The R-matrix Method

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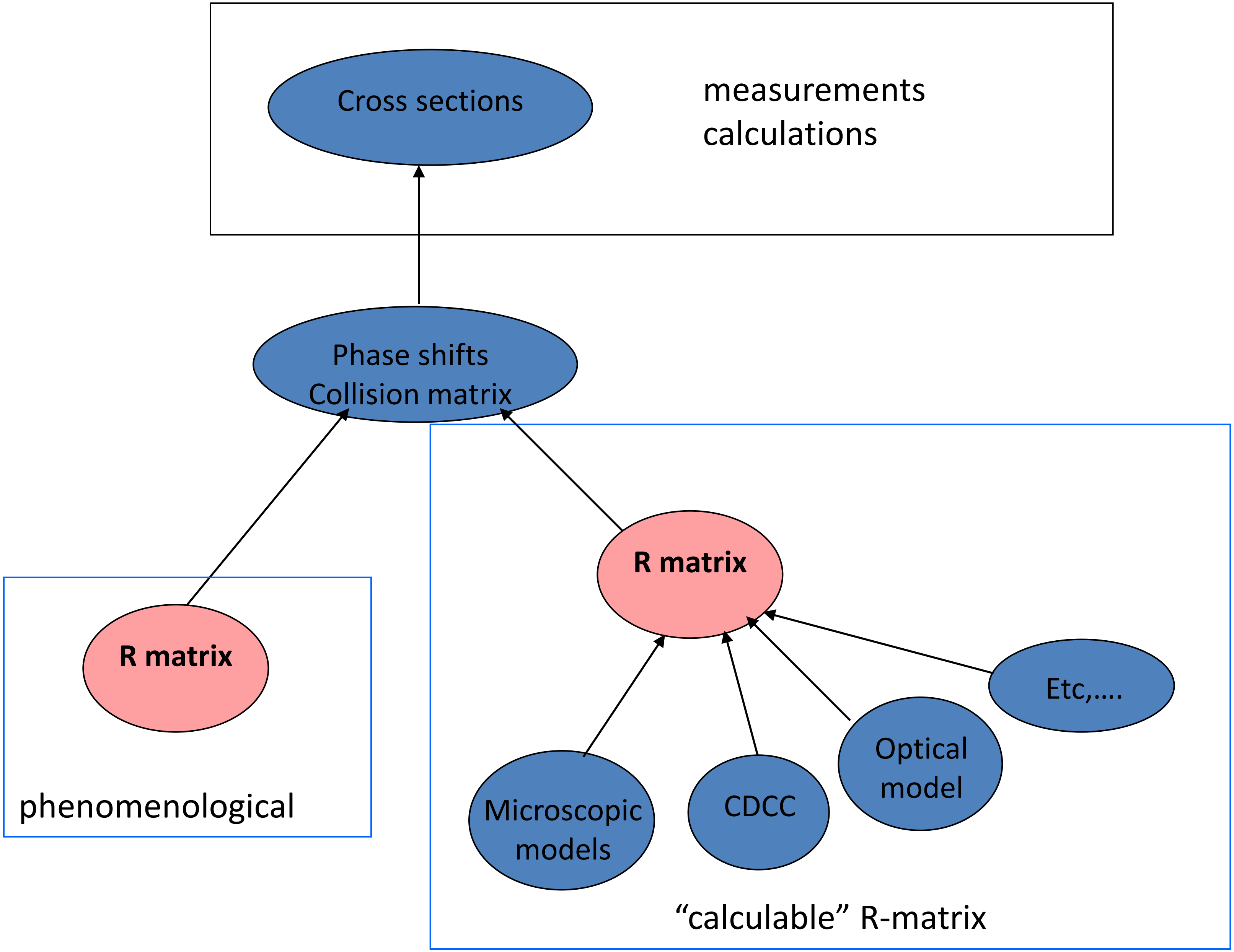
1. Introduction
2. Scattering theory (elastic scattering)
3. General R-matrix formalism
4. Applications of the « calculable » R matrix (theory)
   - Potential model
   - CDCC calculations

1. Introduction



1. Introduction

- Introduced by Wigner (Phys. Rev. 70 (1946) 606) to describe **resonance data**
- Main idea: dividing the space in 2 regions (radius a)
  - Internal region: nuclear, wave function defined on **a basis**
  - External region: Coulomb, wave function exact
- Many applications in atomic and nuclear physics (astrophysics)
- Not limited to resonances
- Main reference: A.M. Lane and R.G. Thomas, Rev. Mod. Phys. 30 (1958) 257
- More ''modern'' reference: P. D., D. Baye, Rep. Prog. Phys. 73 (2010) 036301

- Two directions (common origin!)
  - **Calculable R-matrix**: a tool to extend variational calculations to scattering problems
  - **Phenomenological R-matrix**: a parametrization of cross sections

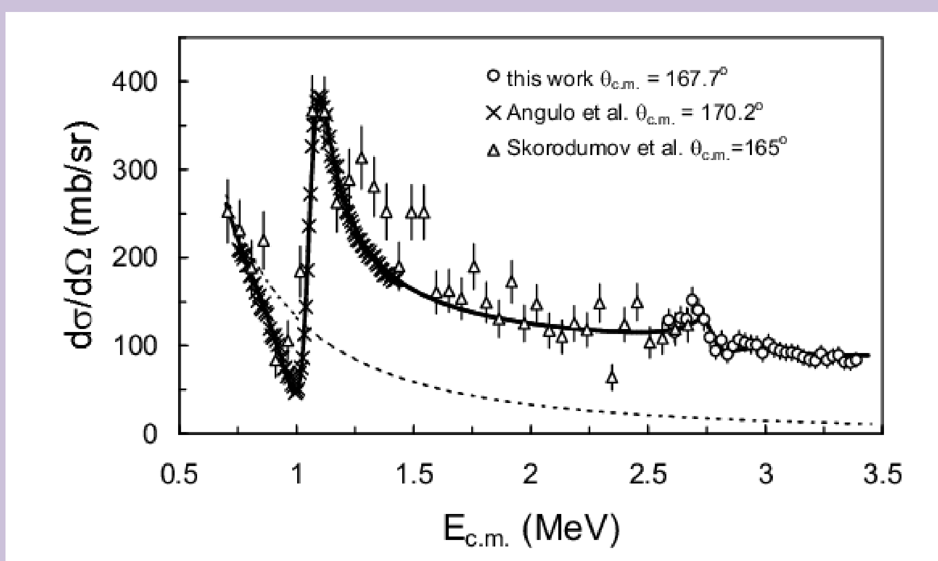
1. Introduction

Theory: solve the Schrödinger equation

$$H\psi(r) = E\psi(r) \quad \text{with } E > 0$$

Calculable

Experiment: analyze cross sections
extrapolate data (astrophysics)
deduce spectroscopy



Phenomenological

R-matrix

1. Introduction

Calculable R-matrix

- Goal: to solve a coupled-channel problem for positive energies

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}\right)u_c^{J\pi}(r)+\sum_{c'} V_{c,c'}^{J\pi}(r)u_{c'}^{J\pi}(r)=(\boldsymbol{E}-E_c)u_c^{J\pi}(r)$$

c= channel
$u_c^{J\pi}(r)$= wave function in channel *c*

- Equation common to many problems (only the potentials $V_{c,c'}^{J\pi}(r)$ are different)
- Negative energies $\boldsymbol{E}$ (bound states): variational methods
- Positive energies $\boldsymbol{E}$ (scattering states, resonances): more difficult

1. Introduction

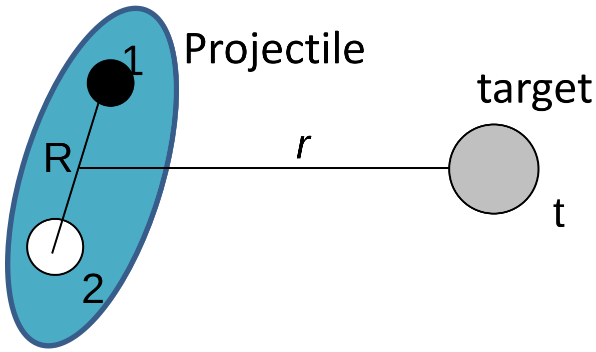
Examples in nuclear physics

- CDCC: Continuum Discretized Coupled Channel

$$\Psi^{JM\pi}(\boldsymbol{r},\boldsymbol{R}) = \sum_{jLn}\left[\Phi_n^j(\boldsymbol{R}) \otimes Y_L(\Omega_r)\right]^{JM} u_{jLn}^{J\pi}(r)$$

2-body wave functions

To be determined



Channel c= spin j, excitation level n, angular momentum L

- Microscopic cluster models: all nucleons are included in the wave function
- Three-body problems: continuum states important

➔ 1st step: Calculation of the coupling potentials
➔ 2nd step: Solving the coupled channel equation → **R-matrix**

Limitations

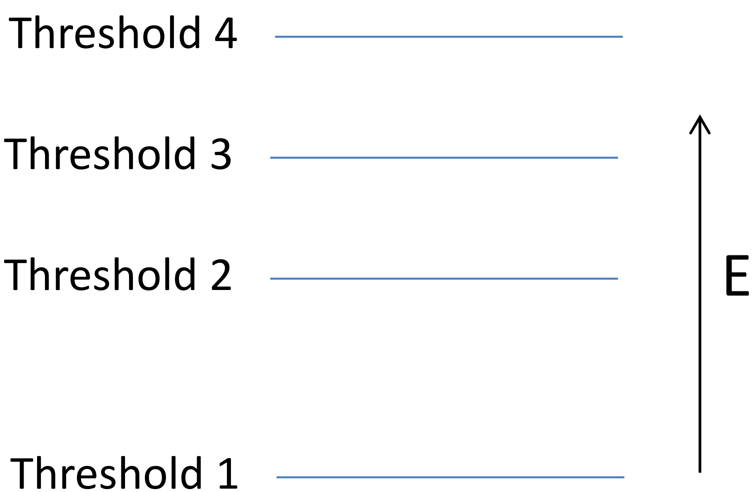
- long-range potentials (require many basis states)
- high energies (fast variations of the wave function)
- number of channels (sometimes several hundreds)

1. Introduction

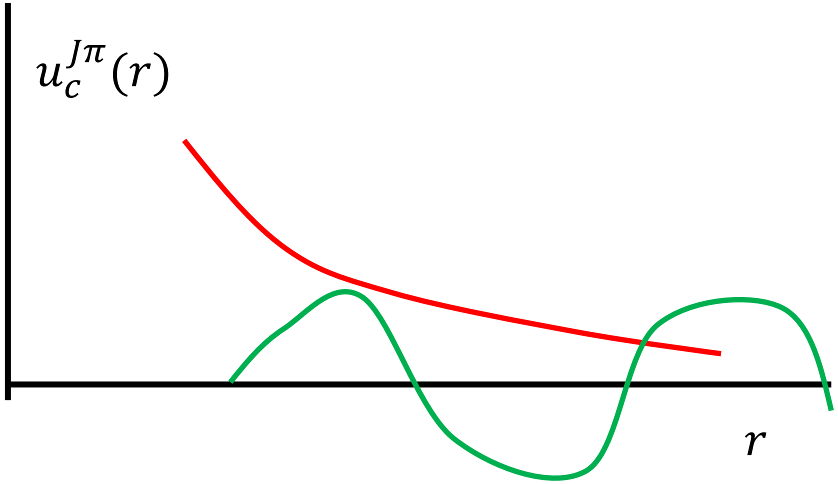
Alternative: discretization method (FRESCO)

R-matrix or discretization method?

- Still an open question…
- Should provide the same results → tests
- Obvious advantage of the R-matrix: treatment of closed channels



Channels 1,2,3: open
Channel 4: closed



Closed channels: $u_c^{J\pi}(r) \to 0$,

- Unstable in discretization methods
- Automatic in the R-matrix

1. Introduction

Phenomenological R-matrix

- Calculation of the R-matrix (one channel) $R(E) = \sum_\lambda \frac{\gamma_\lambda^2}{E_\lambda - E}$
- $\gamma_\lambda^2, E_\lambda$= parameters to be fitted (for each J value)
  → phase shifts
  → cross sections

Examples:

- resonance properties from elastic scattering (^{13}N+p, ^{11}C+p, etc..)
- Nuclear astrophysics: cross section extrapolation
  - ^{12}C(α,γ)^{16}O, ^{18}F(p,α)^{15}O, ^{8}Li(p,α)^{5}He
- beta decay to unbound states (^{8}B→ $\alpha+\alpha$, ^{12}N→ $\alpha+\alpha+\alpha$)

Limitations

- level density
- number of open channels
  → light nuclei
  → low energies (favour angular momenta L=0)

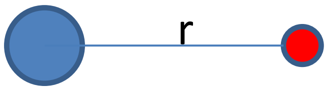
2. Scattering theory

2. Scattering theory

a. Goal: to solve the Schrödinger equation $H\Psi = E\Psi$ for E>0

b. Simplifying assumptions

- 2 structureless particles interacting by a potential V(r)



- elastic scattering only, 1 channel
- Spins 0

c. Wave function $\Psi^{\ell m}(\boldsymbol{r}) = \Psi^{\ell m}(r,\theta,\phi) = \frac{u_\ell(r)}{r} Y_\ell^m(\theta,\phi)$

$Y_\ell^m(\theta,\phi)$=spherical harmonics

$u_\ell(r)$=radial wave function (to be determined from the Schrödinger equation)

$$-\frac{\hbar^2}{2\mu} u_\ell''(r) + V(r)u_\ell(r) = E u_\ell(r)$$

with the potential V(r) defined as

$$V(r) = V_N(r) + \frac{Z_1 Z_2 e^2}{r} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}$$

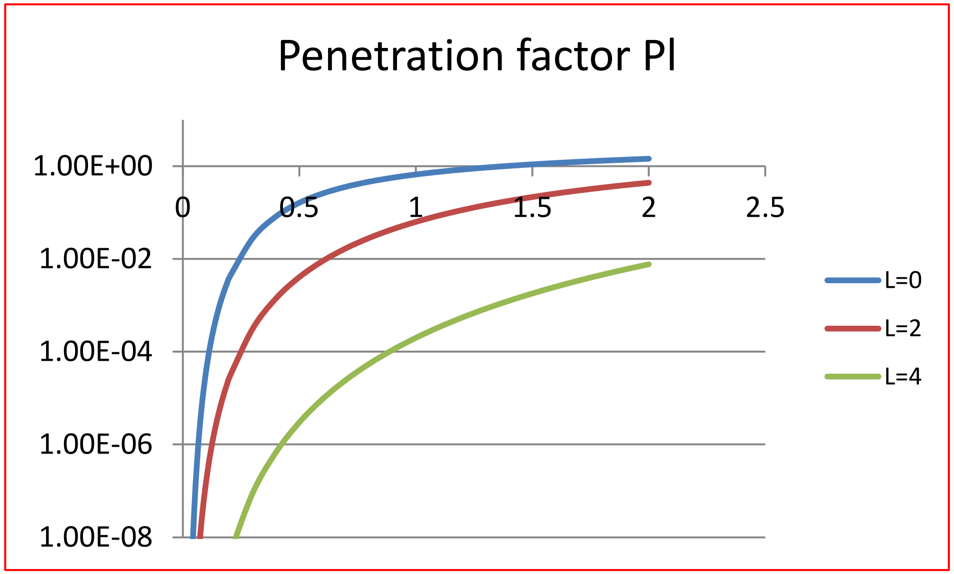
d. Large distances: $r \to \infty$ (V_N(r) is negligible)

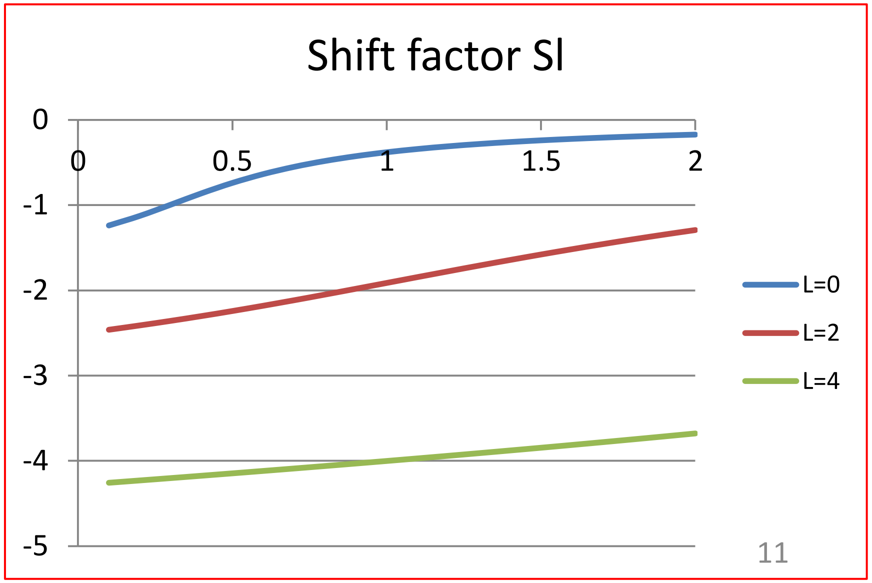
- Coulomb functions $F_\ell(kr,\eta), G_\ell(kr,\eta)$
- Incoming and outgoing functions: $I_\ell = G_\ell - iF_\ell \sim \exp(-ikr)$
  $O_\ell = G_\ell + iF_\ell = I_\ell^* \sim \exp(ikr)$
- Shift and penetration factors at radius a:

$$L_\ell = ka\frac{O'_\ell(ka)}{O_\ell(ka)} = S_\ell + iP_\ell$$

S_ℓ =shift factor (slowly depends on energy)
P_ℓ =penetration factor (fastly depends on energy)

Example: $\alpha + {}^3$He (a=5 fm, Coulomb barrier ~1 MeV)





e. Wave function $u_\ell(r)$ tends to a linear combination of Coulomb functions:

$$u_\ell(r) \to I_\ell(r) - U_\ell O_\ell(r)$$

with $\boldsymbol{U_\ell}$**=collision matrix**$=\exp(2i\delta_\ell)$ (also called « S matrix »)
$\boldsymbol{\delta_\ell}$**=phase shift** (real if the potential is real):
provides the information about the potential
must be calculated for each ℓ

f. Cross sections

- elastic only (single-channel)

- definition: $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$, with $f(\theta) = \frac{1}{k}\sum_\ell (1-\exp(2i\delta_\ell))\,(2\ell+1)P_\ell(\cos\theta)$
  converges very slowly (long range of the Coulomb interaction)
  → separation between nuclear and Coulomb : $\delta_\ell = \delta_\ell^N + \sigma_\ell$

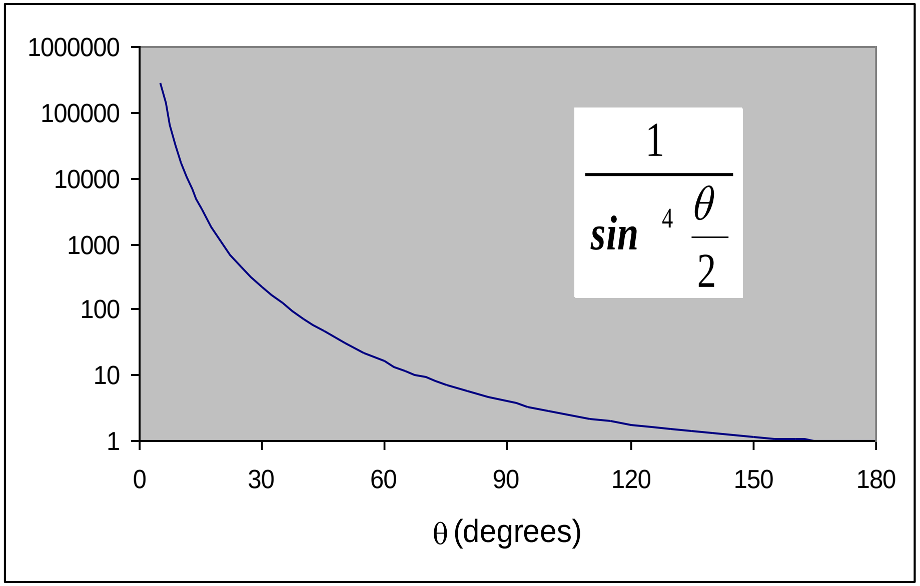
- $\frac{d\sigma}{d\Omega} = |f_C(\theta) + f_N(\theta)|^2$
  - with $f_C(\theta) = -\frac{\eta}{2k\sin^2(\theta/2)}\exp(-i\eta\log\sin^2(\theta/2))$
    =Coulomb amplitude: analytical definition
  - $f_N(\theta) = \frac{1}{k}\sum_\ell (1-\exp(2i\delta_\ell^N))\exp(2i\sigma_\ell)\,(2\ell+1)P_\ell(\cos\theta)$
    = nuclear amplitude, converges rapidly

2. Scattering theory

$$f(\theta) = f_C(\theta) + f_N(\theta)$$

- $f_C(\theta)$: Coulomb part: exact
- $f_N(\theta)$: nuclear part: converges rapidly

$$\frac{d\sigma_C}{d\Omega} = |f_C(\theta)|^2 \sim \frac{1}{E^2} \frac{1}{\sin^4 \frac{\theta}{2}}$$

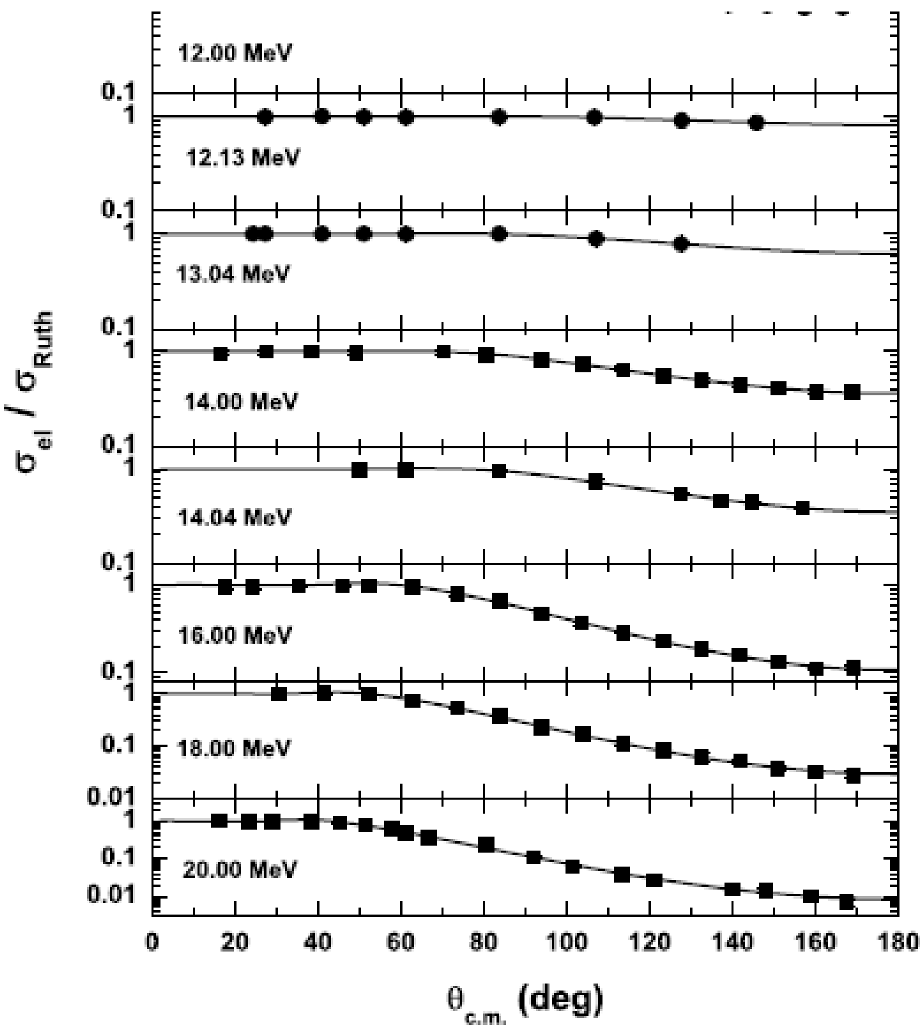


- $\frac{d\sigma_C}{d\Omega}$ =Rutherford cross section
- The total Coulomb cross section is not defined (diverges)
- Coulomb is dominant at small angles
  → used to normalize data
- Increases at low energies
- Minimum at θ=180° → nuclear effect maximum

2. Scattering theory

Cross section: $\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = |f^C(\theta) + f^N(\theta)|^2$

- Coulomb amplitude strongly depends on the angle → $\frac{d\sigma/_{d\Omega}}{d\sigma_C/_{d\Omega}}$



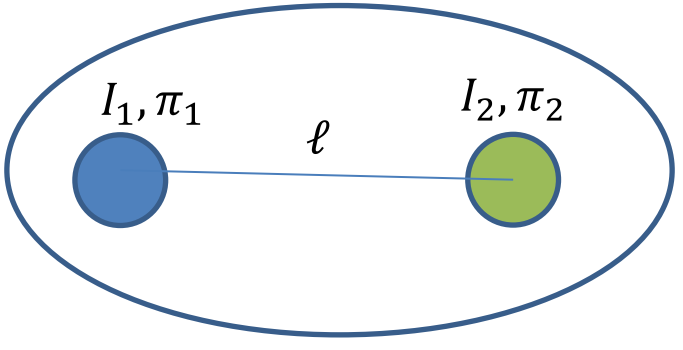
$^6Li + ^{58}Ni$ system

- $E_{cm} = \frac{58}{64} E_{lab}$
- Coulomb barrier
  $$E_B \sim \frac{3 * 28 * 1.44}{7} \sim 17 \text{ MeV}$$
- Below the barrier: $\sigma \sim \sigma_C$
- Above E_B : σ is different from σ_C

g. Extensions to Multichannel calculations:

- $U = \exp(2i\delta) \rightarrow$ matrix $U_{ij} = \eta_{ij}\exp(2i\delta_{ij})$ with $\eta_{ij} < 1$
- $f_N(\theta) \rightarrow f_{N,ij}(\theta)$
- $\frac{d\sigma}{d\Omega} \rightarrow \left(\frac{d\sigma}{d\Omega}\right)_{ij} = \left|f_{N,ij}(\theta)\right|^2$: no Coulomb interference if $i \neq j$!

- One channel: phase shift $\delta \rightarrow U=\exp(2i\delta)$
- Multichannel: *collision matrix* U_{ij}, (symmetric , unitary) with i,j=channels
- Good quantum numbers J=total spin π=total parity
- Channel *i* characterized by $I=I_1 \oplus I_2$ =channel spin
  $J=I \oplus \ell$ ℓ =angular momentum



Good quantum numbers : J, π

Angular-momentum couplings

$$|I_1 - I_2| \leq I \leq I_1 + I_2$$
$$|\ell - I| \leq J \leq \ell + I$$
$$\pi = \pi_1 * \pi_2 * (-1)^\ell$$

2. Scattering theory

Example of quantum numbers

α+^{3}He α=0^+, ^{3}He=$1/2^+$

J	*I*	ℓ	size
1/2+	1/2	0, ~~1~~	1
1/2-	1/2	~~0~~, 1	1
3/2+	1/2	~~1~~, 2	1
3/2-	1/2	1, ~~2~~	1

p+^{7}Be ^{7}Be=$3/2^-$, p=$1/2^+$

J	*I*	ℓ	size
0+	1 2	1 ~~2~~	1
0-	1 2	~~1~~ 2	1
1+	1 2	~~0~~, 1, ~~2~~ 1, ~~2~~, 3	3
1-	1 2	0, ~~1~~, 2 ~~1~~, 2, ~~3~~	3

Cross sections

One channel: $$\frac{d\sigma}{d\Omega}=|f(\theta)|^2, \text{ with } f(\theta)=\frac{1}{2ik}\sum_l (2l+1)(\exp(2i\delta_l)-1)P_l(\cos\theta)$$

Multichannel $$\frac{d\sigma}{d\Omega}=\sum_{K_1,K_2,K_1',K_2'} |f_{K_1K_2,K_1'K_2'}(\theta)|^2$$

With: K_1,K_2=spin orientations in the entrance channel

K'_1,K'_2=spin orientations in the exit channel

$$f_{K_1K_2,K_1'K_2'}(\theta)=\sum_{J,\pi}\sum_{lI,l'I'}\ldots U^{J\pi}_{lI,l'I'}\; Y_{l'}(\theta,0)$$

Collision matrix

- generalization of δ: $U_{ij}=\eta_{ij}\exp(2i\delta_{ij})$
- determines the cross section

3. The R-matrix method: general formalism

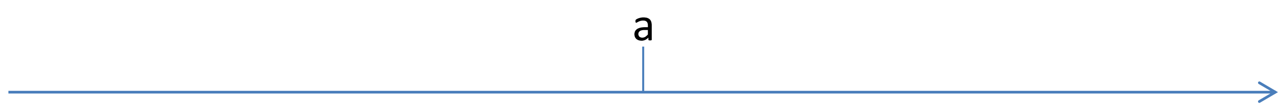
3. The R-matrix method: general formalism

a. Introduction – framework

- Presented for 2 structureless particles
  one channel

- N basis functions $\phi_i(r)$: variational calculations: $u(r) = \sum_{i=1}^{N} c_i \phi_i(r)$
  tend to zero at large distances
  valid at short distances only

- Definition of 2 regions: radius a (**channel radius**)



internal region: $r \leq a$

$$u_{int}(r) = \sum_{i=1}^{N} c_i \phi_i(r)$$

external region: $r \geq a$

$$u_{ext}(r) = I_\ell(r) - U_\ell O_\ell(r)$$

- Schrödinger equation + Matching at $r = a$
  ➔ collision matrix U (~phase shift) and coefficients c_i (wave function)
  !! Channel radius a is not a parameter!!

3. The R-matrix method: general formalism

b. **Procedure**

Step 1: Compute the matrix elements of the Hamiltonian over the internal region

$$H_{ij} =< \phi_i|\, H|\phi_j >_{int}= \int_0^a \phi_i(r)(T+V)\phi_j(r)dr$$

$$N_{ij} =< \phi_i|\phi_j >_{int}= \int_0^a \phi_i(r)\phi_j(r)dr$$

Problem: the kinetic energy is not hermitian over a finite interval [0,a]

$$\int_0^a \phi_i(r)\frac{d^2}{dr^2}\phi_j(r)dr \neq \int_0^a \phi_j(r)\frac{d^2}{dr^2}\phi_i(r)dr$$

→ Bloch operator

$$\mathcal{L}(L) = \frac{\hbar^2}{2\mu a}\delta(r-a)\left(\frac{d}{dr}-\frac{L}{r}\right)r$$

L=arbitrary constant ($L=0$ in most cases)

3. The R-matrix method: general formalism

role of the surface operator $\mathcal{L}(L) = \frac{\hbar^2}{2\mu a}\delta(r-a)\left(\frac{d}{dr} - \frac{L}{r}\right)r$

1. makes $\mathrm{T} + \mathcal{L}(L)$ hermitian

$$< \phi_i | \, T + \mathcal{L}(L) | \phi_j >_{int} = < \phi_j | \, T + \mathcal{L}(L) | \phi_i >_{int}$$

2. The Schrödinger equation

$$(H - E)u_\ell = 0$$

is replaced by the Bloch-Schrödinger equation

$$(H - E + \mathcal{L}(L))u_{int} = \mathcal{L}(L)u_{int} = \mathcal{L}(L)u_{ext}$$

Equivalent to 2 equations: $(H - E)u_{int}$**=0**

$$u'_{int}(a) = u'_{ext}(a)$$

→the Bloch operator ensures $u'_{int}(a) = u'_{ext}(a)$ (for the exact solution)

« Old » use of the R-matrix theory

- No Bloch operator
- Basis states such that $\phi_i{}'(a) = 0$
  - →Hermiticity OK
  - →but the total wave function has always a derivative =0

3. The R-matrix method: general formalism

Determination of the scattering matrix

- We use
$$(H-E+\mathcal{L}(L))u_\ell = \mathcal{L}(L)u_\ell \quad (1)$$
$$u_{int}(r) = \sum_{i=1}^{N} c_i\phi_i(r) \quad (2)$$
$$u_{ext}(r) = A(I_\ell(kr) - U_\ell O_\ell(kr)) \quad (3)$$
$$u_{int}(a) = u_{ext}(a) \quad (4)$$

With (1),(2),(3) →$\sum_{i=1}^{N} c_i < \phi_j\,|H-E+\mathcal{L}(L)|\phi_i >_{int} = < \phi_j\,(r)|\mathcal{L}(L)|u_{ext} >$

matrix D_{ij} → after inversion, provides coefficients c_i

with (4) →$\sum_{i=1}^{N} c_i\phi_i(a) = A(I_\ell(ka) - U_\ell O_\ell(ka))$
From these 2 equations, one gets the collision matrix (=scattering matrix)

$$U(E) = \frac{I(ka)}{O(ka)}\frac{1-L^*R(E)}{1-LR(E)}$$

with $R(E) = \frac{\hbar^2 a}{2\mu}\sum_{ij}\phi_i(a)\,(D^{-1})_{ij}\phi_j(a)$ (R-matrix:1x1 for single-channel calculations)

$L = ka\frac{O'(ka)}{O(ka)} = S(E) + iP(E)$ (L is complex)

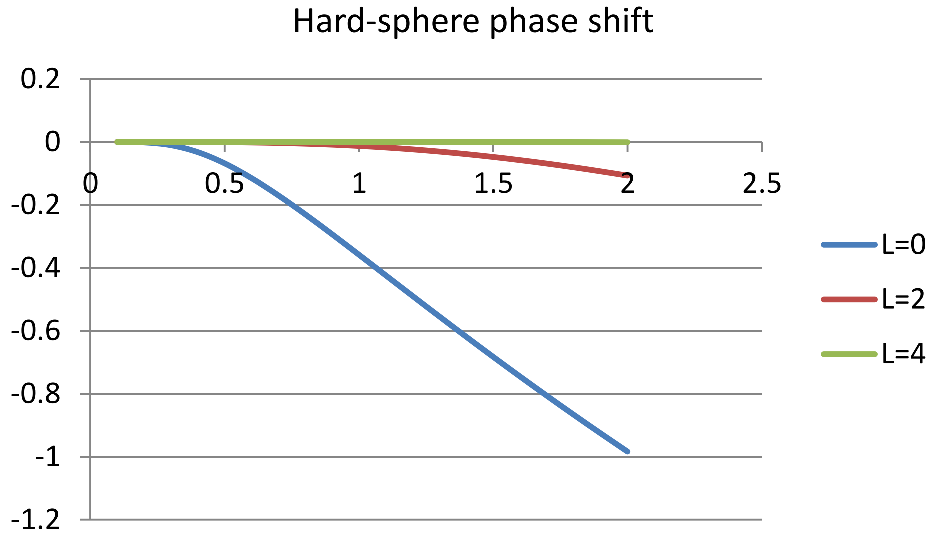
3. The R-matrix method: general formalism

Factorization of U

$$U(E) = \frac{I(ka)}{O(ka)} \frac{1-L^*R(E)}{1-LR(E)} = \exp(2i\delta) = \exp(2i\delta_{HS}) \exp(2i\delta_R)$$

- Hard-sphere phase shift: $\exp(2i\delta_{HS}) = \frac{I(ka)}{O(ka)} \rightarrow \delta_{HS} = -\operatorname{atan}\frac{F(ka)}{G(ka)}$
- R-matrix phase shift: $\exp(2i\delta_R) = \frac{1-L^*R(E)}{1-LR(E)} = \frac{1-SR+iPR}{1-SR-iPR} \rightarrow \delta_R = \operatorname{atan}\frac{PR}{1-SR}$
- δ_{HS} and δ_R depend on a but **the sum should not depend on a**

- Real potentials : R and δ are real and $|U(E)| = 1$
- Complex potentials: R and δ are complex and $|U(E)| < 1$ (sign of imaginary part)



3. The R-matrix method: general formalism

•Coulomb functions $F_\ell(kr,\eta), G_\ell(kr,\eta)$

•Incoming and outgoing functions:

$$I_\ell = G_\ell - iF_\ell \sim \exp(-ikr)$$
$$O_\ell = G_\ell + iF_\ell = I_\ell^* \sim \exp(ikr)$$

•Shift and penetration factors at radius a:

$$L_\ell = ka\frac{O'_\ell(ka)}{O_\ell(ka)} = S_\ell + iP_\ell$$

S_ℓ =shift factor (slowly depends on energy)

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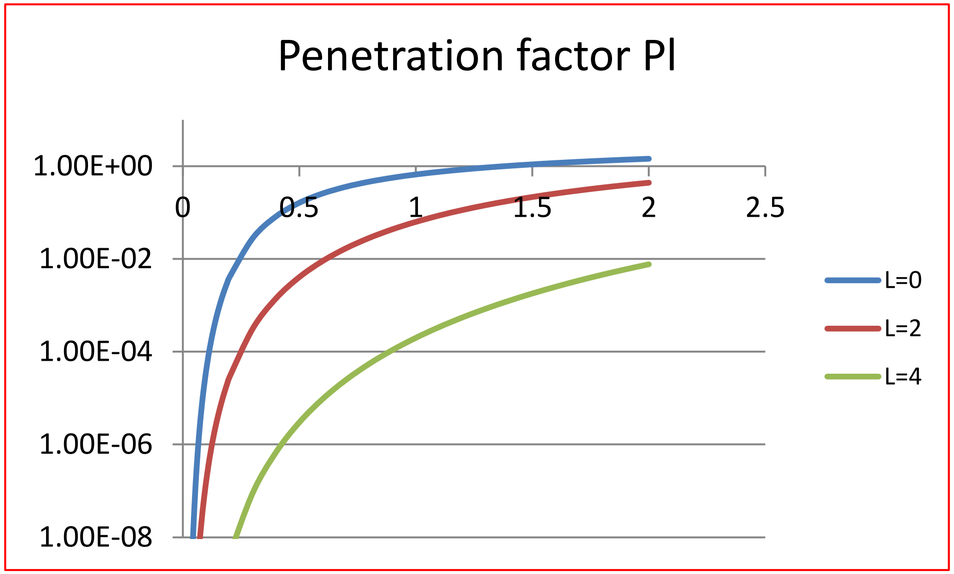
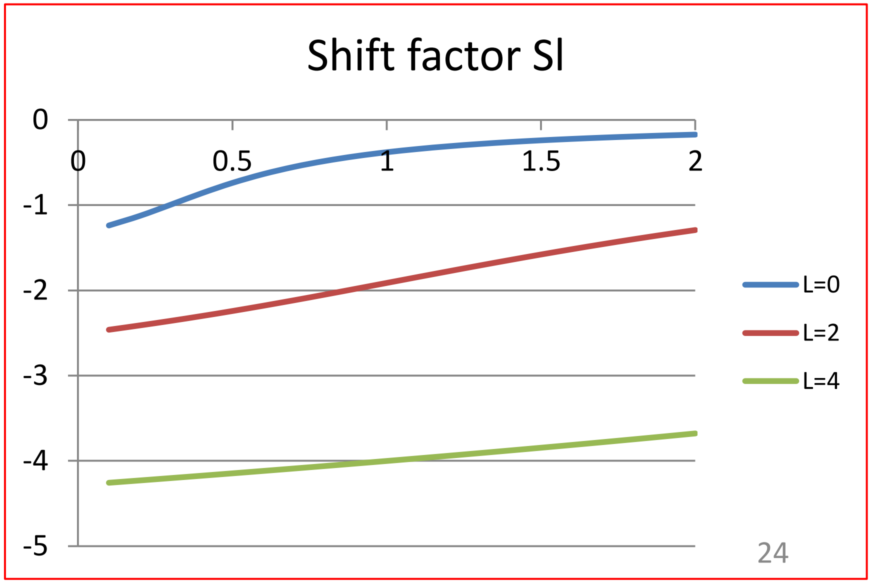
Example: α+^{3}He (a=5 fm, Coulomb barrier ~1 MeV)





4. Applications of the calculable R-matrix

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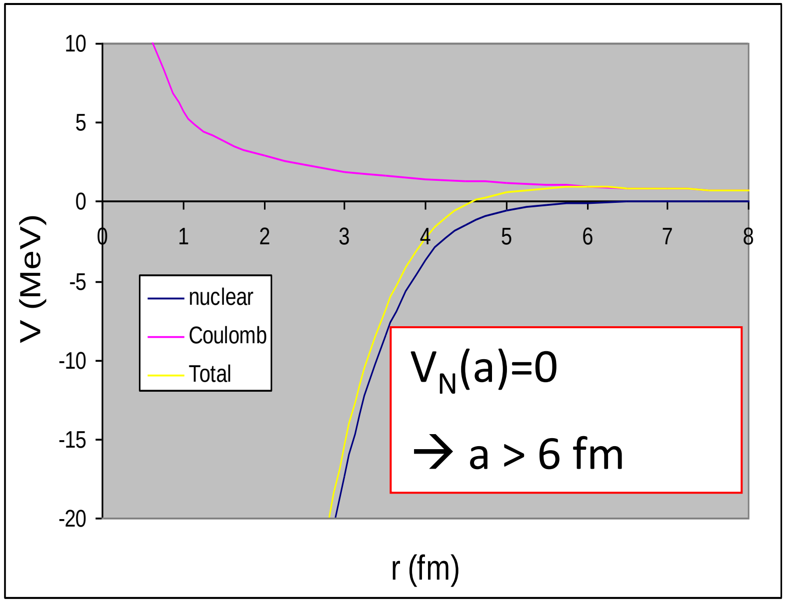
Application to the potential model

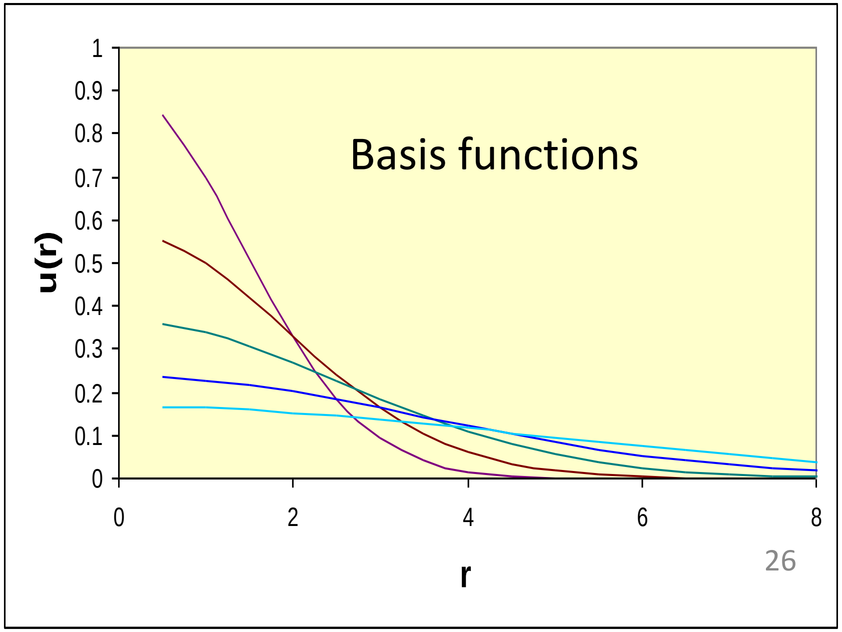
- Solutions of $-\frac{\hbar^2}{2\mu}u_\ell'' + \left(V_N(r) + \frac{Z_1Z_2e^2}{r} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}\right)u_\ell = Eu_\ell$
- Simple integrals for R-matrix calculations
- Exact solution available

$\alpha+\alpha$ phase shifts:

•Nuclear potential : $V_N(r) = -126\exp(-(r/2.13)2)$ (Buck et al., Nucl. Phys. A275 (1977) 246)

•Basis functions: $\phi_i(r) = r^l * \exp(-(r/a_i)^2)$
with $a_i=x_0*a_0^{(i-1)}$ (geometric progression)
typically x_0=0.6 fm, a_0=1.4

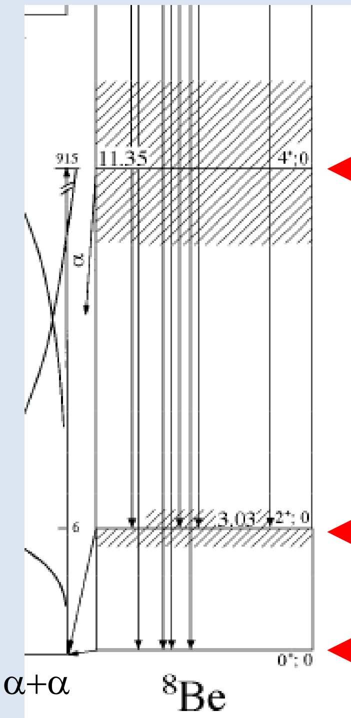




4. Applications of the calculable R-matrix

Example: $\alpha+\alpha$

Experimental spectrum of ^{8}Be

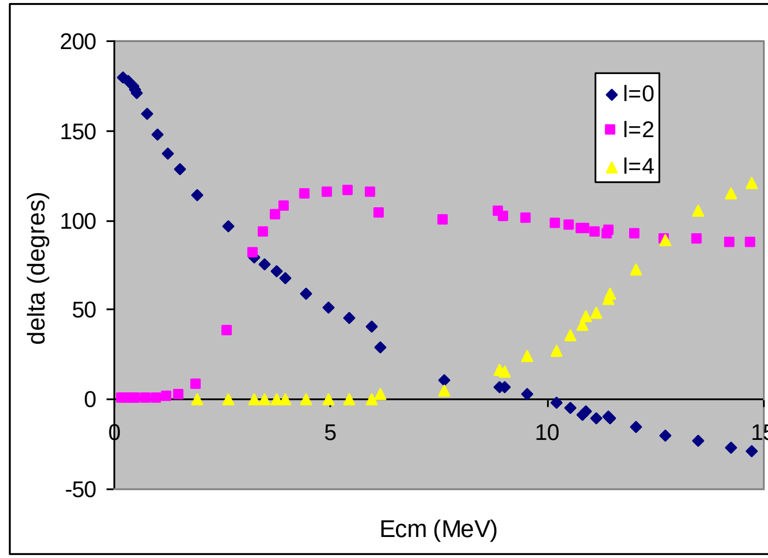


4^+
E~11 MeV
Γ~3.5 MeV

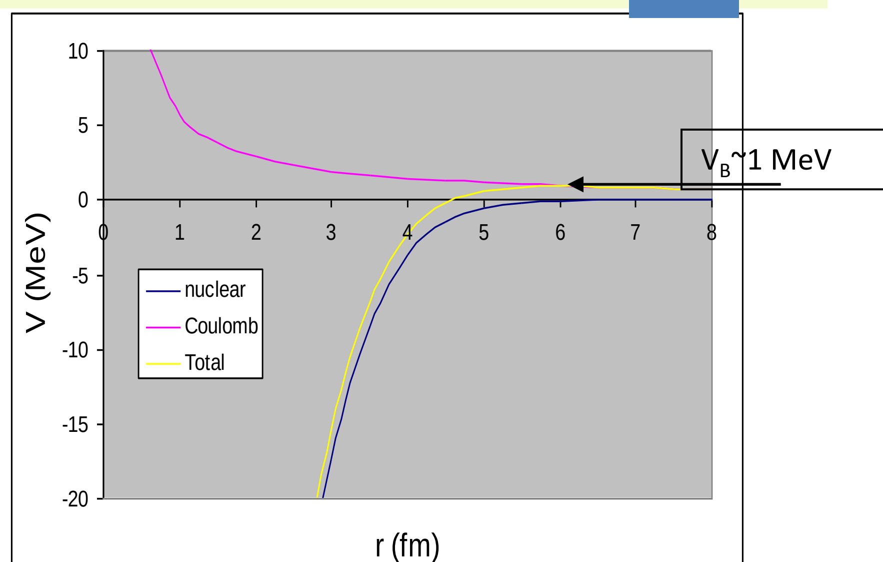
2^+
E~3 MeV
Γ~1.5 MeV

0^+
E=0.09 MeV
Γ=6 eV

Experimental phase shifts



Potential: $V_N(r)=-122.3*\exp(-(r/2.13)^2)$



4. Applications of the calculable R-matrix

Input data

- Potential
- Set of *N* basis functions (here gaussians with different widths)
- Channel radius *a*

Requirements

- *a* large enough : $V_N(a)$~0
- *N* large enough (to reproduce the internal wave functions)
- *N* as small as possible (computer time)

  → compromise

4. Applications of the calculable R-matrix

Procedure: Must be repeated for each ℓ

1) Compute matrix elements of the potential (simple numerical integrals)
2) $D_{ij} =< \phi_i|H - E + \mathcal{L}(L)|\phi_j >_{int}= \int_0^a \phi_i(r)(T + \mathcal{L}(L) + V - E)\phi_j(r)r^2dr$
3) Compute the R matrix

$$R(E) = \frac{\hbar^2 a}{2\mu}\sum_{ij} \phi_i(a)\,(D^{-1})_{ij}\phi_j(a)$$

4) Compute the collision matrix U

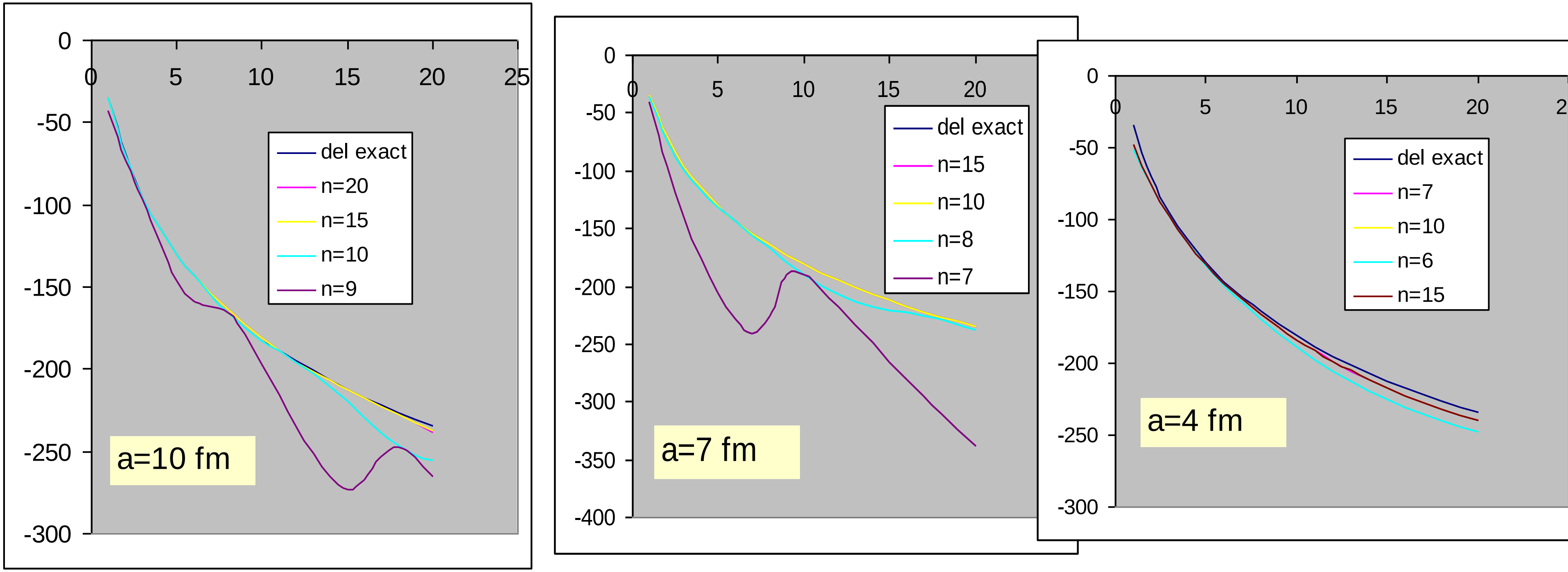
$$U(E) = \frac{I(ka)}{O(ka)}\frac{1 - L^* R(E)}{1 - LR(E)}$$

Tests

- Stability of the phase shift with the channel radius *a*
- Continuity of the derivative of the wave function

4. Applications of the calculable R-matrix

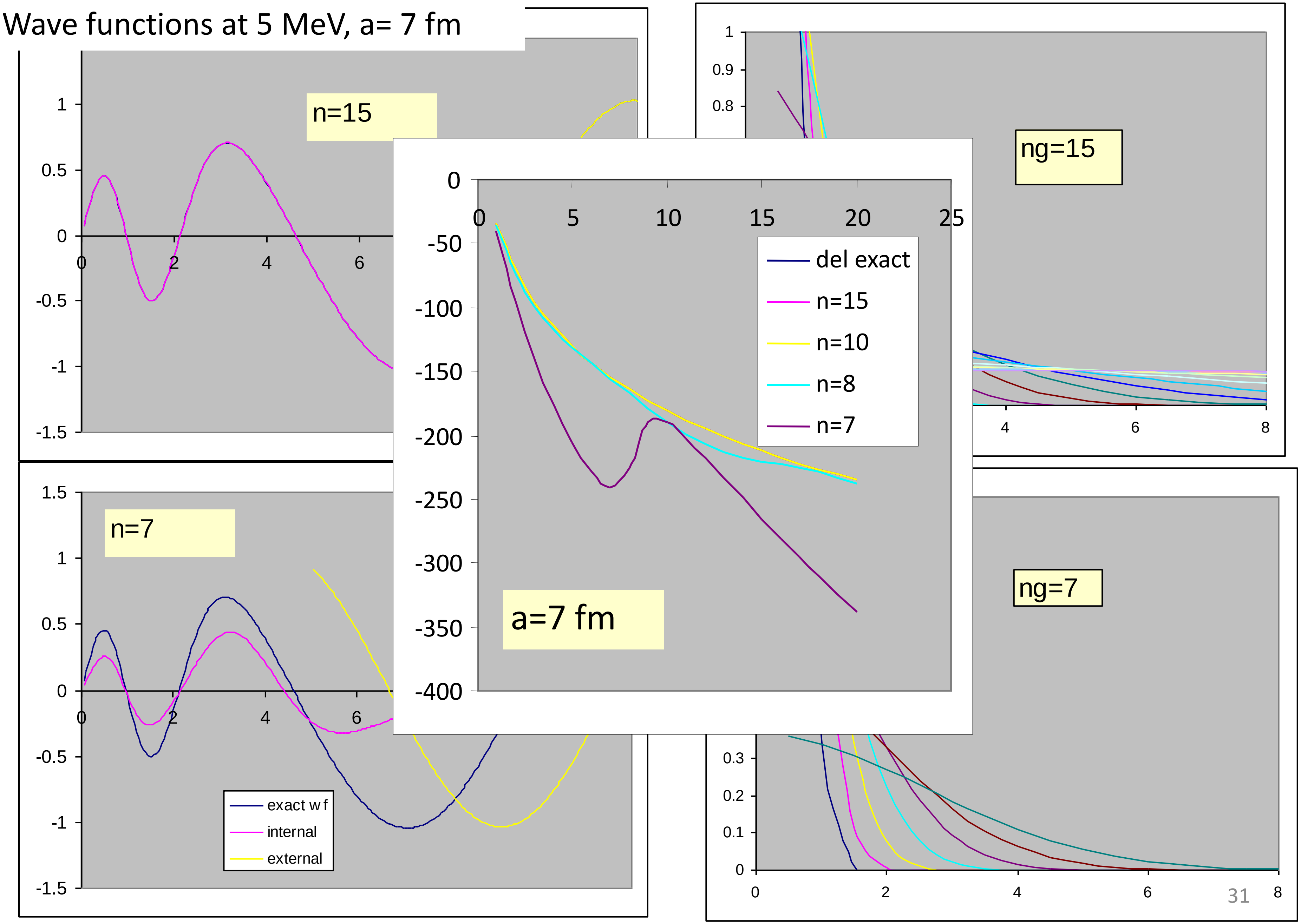
α+α Elastic phase shifts $\ell = 0$



- a=10 fm too large (needs too many basis functions)
- a=4 fm too small (nuclear not negligible)
- a=7 fm is a good compromise

4. Applications of the calculable R-matrix

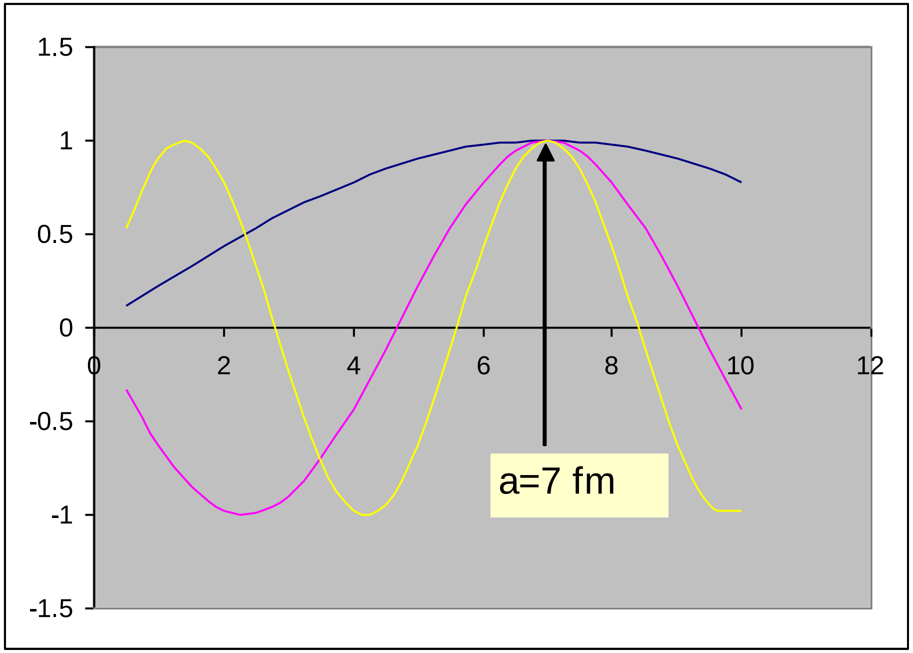
Wave functions at 5 MeV, a= 7 fm

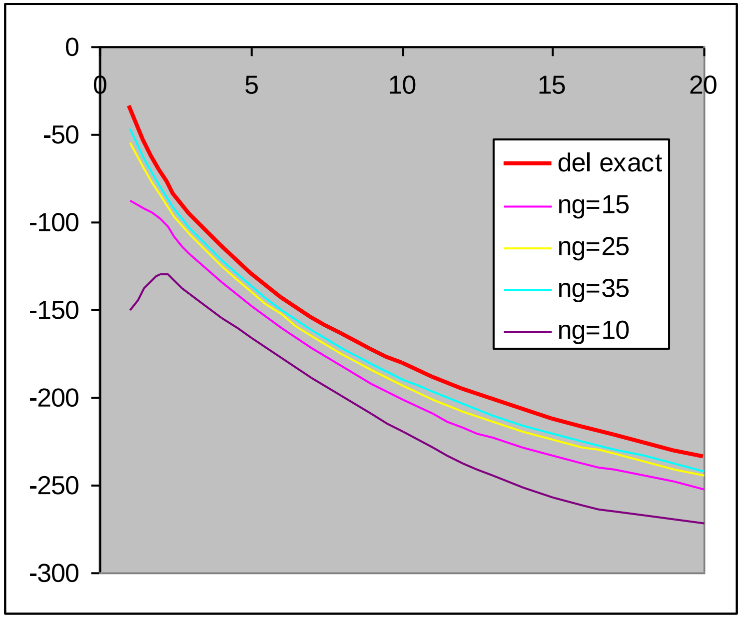


4. Applications of the calculable R-matrix

Other example : sine functions $u_i^\ell(r) = \sin\frac{\pi r}{a}(i-\frac{1}{2})$

- Matrix elements very simple
- Derivative $u_i'(a) = 0$





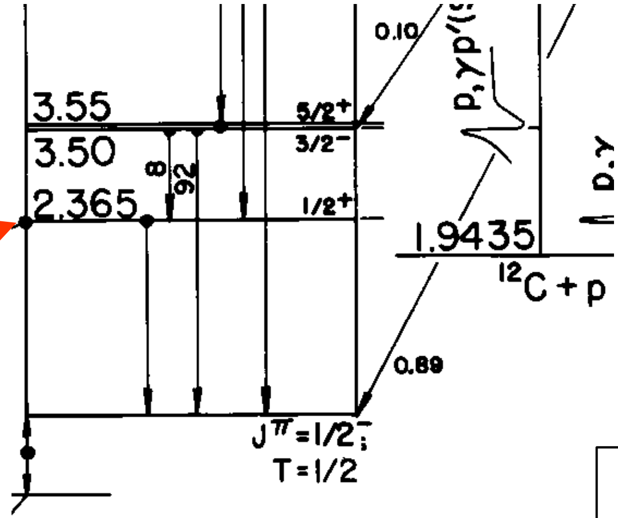
➔ Not a good basis (no flexibility)

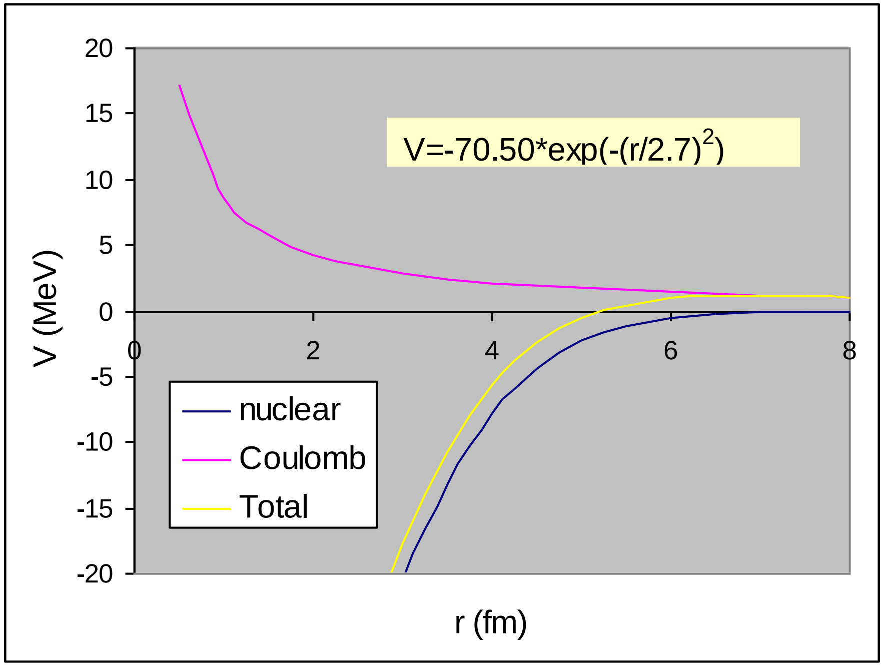
In ref. P. D., D. Baye, Rep. Prog. Phys. 73 (2010) 036301:
Lagrange meshes (simple matrix elements)

4. Applications of the calculable R-matrix

Example of resonant reaction: $^{12}C+p$

Resonance
ℓ=0
E=0.42 MeV
Γ=32 keV

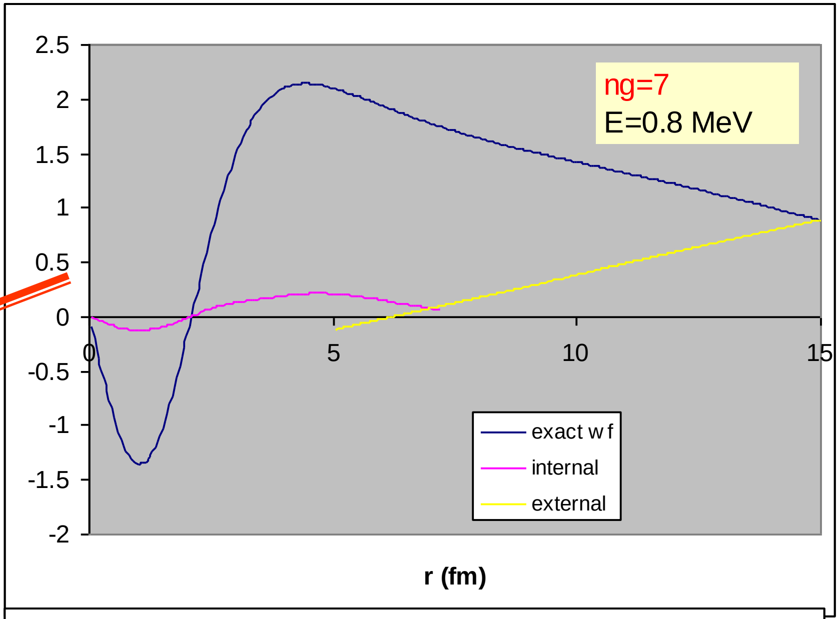




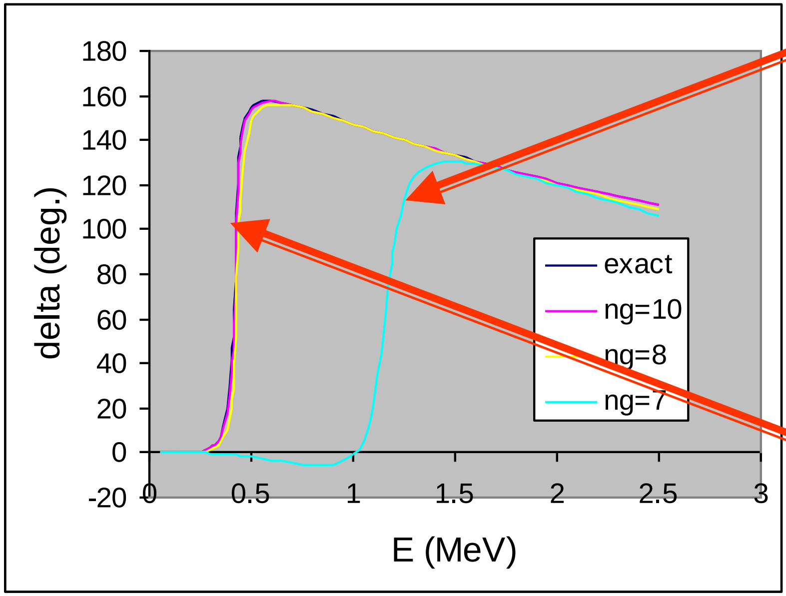
- potential : V=-70.5*exp(-(r/2.70)^2)
- Basis functions: $\phi_i(r) = r^{\ell}\exp(-(r/a_i)^2)$

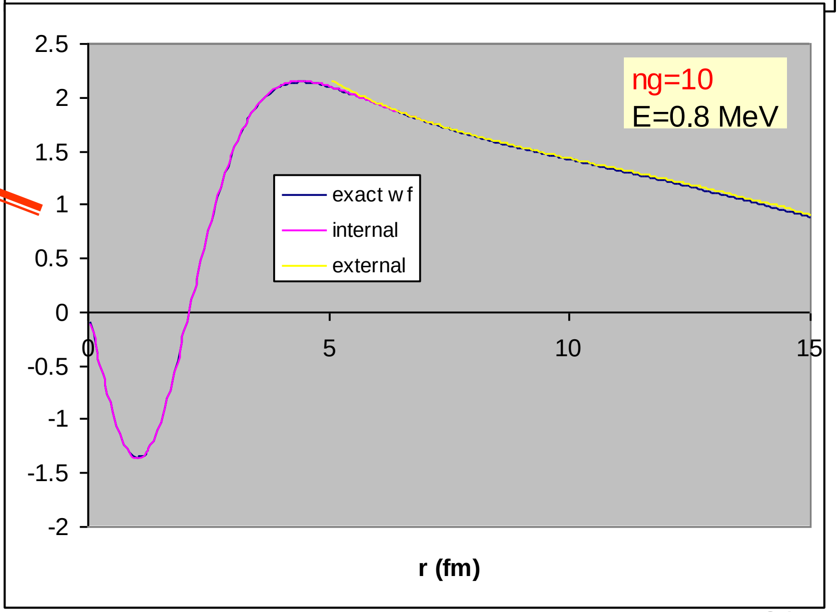
4. Applications of the calculable R-matrix

Wave functions



Phase shifts a=7 fm





4. Applications of the calculable R-matrix

Application of the R-matrix to bound states

Positive energies: $\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - 2\frac{\eta k}{r} + k^2\right) u_\ell = 0$ Coulomb functions $F_\ell(kr), G_\ell(kr)$

Negative energies: $\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - 2\frac{\eta k}{r} - k^2\right) u_\ell = 0$ Whittaker functions $W_{-\eta,\ell+1/2}(2kr)$

Asymptotic behaviour:

$$F_\ell(x) \to \sin(x - \ell\frac{\pi}{2} - \eta \log 2x)$$

$$G_\ell(x) \to \cos(x - \ell\frac{\pi}{2} - \eta \log 2x)$$

$$W_{-\eta,\ell+1/2}(2x) \to \frac{\exp(-x)}{x^\eta}$$

4. Applications of the calculable R-matrix

- R matrix equations for bound states
  We use $(H - E + \mathcal{L}(L))\, u_{int} = \mathcal{L}(L) u_{ext}$ (1)
  $u_{int}(r) = \sum_{i=1}^{N} c_i \phi_i(r)$ (2)
  $u_{ext}(r) = C\, W_{-\eta,\ell+1/2}(2kr)$ (3)

With C=ANC (Asymptotic Normalization Constant): important in "external" processes

- Using (2) in (1) and the continuity equation:

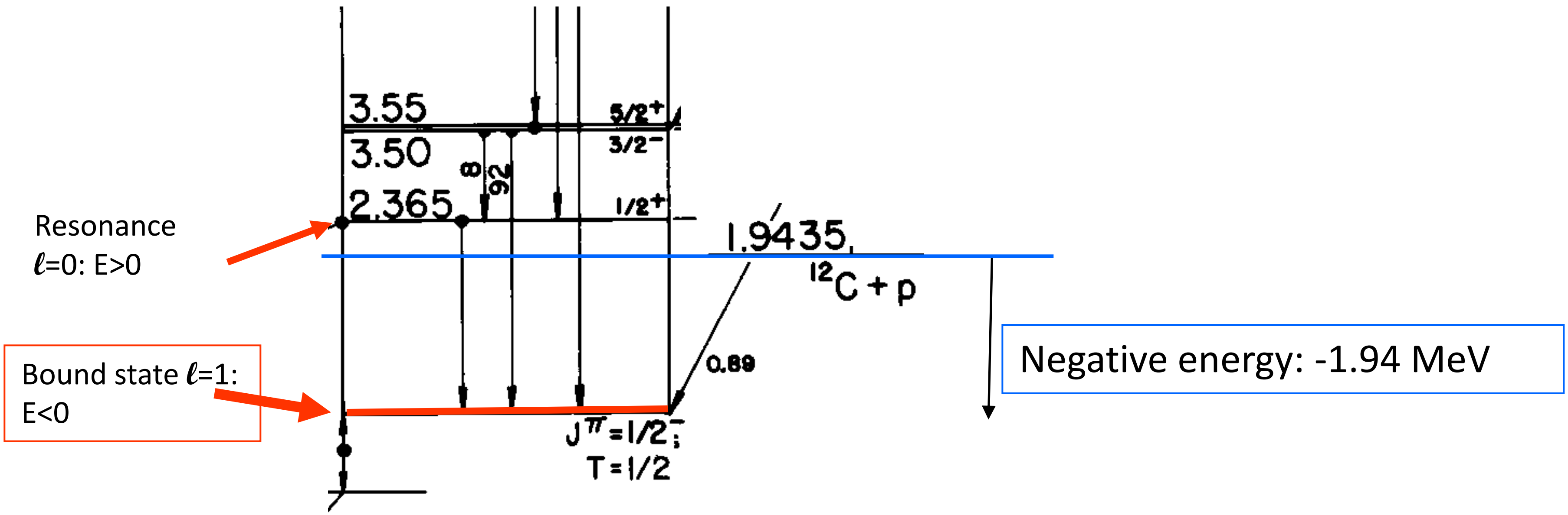
$$\sum_{i=1}^{N} c_i < \phi_j\, |H - E + \mathcal{L}(L)| \phi_i >_{int} = < \phi_j\,(r)|\mathcal{L}(L)|u_{ext} > = 0$$

$$\text{if } L = 2ka\, W'(2ka)/W(ka)$$

- Standard diagonalization problem
- But: L depends on the energy, which is not known → iterative procedure
  First iteration: L=0

4. Applications of the calculable R-matrix

Application to the ground state of $^{13}N = ^{12}C + p$



- Potential : $V=-55.3*\exp(-(r/2.70)^2)$
- Basis functions: $\phi_i(r) = r^\ell \exp(-(r/a_i)^2)$ (as before)

4. Applications of the calculable R-matrix

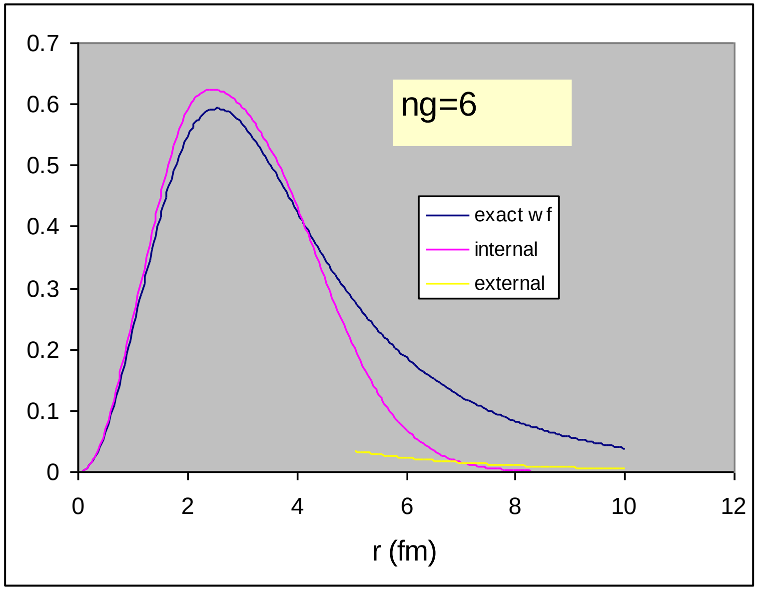
Calculation with a=7 fm

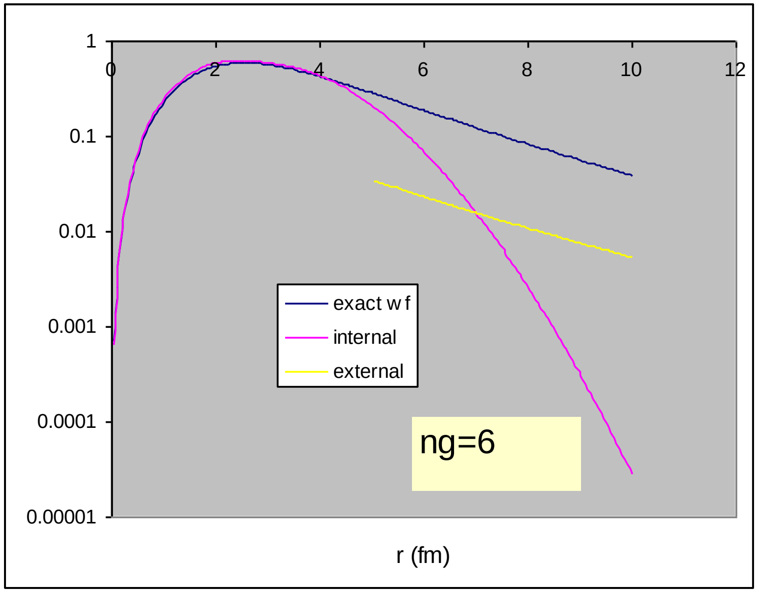
- $N = 6$ (poor results)
- $N = 10$ (good results)

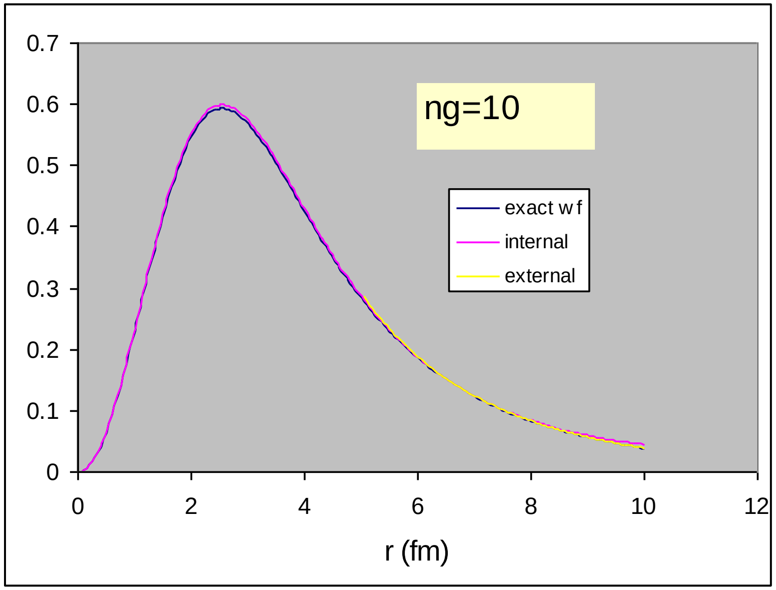
Iteration	$N = 6$	$N = 10$
1	-1.500	-2.190
2	-1.498	-1.937
3	-1.498	-1.942
		-1.942
Final	-1.498	-1.942
Exact	-1.942	
Left derivative	-1.644	-0.405
Right derivative	-0.379	-0.406

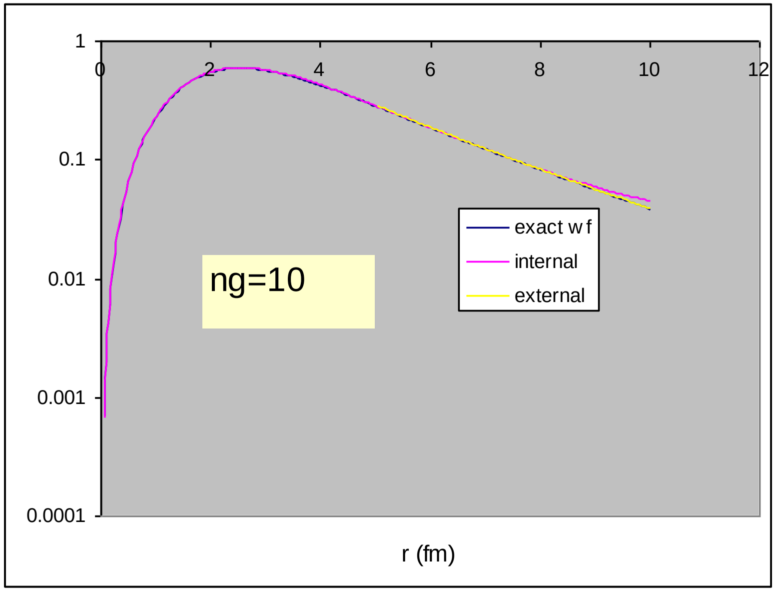
4. Applications of the calculable R-matrix

Wave functions (a=7 fm)









4. Applications of the calculable R-matrix

Other applications of the "calculable" R matrix

- **Microscopic cluster models** (next week):
  include the structure of the nuclei
  use a nucleon-nucleon interaction

- **CDCC calculations:** T. Druet, D. Baye, P.D. J.-M. Sparenberg, Nucl. Phys. A 845 (2010) 88
  Reactions with 2-body projectiles (ex: d+^{58}Ni) or 3-body projectiles (^{6}He)
  set of coupled equations

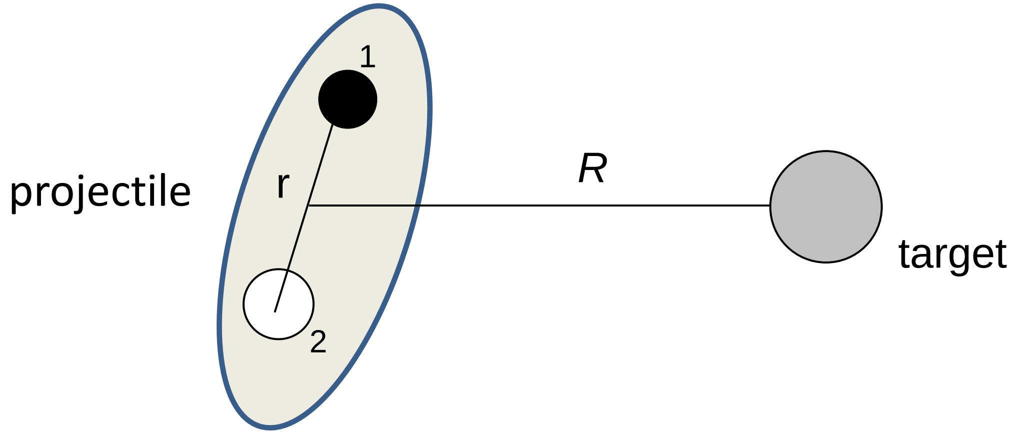
- **Three-body continuum states**: P.D., E. Tursunov, D. Baye, NPA765 (2006) 370
  hyperspherical formalism (ex: α+n+n)
  set of coupled equations

Applicationto the CDCC method

$H\ \Psi^{JM\pi} = E\ \Psi^{JM\pi}$ for E>0

with correct asymptotic conditions (→ collision matrix)

$$H = H_0(r) - \frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{R}} + V_{t1}(\boldsymbol{R} + \frac{A_2}{A_p}\boldsymbol{r}) + V_{t2}(\boldsymbol{R} - \frac{A_1}{A_p}\boldsymbol{r})$$



V_{t1}, V_{t2}= optical potentials
typically: Woods-Saxon

Two steps:
1. Diagonalize H_0 → basis for the projectile
2. Expand the total wave function over this basis
   → system of coupled differential equations

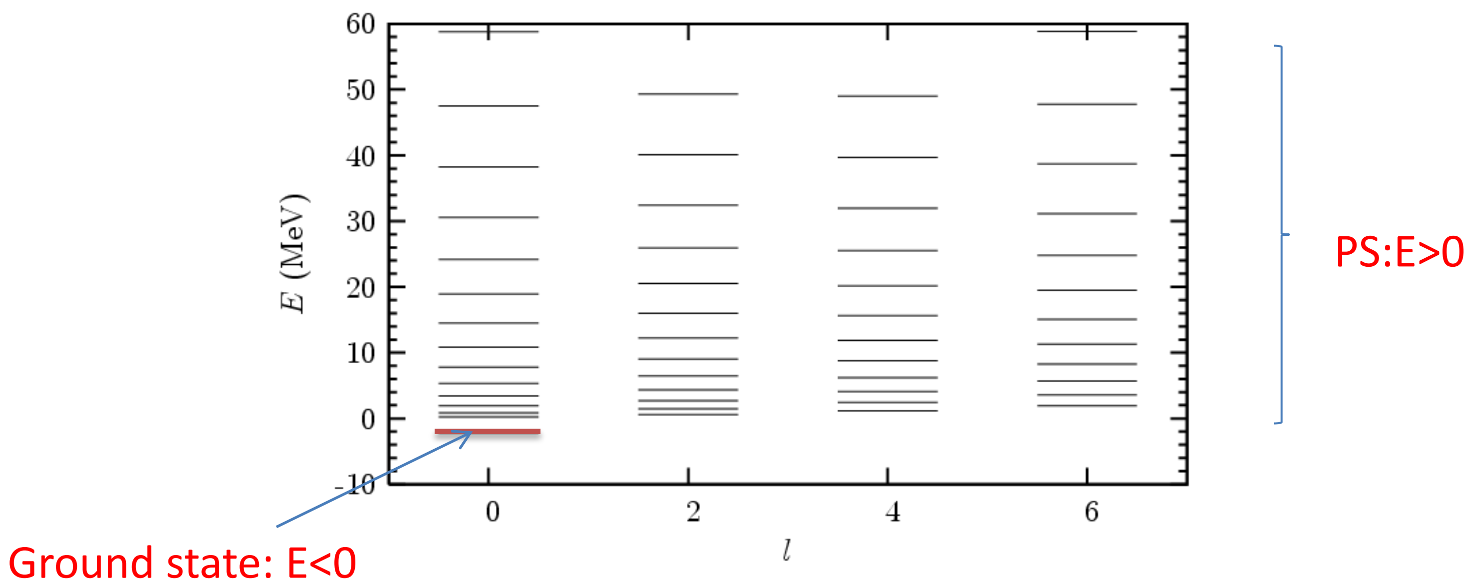
4. Applications of the calculable R-matrix

First step: diagonalization of the **projectile** hamiltonian H_0

$$H_0\Phi_l^{jm}(\boldsymbol{r}) = E_l^j \Phi_l^{jm}(\boldsymbol{r})$$

Two options for positive energies:

1. Expand Φ^{jm} on a basis (traditionally: gaussians, here: Lagrange functions)
   Pseudo-state (PS) method → Φ^{jm} is square-integrable
   Example: deuteron=p+n



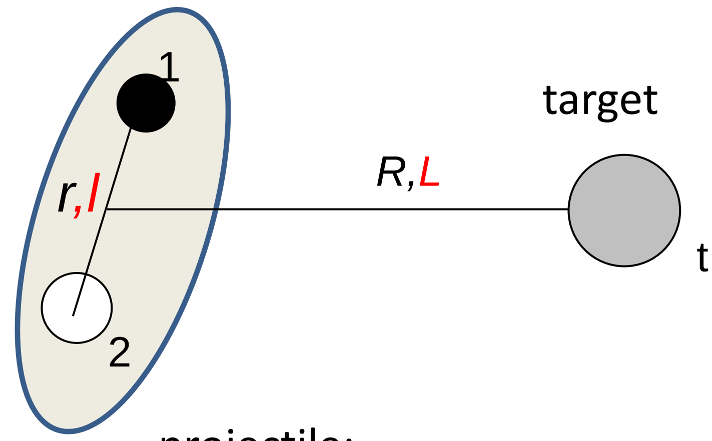
2. The projectile wave functions are described by « bins »

$$\phi_{li}^j(r) = \sqrt{\frac{1}{\Delta_i}} \int_{k_{i-1}}^{k_i} \tilde{\phi}_l^j(k_r, r)\, dk_r$$

2nd step: expand the total wave function

$$\Psi^{JM\pi}(\boldsymbol{R},\boldsymbol{r}) = \sum_{ljLi} u^{J\pi}_{ljLi}(R)\, \phi^{j}_{li}(r)\, Y^{JM}_{ljL}(\Omega_R,\Omega_r),$$

- $u^{J\pi}_{ljLi}(R)$: To be determined
- $\phi^{j}_{li}(r)$: 2-body wave functions
- $Y^{JM}_{ljL}(\Omega_R,\Omega_r)$: Angular functions



Expand the potential in multipoles (numerical integration over the angle)

$$V_{t1}(\boldsymbol{R}+\frac{A_2}{A_p}\boldsymbol{r}) + V_{t2}(\boldsymbol{R}-\frac{A_1}{A_p}\boldsymbol{r}) = \sum_{\lambda} V_{\lambda}(r,R) P_{\lambda}(\cos\theta_{Rr})$$

Insert both expansions in the Schrödinger associated with H

$$H = H_0 + T_R + V_{t1}(\boldsymbol{R}+\frac{A_2}{A_p}\boldsymbol{r}) + V_{t2}(\boldsymbol{R}-\frac{A_1}{A_p}\boldsymbol{r})$$

4. Applications of the calculable R-matrix

Finally: system of coupled equations→ provides radial functions $u^{J\pi}(R)$

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR^2}-\frac{L(L+1)}{R^2}\right)+E_c-E\right]u_c^{J\pi}(R)+\sum_{c'}V_{c,c'}^{J\pi}(R)u_{c'}^{J\pi}(R)=0$$

With potentials obtained from

$$V_{c,c'}^{J\pi}(R)\sim\int_0^\infty \phi_{li}^{j}(r)\,V_\lambda(r,R)\,\phi_{l'i'}^{j'}(r)dr$$

+ factors (6j, Clebsch-Gordan,…)

Channel c= l,j projectile quantum numbers
i: excitation level of the projectile [physical state (E<0) or PS (E>0)]
L : orbital angular momentum between projectile and target

Number of c values: typically ~100-200

Common procedure for CDCC

- Two-body states $\Phi^j(r)$ ➔ Lagrange functions for the projectile (coordinate r)
- Determination of the potentials $V_{cc'}(R)$➔ Lagrange functions for the p-t (coordinate R)
- Solution of the scattering system ➔ R matrix

Alternative method: Numerov algorithm (FRESCO)

4. Applications of the calculable R-matrix

The Lagrange-mesh method (*D. Baye, Phys. Stat. Sol. 243 (2006) 1095*)

- Gauss approximation: $\int_0^a g(x)dx \approx \sum_{k=1}^{N} \lambda_k g(x_k)$
  - N= order of the Gauss approximation
  - x_k=roots of an orthogonal polynomial, λ_k=weights
  - If interval [0,*a*]: Legendre polynomials
    [0,∞]: Laguerre polynomials

- Lagrange functions for [0,1]: $f_i(x) \sim P_N(2x-1)/(x-x_i)$
  - x_i are roots of $P_N(2x_i-1)=0$
  - with the Lagrange property: $f_i(x_j) = \lambda_i^{-1/2}\,\delta_{ij}$

- Matrix elements with Lagrange functions: Gauss approximation is used

$$< f_i|f_j >= \int f_i(x)f_j(x)dx \approx \sum_{k=1}^{N} \lambda_k f_i(x_k)f_j(x_k) \approx \delta_{ij}$$

$< f_i|T|f_j >$ analytical

$$< f_i|V|f_j >= \int f_i(x)V(x)f_j(x)dx \approx V(x_i)\delta_{ij}$$

⇒ **no integral needed**
very simple!

4. Applications of the calculable R-matrix

Application to CDCC

T. Druet, D. Baye, P.D. J.-M. Sparenberg, Nucl. Phys. A 845 (2010) 88

- 2-body states defined in a Lagrange basis

$$\phi^{j}_{li}(r) = \sum_{k=1}^{N} c^{j}_{li,k} f_k(r)$$

With coefficients c_k determined from the 2-body Schrödinger equation

- Coupling potentials for CDCC: obtained from previous functions

$$\begin{aligned} V^{J\pi}_{c,c'}(R) &\sim \int_0^\infty \phi^{j}_{li}(r)\, V_\lambda(r,R)\, \phi^{j'}_{l'i'}(r) dr \\ &\sim \sum_k c^{j}_{li,k} c^{j'}_{l'i',k} V_\lambda(r_k, R) \end{aligned}$$

➔ **no integral,** simple calculation of the coupling potentials
➔ can be easily extended to **non-local potentials**

Matrix elements

$$C^{J\pi}_{cn,c'n'} = \langle \varphi_n \mid (T_c + \mathcal{L}_c + E_c - E)\delta_{cc'} + V^{J\pi}_{cc'} \mid \varphi_{n'} \rangle_{\text{int}}$$

- In general: integral over *R* (from *R=0* to *R=a*)
  Lagrange mesh: value of the potential at the mesh points ➔ very fast
- From matrix ***C*** → R matrix

$$R^{J\pi}_{c,c'} = \sum_{n,n'} (C^{J\pi})^{-1}_{cn,c'n'} \, \varphi_n(a) \, \varphi_{n'}(a)$$

→ Collision matrix ***U*** → phase shifts, cross sections

- Typical sizes: ~100-200 channels c, N~30-40
- Test: collision matrix ***U*** does not depend on *N, a*
- Choice of *a*: compromize (*a* too small: R-matrix not valid, *a* too large: *N* large)

- Some remarks

  ☺ Fast (no integral), accurate

  ☺ The basis is defined by *N* and *a* only : no further parameter (≠ for gaussians)

  ☹ Legendre functions: more zeros near *R=0*, and *R=a* → not optimal

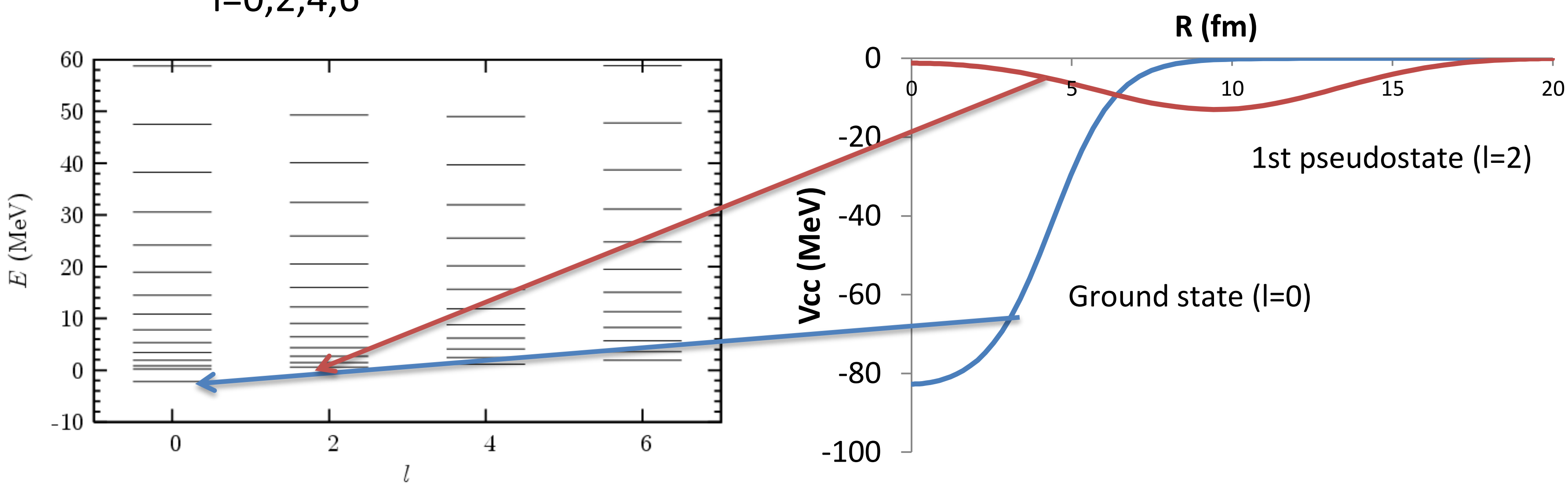
4. Applications of the calculable R-matrix

Test case: d+^{58}Ni at E_{lab}=80 MeV

- Standard benchmark in the literature
- p+n: gaussian potential (reproduces E_d=-2.22 MeV)
- p+^{58}Ni, n+^{58}Ni: optical potentials
- Elastic scattering and breakup

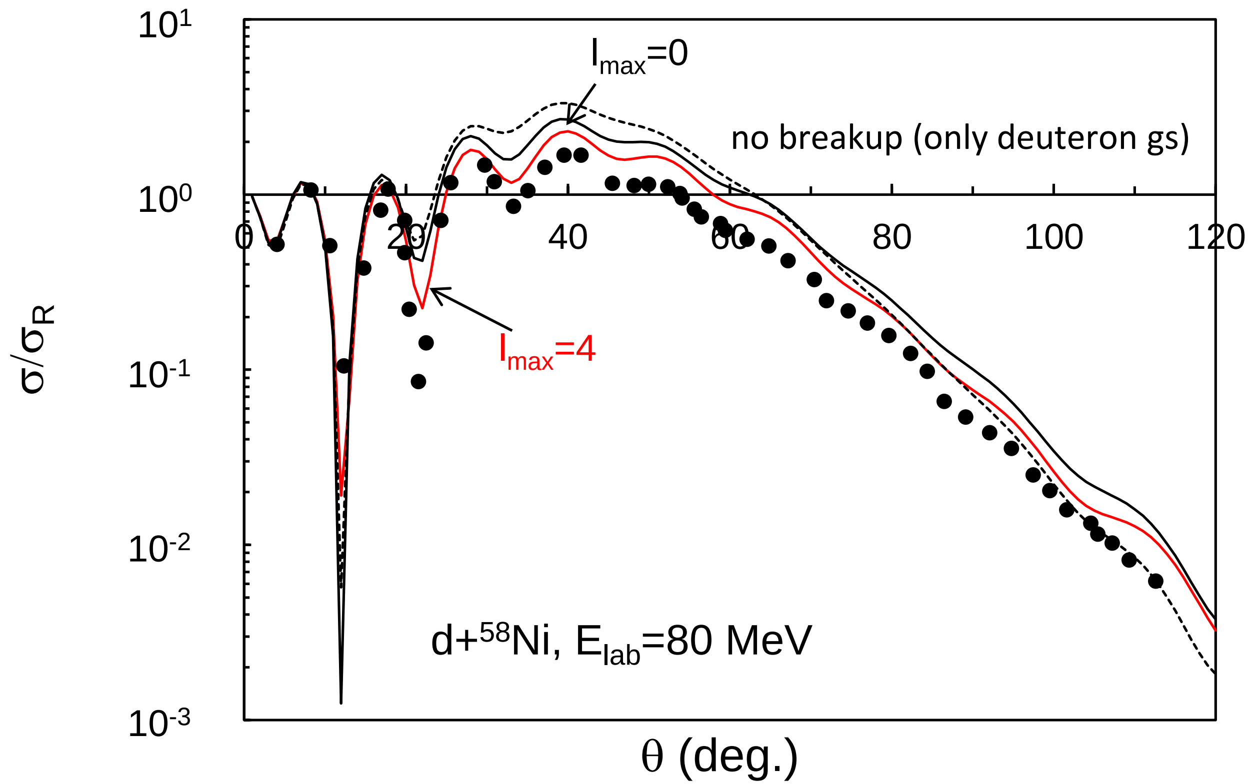
deuteron basis:
l=0,2,4,6

d+^{58}Ni potentials (nuclear)



→ long range for PS
→ radius a≥ 15 fm

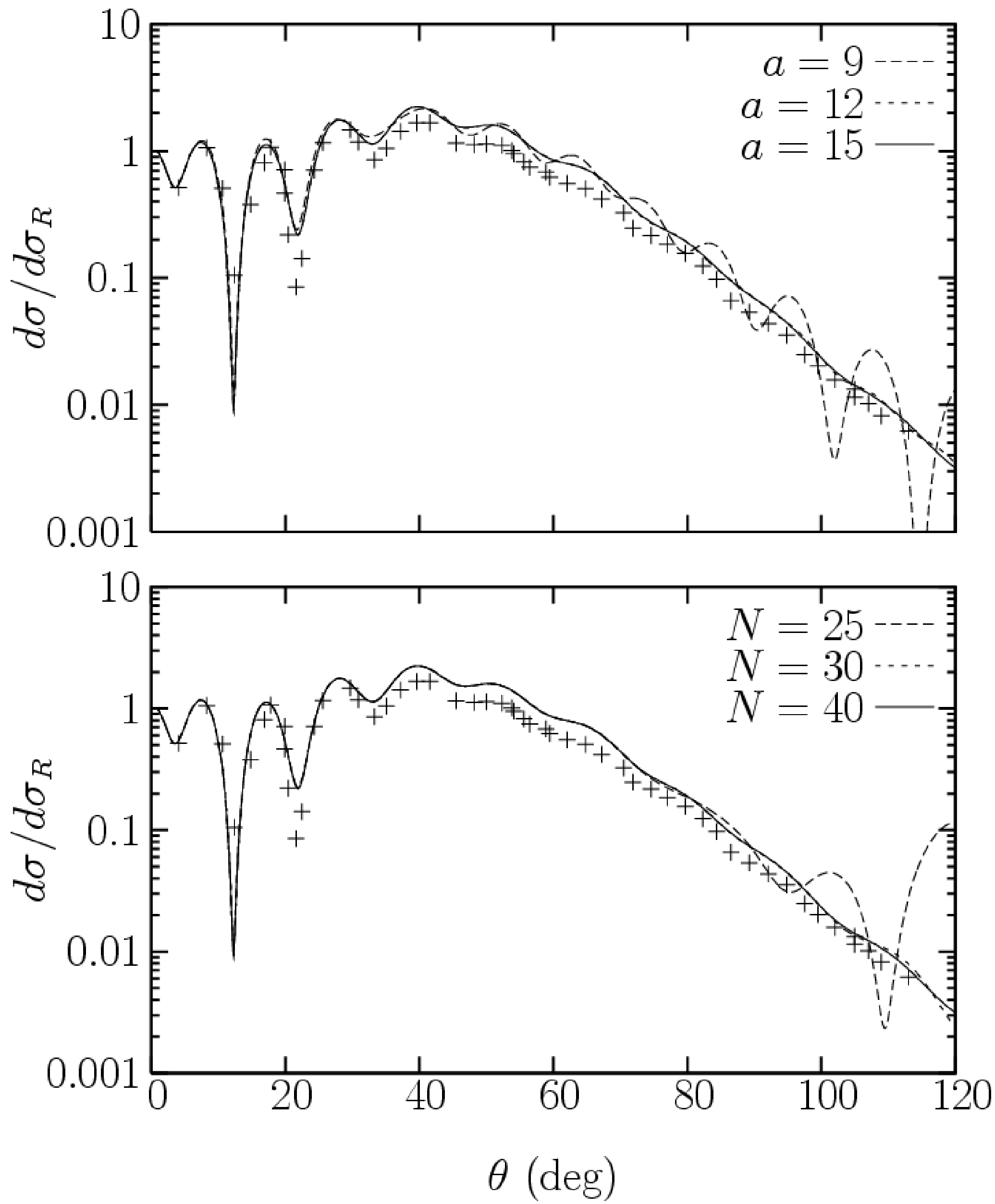
Convergence with the p+n angular momentum



➔ importance of p+n breakup channels

4. Applications of the calculable R-matrix

Convergence with R-matrix parameters



channel radius *a (N=30)*

Number of basis (Lagrange) functions *N (a=15* fm)

Propagation techniques

Computer time: 2 main parts

- Matrix elements: very fast with Lagrange functions
- Inversion of (complex) matrix C → R-matrix (long times for large matrices)

For reactions involving halo nuclei:

- Long range of the potentials (Coulomb)

$$\frac{Z_1 Z_t e^2}{\boldsymbol{R} + \frac{A_2}{A_p}\boldsymbol{r}} + \frac{Z_2 Z_t e^2}{\boldsymbol{R} - \frac{A_1}{A_p}\boldsymbol{r}} = \sum_\lambda V_\lambda(r, R) P_\lambda(\cos\theta_{Rr})$$

$$V_{cc'}(R) \approx \frac{Z_p Z_t e^2}{R} + \frac{Z_t Q_p}{R^3} + \dots$$

Can be large (large quadrupole moments of PS)

- Radius *a* must be large
- Many basis functions (*N* large)

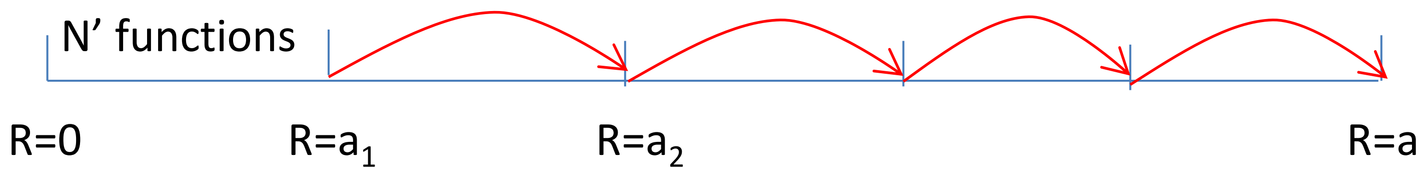
→ Propagation techniques (well known in atomic physics)

Ref.: Baluja et al. Comp. Phys. Comm. 27 (1982) 299

Without propagation

- Matrix elements integrated over [0,a]
- Inversion of a matrix of dimension N x N_c

With propagation



- The interval [0,a] is split in N_S subintervals
- In each subinterval N'~N/N_S: $\langle \varphi_n \mid (T_c + \mathcal{L}_c + E_c - E)\delta_{cc'} + V_{cc'}^{J\pi} \mid \varphi_{n'} \rangle_{a_i - a_{i+1}}$
  - Interval 1: determine R(a_1)
  - Interval 2 : R(a_2) from R(a_1)
  - Interval N_S: R(a) from R(a_{NS-1})

  } (inversion of a matrix with size N' x N_c)

➔ N_S smaller calculations:

Lagrange functions well adapted to matrix elements over [a_i,a_{i+1}]