g.

http://ie.lbl.gov/toi2003/MassSearch.asp

Bound states – real potentials

$$U(r) = V_C(r) + V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

$$V(r) = -\frac{V_R}{[1 + \exp(X_R)]}, \qquad X_R = \frac{r - R_R}{a_R}$$



Bound states – potential conventions

$$U(r) = V_C(r) + V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

$$V(r) = -\frac{V_R}{[1 + \exp(X_R)]}, \qquad X_i = \frac{r - R_i}{|a_i|}$$

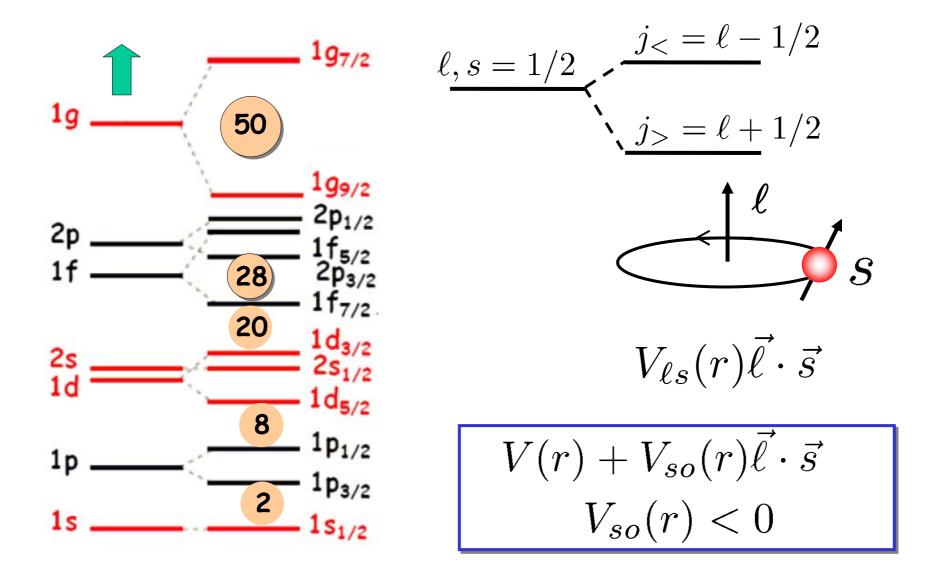
$$V_{so}(r) = -rac{2}{r} rac{V_{so}}{a_{so}} rac{\exp(X_{so})}{[1 + \exp(X_{so})]^2} \; ,$$
 Conventions

$$R_i = r_i A_2^{1/3}$$
 or $R_i = r_i \left[A_1^{1/3} + A_2^{1/3} \right]$

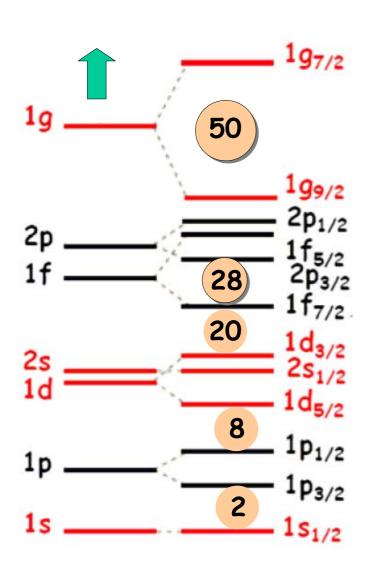
$$V_C(r) = Z_1 Z_2 e^2 / r, r > R_C$$

$$= \frac{Z_1 Z_2 e^2}{2R_C} \left[3 - \left(\frac{r}{R_C}\right)^2 \right], r \le R_C$$

Bound states – nuclear single particle structures



Bound states – for nucleons - conventions



Conventions

$$\phi_{n\ell j}^m(\vec{r})$$

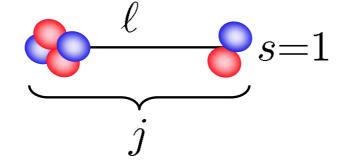
With this potential, and using sensible parameters, we will obtain the independent-particle shell model level orderings, shell closures with spin-orbit splitting.

NB: In diagram $2d_{5/2}$ means the second $d_{5/2}$ state. Defined this way, n>0 and n-1 is the number of nodes in the radial wave function. This is the convention used in e.g. FRESCO but many codes ask for the actual number of nodes. Care is needed.

Direct reactions – requirements (2)

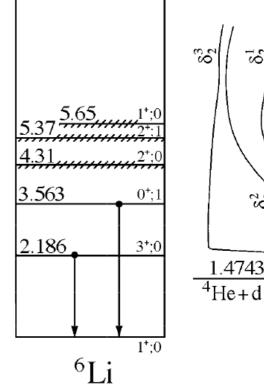
<u>Description of wave functions for unbound (often light)</u>
<u>systems</u> (nucleons or clusters) with low relative energy:
<u>Usually have low nuclear level density</u> of isolated
resonances. Use the same real potential model as
binds the system → scattering wave functions in this
potential. Also '<u>bin</u>' wave functions.

⁶Li (α+d)



$$U(r) = V_C(r) + V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

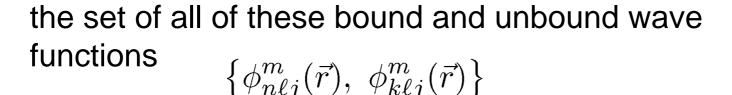
$$\phi_{k\ell j}^{m}(\vec{r}) = \sum_{\lambda=1}^{\infty} (\ell \lambda s \sigma | jm) \frac{u_{k\ell j}(r)}{kr} Y_{\ell}^{\lambda}(\hat{r}) \chi_{s}^{\sigma}$$



Completeness and orthogonality

Given a fixed two-body Hamiltonian

$$H = T + U(r) = T + V_C(r) + V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$



form a complete and orthogonal set, and specifically

$$\langle \phi_{n\ell j}^m(\vec{r}) | \phi_{k\ell j}^m(\vec{r}) \rangle = 0$$

When including coupling of bound to unbound states it is essential we use a <u>fixed</u> Hamiltonian for both the bound and unbound states (in each ℓ *j* channel) else we lose the orthogonality and the states will couple even without a perturbation or interaction with the target.

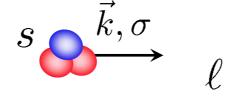
Direct reactions – requirements (3)

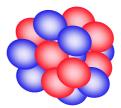
Description of wave functions for scattering of nucleons or clusters from a heavier target and/or at higher energies:

(a) high nuclear level density and broad overlapping resonances, (b) many open reaction channels, inelasticity and absorption. Use a complex (absorptive) optical model potential – from theory or simply fitted to elastic scattering data for the system and the energy of interest.

Distorted waves:

$$\chi_{\vec{k},\sigma}(\vec{r})$$





$$U(r) = V_C(r) + V(R) + iW(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

Optical potentials – the role of the imaginary part

$$k^{2} = \frac{2\mu}{\hbar^{2}} \underbrace{(E + V_{0})}_{-V_{0}} \qquad \underbrace{\frac{\bar{\psi}(x) = e^{i\bar{k}x}}{\bar{\psi}(x) = e^{i\bar{k}x}}}_{\bar{\psi}(x) = e^{i\bar{k}x}} E$$

$$-V_{0} \qquad \underbrace{-V_{0} - iW_{0}}_{\bar{\psi}(x) = e^{i\bar{k}x}}$$

$$\bar{k}^2 = \frac{2\mu}{\hbar^2} (E + V_0 + iW_0) = \frac{2\mu}{\hbar^2} (E + V_0) \left[1 + \frac{iW_0}{E + V_0} \right]$$

$$\bar{k} = k \left[1 + \frac{iW_0}{E + V_0} \right]^{1/2} \approx k \left[1 + \frac{iW_0}{2(E + V_0)} \right], \quad W_0 \ll E, V_0$$

So, for $W_0 > 0$, $\bar{k} = k + ik_i/2$, $k_i = kW_0/(E + V_0) > 0$,

$$\bar{\psi}(x) = e^{i\bar{k}x} = e^{ikx}e^{-\frac{1}{2}k_ix}, \quad |\bar{\psi}(x)|^2 = e^{-k_ix}$$

Optical potentials - parameter conventions

$$U(r) = V_C(r) + V(r) + iW(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

$$V(r) = -\frac{V_R}{[1 + \exp(X_R)]}, \qquad X_i = \frac{r - R_i}{a_i}$$

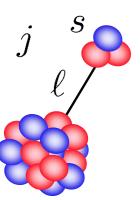
$$V_{so}(r) = -\frac{2V_{so}}{r a_{so}} \frac{\exp(X_{so})}{[1 + \exp(X_{so})]^2}$$
, FRESCO conventions

$$W(r) = -\frac{W_V}{[1 + \exp(X_V)]} - \frac{4W_S \exp(X_S)}{[1 + \exp(X_S)]^2} ,$$

$$R_i = r_i A_2^{1/3}$$
 or $R_i = r_i \left[A_1^{1/3} + A_2^{1/3} \right]$

The Schrodinger equation (1)

So, using usual notation



$$\int_{\ell} \int_{\ell} \int_{$$

and defining
$$\phi_{\ell j}^m(\vec{r}) = \sum_{\lambda \sigma} (\ell \lambda s \sigma | j m) \frac{u_{\ell j}(r)}{r} Y_\ell^\lambda(\hat{r}) \chi_s^\sigma$$

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2} [E_{cm} - U_{\ell j}(r)]\right) u_{\ell j}(r) = 0$$

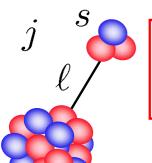
bound states $E_{cm} < 0$ scattering states $E_{cm} > 0$

With
$$U(r) = V_C(r) + V(r) + i \overline{W(r)} + V_{so}(r) \vec{\ell} \cdot \vec{s}$$

$$U_{\ell j}(r) = V_C(r) + V(r) + iW(r) + iW(r) + V_{so}(r)[j(j+1) - \ell(\ell+1) - s(s+1)]/2$$

The Schrodinger equation (2)

Must solve



$$\int_{\ell}^{s} \left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2} [E_{cm} - U_{\ell j}(r)] \right) u_{\ell j}(r) = 0$$

$$E_{cm} < 0 \quad \kappa_b$$

bound states
$$E_{cm} < 0$$
 $\kappa_b = \sqrt{\frac{2\mu |E_{cm}|}{\hbar^2}}$

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu}{\hbar^2} U_{\ell j}(r) - \kappa_b^2\right) u_{n\ell j}(r) = 0 \qquad \text{Discrete spectrum}$$

$$E_{cm} > 0$$

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

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu}{\hbar^2} U_{\ell j}(r) + k^2\right) u_{k\ell j}(r) = 0$$
 Continuous spectrum

Large r: The Asymptotic Normalisation Coefficient



$$E_{cm} < 0 \quad \kappa_b = \sqrt{\frac{2\mu |E_{cm}|}{\hbar^2}}$$

Bound states
$$E_{cm} < 0 \quad \kappa_b = \sqrt{\frac{2\mu|E_{cm}|}{\hbar^2}}$$

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu}{\hbar^2} U_{\ell j}(r) - \kappa_b^2\right) u_{n\ell j}(r) = 0$$

but beyond the range of the nuclear forces, then

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\eta_b \kappa_b}{r} - \kappa_b^2\right) u_{n\ell j}(r) = 0, \quad \eta_b = \frac{\mu Z_c Z_v e^2}{\hbar \kappa_b}$$

$$u_{n\ell j}(r) o C_{\ell j} W_{-\eta_b,\ell+1/2}(2\kappa_b r) \longrightarrow C_{\ell j} \exp(-\kappa_b r)$$
 Whittaker function $r \to \infty$

 $C_{\ell j}$ | ANC completely determines the wave function outside of the range of the nuclear potential - only requirement if a reaction probes only these radii

Large r: The phase shift and partial wave S-matrix

Scattering states

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

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu}{\hbar^2} U_{\ell j}(r) + k^2\right) u_{k\ell j}(r) = 0$$

and beyond the range of the nuclear forces, then

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\eta k}{r} + k^2\right) u_{k\ell j}(r) = 0, \quad \eta = \frac{\mu Z_c Z_v e^2}{\hbar k}$$

 $F_{\ell}(\eta, kr), \ G_{\ell}(\eta, kr)$ regular and irregular Coulomb functions

$$u_{k\ell j}(r) \rightarrow e^{i\delta_{\ell j}} \left[\cos \delta_{\ell j} F_{\ell}(\eta, kr) + \sin \delta_{\ell j} G_{\ell}(\eta, kr)\right]$$

$$\rightarrow (i/2) \left[H_{\ell}^{(-)}(\eta, kr) - S_{\ell j} H_{\ell}^{(+)}(\eta, kr)\right]$$

$$H_{\ell}^{(\pm)}(\eta,kr) = G_{\ell}(\eta,kr) \pm iF_{\ell}(\eta,kr)$$

Phase shift and partial wave S-matrix: Recall

$$u_{k\ell j}(r) \rightarrow e^{i\delta_{\ell j}} [\cos \delta_{\ell j} F_{\ell}(\eta, kr) + \sin \delta_{\ell j} G_{\ell}(\eta, kr)]$$

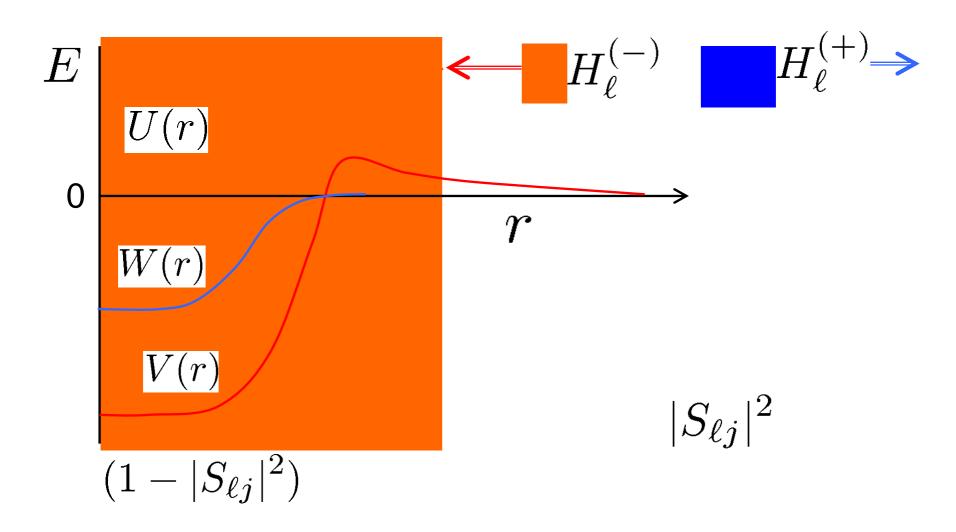
If U(r) is real, the phase shifts $\delta_{\ell j}$ are real, and [...] also

$$u_{k\ell j}(r)
ightarrow (i/2)[H_{\ell}^{(-)}(\eta,kr)-S_{\ell j}H_{\ell}^{(+)}(\eta,kr)]$$
 $S_{\ell j}=e^{2i\delta_{\ell j}}
ightarrow rac{\mathrm{Ingoing}}{\mathrm{waves}} rac{\mathrm{outgoing}}{\mathrm{waves}} \ |S_{\ell j}|^2 \qquad \mathrm{survival\ probability\ in\ the\ scattering} \ (1-|S_{\ell j}|^2) \ \mathrm{absorption\ probability\ in\ the\ scattering}$

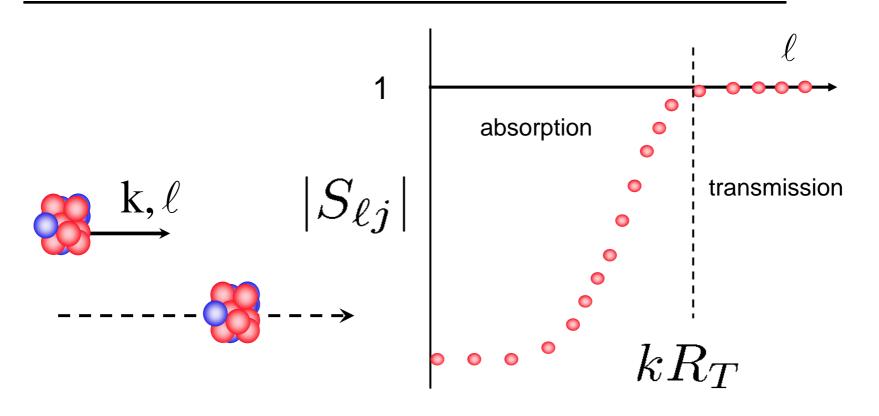
Having calculate the phase shifts and the partial wave S-matrix elements we can then compute all scattering observables for this energy and potential (but later).

Ingoing and outgoing waves amplitudes

$$u_{k\ell j}(r) \to (i/2)[H_{\ell}^{(-)} - H_{\ell}^{(+)}]$$



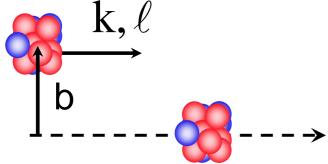
S-matrix with absorption



$$u_{k\ell j}(r) \to (i/2)[H_{\ell}^{(-)} - S_{\ell j}H_{\ell}^{(+)}]$$

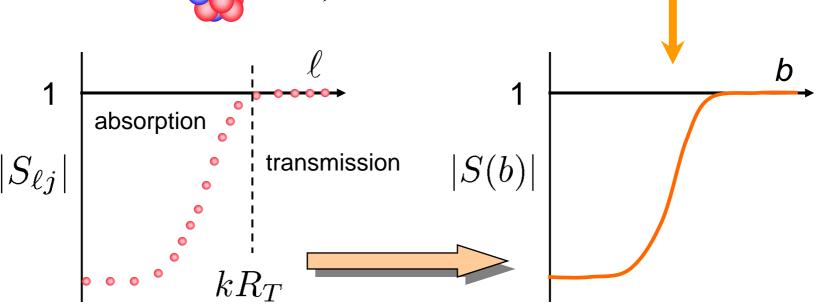
Semi-classical models for the S-matrix - S(b)

b=impact parameter



for high energy/or large mass, semi-classical ideas are good

 $kb \cong \ell$, actually $\Rightarrow \ell+1/2$



Point particle scattering – cross sections

All cross sections, etc. can be computed from the S-matrix, in either the partial wave or the semi-classical (impact parameter) representation, for example (spinless case):

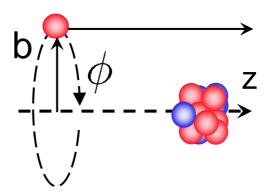
$$\sigma_{el} = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1)|1 - S_{\ell}|^2 \approx \int d^2\vec{b} |1 - S(b)|^2$$

$$\sigma_R = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1)(1 - |S_{\ell}|^2) \approx \int d^2\vec{b} (1 - |S(b)|^2)$$

$$\sigma_{tot} = \sigma_{el} + \sigma_R = 2 \int d^2 \vec{b} \left[1 - \text{Re.} S(b) \right]$$
 etc.

and where (cylindrical coordinates)

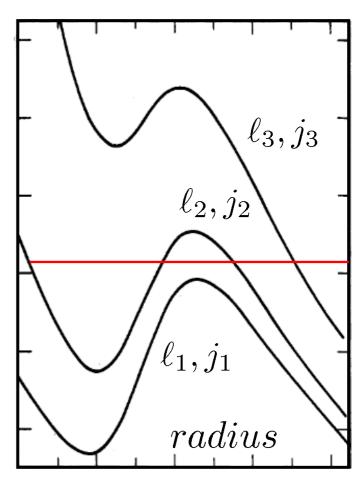
and where (cylindrical coordinates)
$$\int d^2\vec{b} \equiv \int_0^\infty bdb \int_0^{2\pi} d\phi = 2\pi \int_0^\infty bdb$$



Phase shifts and S-matrix: Resonant behaviour

In real potentials, at low energies, the combination of an attractive nuclear, repulsive Coulomb and/or centrifugal terms can lead to potential pockets and resonant behaviour – the system being able to trapped in the pocket for some (life)time τ .

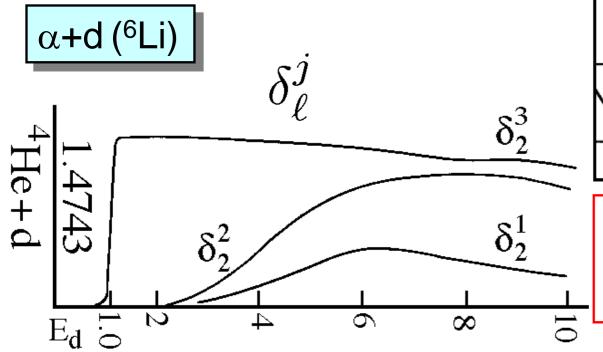
$$\frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + U_{\ell j}(r)$$

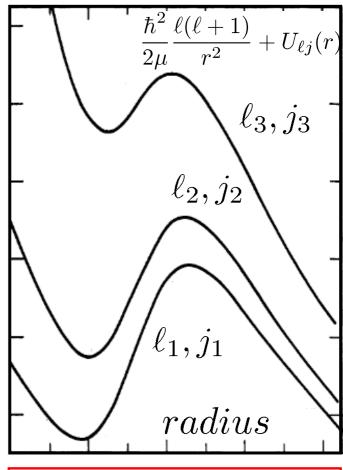


Phase shifts and S-matrix: Resonant behaviour

Potential pockets can lead to resonant behaviour – the system being able to trapped in the pocket for some (life)time τ .

Clearest signal is the rise of the phase shift through 90 degrees.





Potential parameters should describe any known resonances

Bound states potential parameters - nucleons

$$U(r) = V_C(r) + V(r) + V_{so}(r)\vec{\ell} \cdot \vec{s}$$

$$V(r) = -\frac{V_R}{[1 + \exp(X_R)]}, \qquad X_i = \frac{r - R_i}{a_i}$$

$$V_{so}(r) = -\frac{2 V_{so}}{r a_{so}} \frac{\exp(X_{so})}{[1 + \exp(X_{so})]^2} ,$$

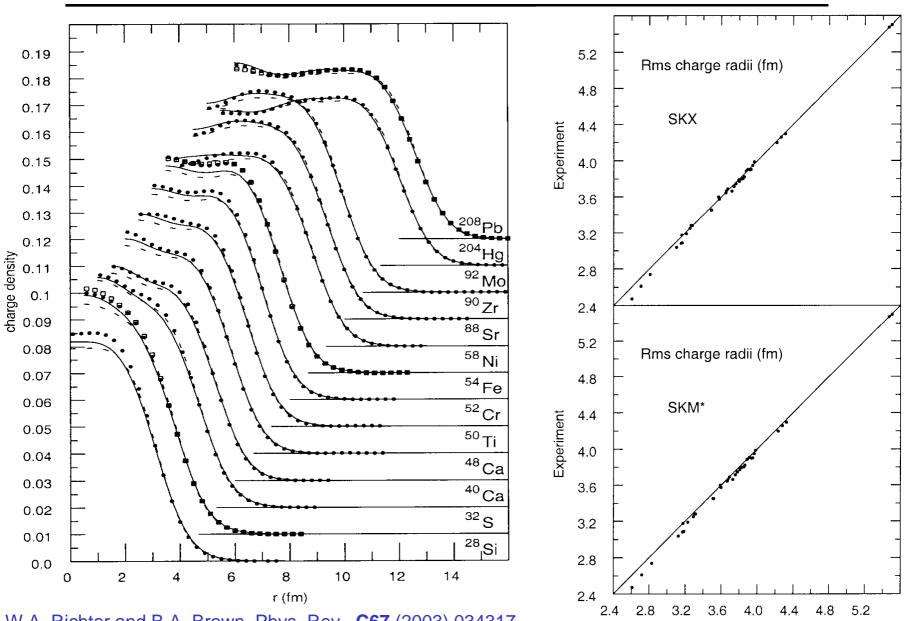
$$R_i = r_i A_2^{1/3}$$

$$r_R = r_C = r_{so} \approx 1.25 \text{fm}$$

$$a_R = a_{so} \approx 0.65 - 0.7 \text{fm}$$

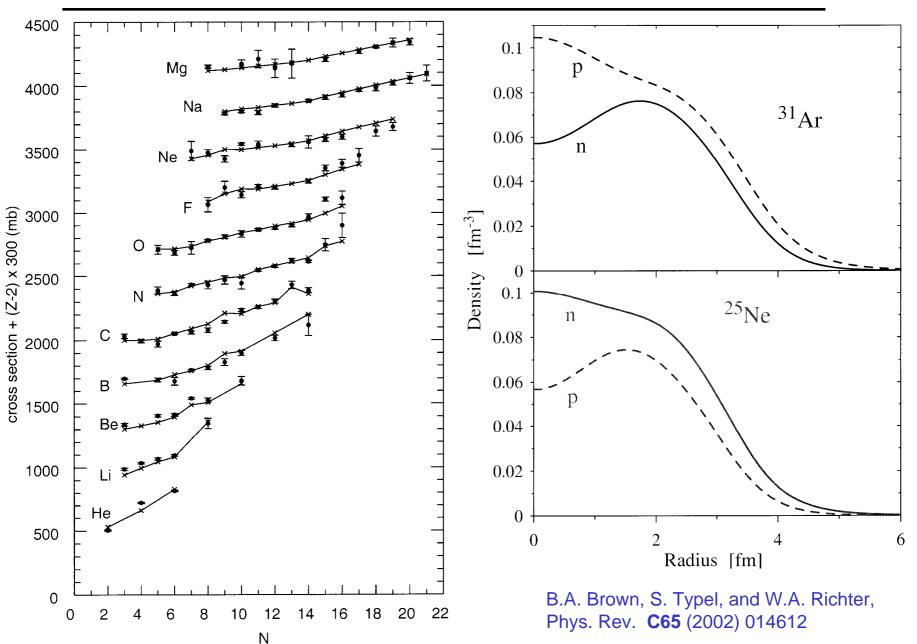
Theory

Sizes - Skyrme Hartree-Fock radii and densities



W.A. Richter and B.A. Brown, Phys. Rev. C67 (2003) 034317

Sizes - Skyrme Hartree-Fock radii and densities



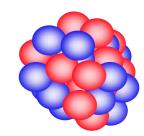
Bound states - use mean field information

```
INPUT VALUES
                 IA,IZ =
 ---- Neutron bound state results
 k n l
                  IE
                      OCC
 1 1 s 1/2 -26.757 1
                     2.00
                            36.70
                                   35.28
 2 1 p 3/2 -16.883 1
                     4.00
                            36.70
                                   35.80
 3 1 p 1/2 -12.396 1
                     2.00
                            36.70
                                   36.04
 4 1 d 5/2 -6.166 1
                     6.00
                            36.70
                                  36.37
 5 1 d 3/2 -0.109 1 0.00 36.70
                                  36.69
 6 2 s 1/2 -3.360 1 2.00
                            36.70
                                  36.52
 7 1 f 7/2 -0.200 3
                      0.00
                            46.02
                                  46.01
 8 1 f 5/2 -0.200 3
                      0.00
                            60.56
                                  60.55
 9 2 p 3/2
            -0.2003
                      0.00
                            48.10
                                   48.09
---- Neutron single-particle radii -----
```

But must make small correction as HF is a fixed centre calculation

$$\langle r^2 \rangle = \frac{A}{A-1} \langle r^2 \rangle_{HF}$$

```
rho(8.9) rho(9.9) rho(10.9)
            R(2)
                   R(4)
                          OCC
1 1 s 1/2 2.274
                                0.848E-09 0.706E-10 0.600E-11
                  2.575
                         2.000
2 1 p 3/2
                  3.133
         2.863
                         4.000
                                0.188E-07 0.244E-08 0.325E-09
3 1 p 1/2
          2.954
                  3.268
                         2.000
                                0.727E-07 0.122E-07 0.210E-08
4 1 d 5/2
           3.434
                         6.000
                                0.524E-06 0.129E-06 0.327E-07
                  3.757
5 1 d 3/2 4.662 6.063
                         0.000
                                0.131E-04 0.675E-05 0.371E-05
6 2 s 1/2
           4.172 4.895
                         2.000
                                0.769E-05 0.278E-05 0.102E-05
7 1 f 7/2
                         0.000
           3.865
                4.440
                                0.324E-05 0.134E-05 0.600E-06
8 1 f 5/2
         3.890
                 4.477
                         0.000
                                0.341E-05 0.141E-05 0.631E-06
9 2 p 3/2
           6.815
                8.635
                         0.000
                                0.451E-04 0.270E-04 0.167E-04
```



$$^{24}O(g.s.)$$

Bound states – for clusters – conventions (1)

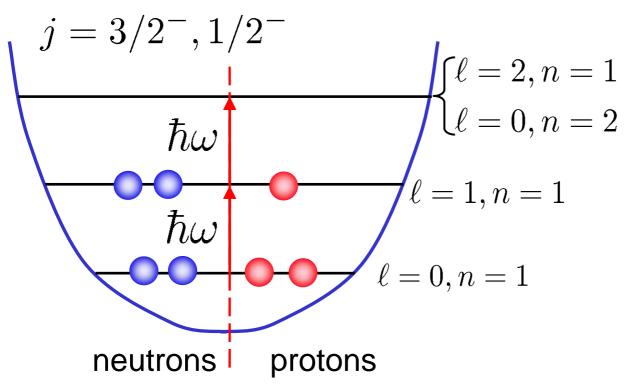
How many nodes for cluster states?

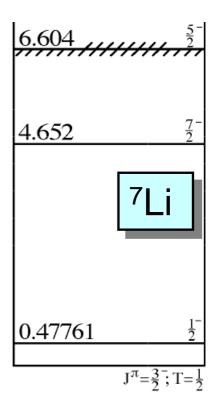
$$\phi^m_{n\ell j}(\vec{r})$$

Usually guided by what the 3D harmonic oscillator potential requires - so as not to violate the Pauli Principle.

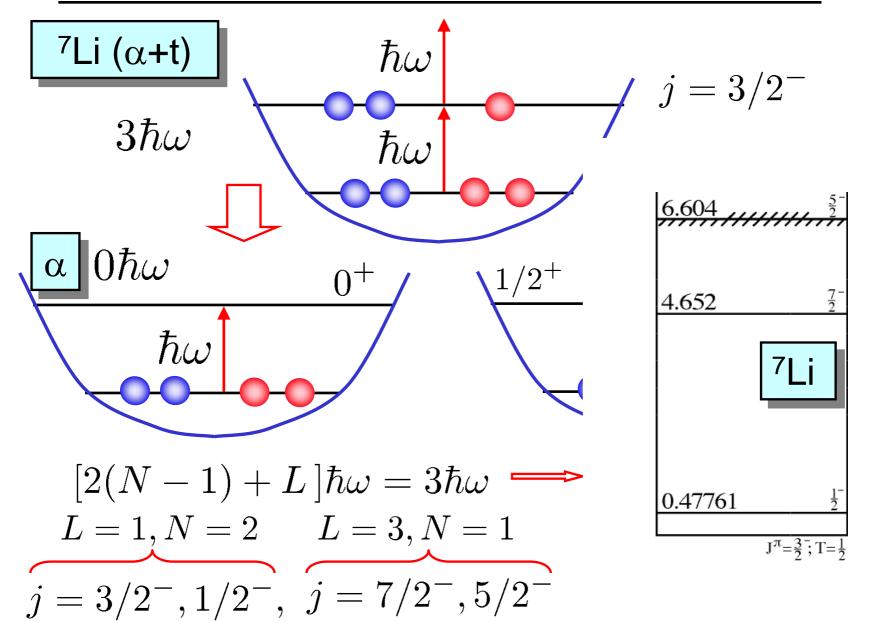
$$[2(n-1)+\ell]\hbar\omega$$

 $[2(n-1)+\ell]\hbar\omega\left\{ egin{array}{l} \mbox{Excitation of a} \\ \mbox{nucleon in this state} \end{array}
ight.$





Bound states - for clusters - conventions (2)



Bound states – spectroscopic factors

In a potential model it is natural to define <u>normalised</u> bound state wave functions. $A_{\mathbf{V}}(I^{\pi})$

$$\phi_{n\ell j}^{m}(\vec{r}) = \sum_{\lambda \sigma} (\ell \lambda s \sigma | jm) \frac{u_{n\ell j}(r)}{r} Y_{\ell}^{\lambda}(\hat{r}) \chi_{s}^{\sigma},$$

$$\int_{0}^{\infty} [u_{n\ell j}(r)]^{2} dr = 1$$

$$n\ell_{j}$$

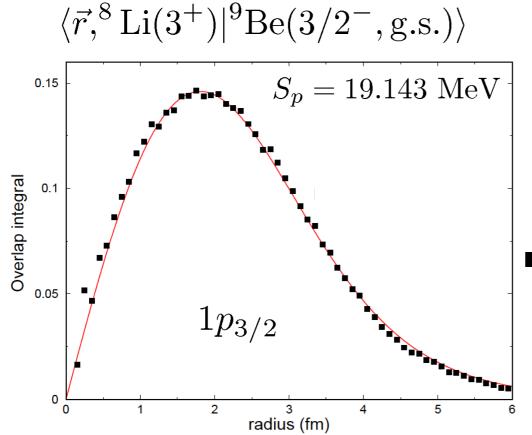
$$A-1 \chi(J_{f}^{\pi})$$

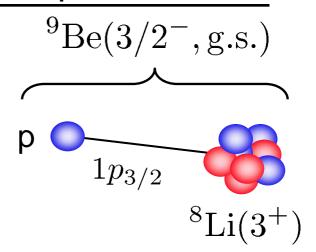
The potential model wave function approximates the <u>overlap function</u> of the A and A–1 body wave functions (A and A–n in the case of an n-body cluster) i.e. the overlap

$$\langle \ell j, \vec{r}, A^{A-1} X(J_f^{\pi}) | A Y(J_i^{\pi}) \rangle \to I_{\ell j}(r), \quad \int_0^{\infty} [I_{\ell j}(r)]^2 dr = S(J_i, J_f \ell j)$$

S(...) is the <u>spectroscopic factor</u> \leftarrow a structure calculation

Bound states – microscopic overlaps





■ Microscopic overlap from Argonne 9- and 8-body wave functions (Bob Wiringa et al.) Available for a few cases

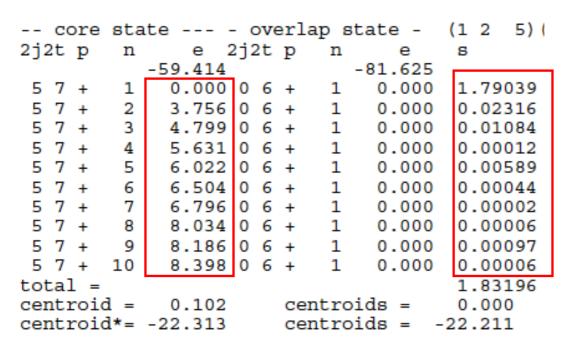
Normalised bound state in Woods-Saxon potential well x (0.23)^{1/2} Spectroscopic factor

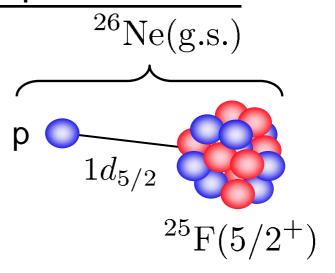
$$r_V = r_{so} = \text{fitted}, \ a_V = a_{so} = \text{fitted}, \ V_{so} = 6.0$$

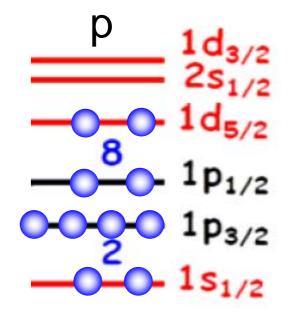
Bound states – shell model overlaps

$$\langle \vec{r},^{25} \text{Ne}(5/2^+, E^*)|^{26} \text{Ne}(0^+, \text{g.s.}) \rangle$$

USDA sd-shell model overlap from e.g. OXBASH (*Alex Brown et al.*). Provides spectroscopic factors but **not** the bound state radial wave function.



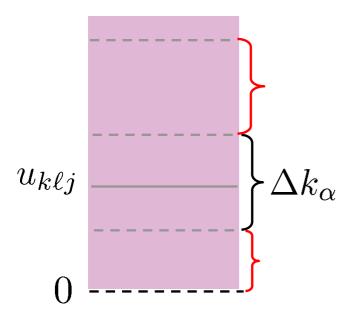




Neither bound nor scattering – continuum bins

Scattering states

$$u_{k\ell j}(r) \rightarrow e^{i\delta_{\ell j}} [\cos \delta_{\ell j} F_{\ell}(\eta, kr) + \sin \delta_{\ell j} G_{\ell}(\eta, kr)]$$



$$\int_0^\infty dr \, u_{k\ell j}(r) \, u_{k'\ell j}^*(r) = \frac{\pi}{2} \delta(k - k')$$

$$\begin{cases} \Delta k_{\alpha} & \hat{u}_{\alpha\ell j}(r) = \sqrt{\frac{2}{\pi N_{\alpha}}} \int_{\Delta k_{\alpha}} dk \, g(k) \, u_{k\ell j}(r) \\ N_{\alpha} = \int_{\Delta k_{\alpha}} dk \, [g(k)]^2 & \text{weight} \\ \text{function} \end{cases}$$

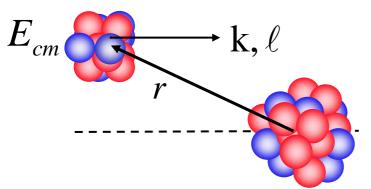
$$N_{lpha} = \int_{\Delta k_{lpha}} dk \, [g(k)]^2$$
 weight function

set

orthonormal set
$$\int_0^\infty\!\!dr\,\hat{u}_{\alpha\ell j}^*(r)\,\hat{u}_{\beta\ell j}(r)=\delta_{\alpha\beta}$$

$$g(k)=1 \qquad g(k)=\sin\delta_{\ell j}$$

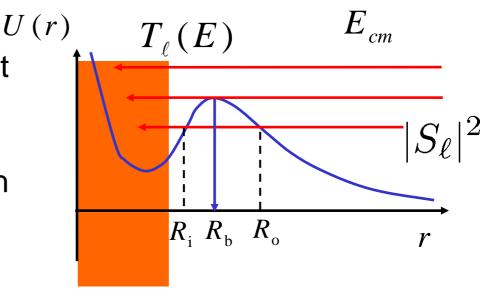
Barrier passing models of fusion



an imaginary part in *U(r)*, at short distances, can be included to absorb all flux that passes over or through the barrier – assumed to

result in fusion

Gives basis also for simple (barrier passing) models of nucleus-nucleus fusion reactions



$$\sigma(E) = \sum_{\ell=0}^{\infty} \sigma_{\ell}(E) = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1)(1 - |S_{\ell}|^2)$$

Code is available - to practice these ideas

bound (bound states solver - see bound.outline)

scatter (spin-independent scattering solver, range of ℓ or energy - see scatter.outline)

scat (single ℓ , j, scattering as a function of energy – see scat.outline)

 $scat_{one}$ (single ℓ , j, and single energy scattering)

bins (single ℓ , j, continuum bin state constructor — see bins.outline)

dens (Alex Brown Hartree Fock solver– for mean field wave functions and densities)