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R-matrix theory of nuclear reactions.

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R-matrix theory of nuclear reactions

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- 1. Introduction
- 2. General collision theory: elastic scattering
- 3. Phase-shift method
- 4. R-matrix theory (\rightarrow theory)
- 5. Phenomenological R matrix (\rightarrow experiment)
- 6. Conclusions

1.Introduction

General context: two-body systems

- Low energies (E \leq Coulomb barrier), few open channels (one)
- Low masses (A \lesssim 15-20)
- Low level densities (\lesssim a few levels/MeV)
- Reactions with neutrons AND charged particles



Low-energy reactions				
ransmission ("tunnelling") decreases with $\ell \to$ few partial waves \to semi-classic theories not valid				
 astrophysics 				
thermal neutrons				
• Wavelength λ=ħc/E λ(fm)~197/E(MeV)				
example: 1 MeV: λ ~200 fm radius ~ 2-4 fm → quantum effects important				

Some references:

•C. Joachain: Quantum Collision Theory, North Holland 1987

•L. Rodberg, R. Thaler: Introduction to the quantum theory of scattering, Academic Press 1967

•J. Taylor : Scattering Theory: the quantum theory on nonrelativistic collisions, John Wiley 1972

Different types of reactions



 $A+B \rightarrow A+B: Q=0$

2. Inelastic collision ($Q \neq 0$) $A+B \rightarrow A^*+B$ (A*=excited state) $A+B \rightarrow A+B^*$ $A+B \rightarrow A^*+B^*$ etc.. 3. Transfer reactions $A+B \rightarrow C+D$ $A+B \rightarrow C+D+E$ $A+B \rightarrow C^*+D$ etc... 4. radiative capture reactions $A+B \rightarrow C + \gamma$

covered here

NOT covered here

2. Collision theory: elastic scattering



Center-of-mass system

Scattering wave functions

Schrödinger equation: V(r)=interaction potential

$$H\psi(r) = \left[-\frac{\hbar^2}{2\mu}\Delta + V(r)\right]\psi(r) = E\psi(r)$$
 with $E > 0$

Assumption: the potential is real and decreases faster than 1/r

A large distances : V(r)
$$\rightarrow$$
 0
2 independent solutions : $\psi(r) \rightarrow A\left(\exp(i\mathbf{k} \cdot \mathbf{r}) + f(\theta) \frac{\exp(ikr)}{r}\right)$
Incoming plane wave Outgoing spherical wave

where: k=wave number: $k^2=2\mu E/\hbar^2$

A=amplitude (scattering wave function is not normalized) $f(\theta)$ =scattering amplitude (length)

Cross sections



- Cross section obtained from the asymptotic part of the wave function
- "Direct" problem: determine σ from the potential
- "Inverse" problem : determine the potential V from σ
- Angular distribution: E fixed, θ variable
- Excitation function: θ variable, E fixed,

How to solve the Schrödinger equation for E>0?

$$H\psi(r) = (-\frac{\hbar^2}{2\mu}\Delta + V(r))\psi(r) = E\psi(r)$$

With $\psi(\mathbf{r}) \rightarrow \exp(ikz) + f(\theta) \frac{\exp(ikr)}{r}$ (z along the beam axis)

Several methods:

- Formal theory: Lippman-Schwinger equation → approximations
 - Eikonal approximation
 - Born approximation
- Phase shift method: well adapted to low energies
- Etc...

Lippman-Schwinger equation:

$$\psi(\mathbf{r}) \to \exp(ikz) + f(\theta) \frac{\exp(ikr)}{r}$$

$$\psi(\mathbf{r}) = \exp(ikz) + \int G(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') \psi(\mathbf{r}') d\mathbf{r}' \quad \text{is solution of the Schrödinger equation}$$
With $G(\mathbf{r}, \mathbf{r}') = -\frac{2\mu}{\hbar^2} \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{4\pi|\mathbf{r} - \mathbf{r}'|} = -\text{Green function}$

r is supposed to be large (r >> r')

$$f(heta) = -rac{2\mu}{4\pi\hbar^2}\int \exp(-ikr'\cos heta)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}'$$

- $\Psi(r)$ must be known
- $\Psi(r)$ only needed where V(r) \neq 0 \rightarrow approximations are possible
- Born approximation : $\psi(\mathbf{r}) = \exp(ikz)$
- Eikonal approximation: $\psi(\mathbf{r}) = \exp(ikz) \times \hat{\psi}(\mathbf{r})$

Valid at high energies: $V(r) \ll E$

3. Phase-shift method

a. Definitions, cross sections

Simple conditions:

neutral systems spins 0 single-channel

- b. Extension to charged systems
- c. Extension to multichannel problems
- d. Low energy properties
- e. General calculation
- f. Optical model

3.a Definition, cross section

The wave function is expanded as

$$\Psi(\mathbf{r}) = \sum_{l,m} \frac{u_l(r)}{r} Y_l^m(\Omega)$$

When inserted in the Schrödinger equation

$$-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) u_l(r) + V(r)u_l(r) = Eu_l(r)$$

To be solved for any potential (real)

For
$$\mathbf{r} \rightarrow \infty$$
 V(r) =0

$$\begin{cases}
u_l'' - \frac{l(l+1)}{r^2} u_l(r) + k^2 u_l(r) = 0, & \text{with } k^2 = \frac{2\mu E}{\hbar^2} \\
= \text{Bessel equation } \rightarrow u_l(r) = j_l(kr), & n_l(kr)
\end{cases}$$

For small x
$$j_l(x) \rightarrow \frac{x^l}{(2l+1)!!}$$
 For large x $j_l(x) \rightarrow \frac{1}{x} \sin(x - l\pi/2)$
 $n_l(x) \rightarrow -\frac{(2l-1)!!}{x^{l+1}}$ For large x $j_l(x) \rightarrow \frac{1}{x} \cos(x - l\pi/2)$

Examples:
$$j_0(x) = \frac{\sin(x)}{x}$$
, $n_0(x) = -\frac{\cos(x)}{x}$

At large distances: $u_{l}(r)$ is a linear combination of $j_{l}(kr)$ and $n_{l}(kr)$:

$$u_{l}(r) \rightarrow j_{l}(kr) - \tan \delta_{l} * n_{l}(kr)$$
With δ_{l} = phase shift (information
about the potential)
If $V=0 \rightarrow \delta=0$
Cross section:

$$\frac{d\sigma}{d\Omega} = |f(\theta, E)|^{2}, \text{ with } f(\theta, E) = \frac{1}{2ik} \sum_{l} (2l+1) [\exp(2i\delta_{l}(E)) - 1] P_{l}(\cos \theta)$$
Provide the cross section

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$$\frac{d\sigma}{d\Omega} = |f(\theta, E)|^2, \text{ with } f(\theta, E) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [\exp(2i\delta_l(E)) - 1] P_l(\cos\theta)$$

→ factorization of the dependences in E and θ

General properties of the phase shifts

- 1. Expansion useful at low energies: small number of *l* values
- 2. The phase shift (and all derivatives) are continuous functions of E
- 3. The phase shift is known within $n\pi: exp(2i\delta) = exp(2i(\delta + n\pi))$
- 4. Levinson theorem
 - $\delta_{l}(E=0)$ is arbitrary
 - $\delta(E=0) \delta(E=\infty) = N\pi$, where N is the number of bound states
 - Example: p+n, ℓ =0: δ (E=0) δ (E= ∞)= π (bound deuteron)

Interpretation of the phase shift from the wave function





Example: ¹²C+p

With resonance: E_R =0.42 MeV, Γ =32 keV \rightarrow lifetime: t=}/ Γ ~2x10⁻²⁰ s

Without resonance: interaction range d~10 fm \rightarrow interaction time t=d/v ~1.1x10⁻²¹ s

3.b Generalization to the Coulomb potential

The asymtotic behaviour $\Psi(r) \rightarrow \exp(ikz) + f(\theta)^* \exp(ikr)/r$

Becomes: $\Psi(r) \rightarrow \exp(ikz + \eta \log(kr)) + f(\theta)^* \exp(ikr - \eta \log(2kr))/r$

With $\eta = Z_1 Z_2 e^2/\hbar v$ =Sommerfeld parameter, v=velocity

Bessel equation:

$$u_{l}^{"} - \frac{l(l+1)}{r^{2}}u_{l}(r) + k^{2}u_{l}(r) = 0$$
Coulomb
equation

$$u_{l}^{"} - \frac{l(l+1)}{r^{2}}u_{l}(r) + (k^{2} - 2k\eta)u_{l}(r) = 0$$

$$u_{l}(r) \rightarrow F_{l}(kr) + \tan \delta_{l} * G_{l}(kr)$$

$$\rightarrow I_{l}(kr) - U_{l} * O_{l}(kr), \text{ with } U_{l} = \exp(2i\delta_{l})$$

$$\rightarrow F_{l}(kr) * \cos \delta_{l} + G_{l}(kr) * \sin \delta_{l}$$

Solutions:
$$F_{l}(\eta,kr)$$
: regular, $G_{l}(\eta,kr)$: irregular
Ingoing, outgoing functions: $I_{l} = G_{l} - iF_{l}$, $O_{l} = G_{l} + iF_{l}$
 $I_{l}(x) \rightarrow \exp(-ix)$
 $O_{l}(x) \rightarrow \exp(-ix)$ 16

Example: hard sphere



Special case: Neutrons, with ℓ =0: $F_0(x)=sin(x), G_0(x)=cos(x)$ $\rightarrow \delta$ =-ka

example : α +n phase shift ℓ =0

R. A. ARNDT AND L. D. ROPER



→ hard sphere is a good approximation

Elastic cross section with Coulomb:

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

Still valid, but converges very slowly.

$$f(\boldsymbol{\theta}) = f_{C}(\boldsymbol{\theta}) + f_{N}(\boldsymbol{\theta})$$

•f_C(θ): Coulomb part: exact
•f_N(θ): nuclear part: converges rapidly

$$\frac{d\sigma_{c}}{d\Omega} = |f_{c}(\theta)|^{2} \sim \frac{1}{E^{2}} \frac{1}{\sin^{4} \frac{\theta}{2}}$$



- 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 $\theta = 180^{\circ} \rightarrow$ nuclear effect maximum

3.c Extension to multichannel problems

- 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

• Selection rules:
$$|I_1 - I_2| \le I \le I_1 + I_2$$

 $|\ell - I| \le J \le \ell + I$
 $\pi = \pi_1 * \pi_2 * (-1)^{\ell}$

Example of quantum numbers

 α +³He α =0⁺, ³He=1/2⁺

p+⁷Be ⁷Be=3/2⁻, p=1/2⁺

J	1	l	size
1/2+	1/2	0, 🗶	1
1/2-	1/2	<u>X</u> , 1	1
3/2+	1/2	X , 2	1
3/2-	1/2	1, 🎗	1

J	1	l	size
0+	1 2	1 X	1
0-	1 2	<mark>Ж</mark> 2	1
1+	1 2	<mark>隊</mark> , 1, ∦ 1, ≵ 3	3
1-	1 2	0, <u>1</u> , 2 <u>1</u> , 2, <u>3</u>	3

Cross sections

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

Multichannel $\frac{dc}{dS}$

$$\frac{\sigma}{\Omega} = \sum_{K_1, K_2, K'_1, K'_2} |f_{K_1 K_2, K'_1 K'_2}(\theta)|^2$$

With: K_1, K_2 =spin orientations in the entrance channel K'_1, K'_2=spin orientations in the exit channel

$$f_{K_{1}K_{2},K_{1}'K_{2}'}(\theta) = \sum_{J,\pi} \sum_{II,I'I'} \dots U_{II,I'I'}^{J\pi} Y_{I'}(\theta,0)$$

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

3.d Low-energy properties of the phase shifts

One defines $\gamma = \frac{1}{u(a)} \left(\frac{du}{dr}\right)_{r=a}$ =logarithmic derivative at *r*=*a* (*a* large)

Then, for very low E (neutral system): $\tan \delta_{\ell} \approx \frac{(ka)^{2\ell+1}}{(2\ell+1)!!(2\ell-1)!!} \left[\frac{\ell - \gamma a}{\gamma a + \ell + 1} \right]$

For
$$l=0$$
: $\alpha = -\lim_{k \to 0} \frac{\tan \delta_0(k)}{k} = \text{scattering length}$



Cross section at low E: $\sigma = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \sin^2 \delta_{\ell} \xrightarrow[k \to 0]{} 4\pi \alpha^2$ (isotropic)

In general (neutrons):
$$\delta \sim k^{2\ell+1}$$

 $\sigma \sim k^{4\ell}$

Thermal neutrons (T=300K, E=25 meV): only *l*=0 contributes





example : α +n phase shift ℓ =0 At low E: δ ~-k α with α >0 \rightarrow replusive

3.e General calculation

For some potentials: analytic solution of the Schrödinger equation In general: no analytic solution \rightarrow numerical approach

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u_{\ell}(r) + (V(r) - E)u_{\ell}(r) = 0$$

with: $V(r) = V_N(r) + \frac{Z_1Z_2e^2}{r} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}$ $u_{\ell}(r) \to F_{\ell}(kr,\eta)\cos\delta_{\ell} + G_{\ell}(kr,\eta)\sin\delta_{\ell}$

Numerical solution : discretization N points, with mesh size h

- u_ℓ(0)=0
- u_l(h)=1 (or any constant)
- $u_{\ell}(2h)$ is determined numerically from $u_{\ell}(0)$ and $u_{\ell}(h)$ (Numerov algorithm)
- u_ℓ(3h),... u_ℓ(Nh)
- for large r: matching to the asymptotic behaviour \rightarrow phase shift

Bound states: same idea

Example: $\alpha + \alpha$



Experimental phase shifts





3.f Optical model

Goal: to simulate absorption channels



High energies:

- many open channels
- strong absorption
- potential model extended to complex potentials (« optical »)

Phase shift is complex: $\delta = \delta_{R} + i\delta_{I}$ collision matrix: $U = \exp(2i\delta) = \eta \exp(2i\delta_{R})$ where $\eta = \exp(-2\delta_{I}) < 1$ Elastic cross section $\frac{d\sigma}{d\Omega} = \frac{1}{4k^{2}} \left| \sum_{\ell} (2\ell + 1)(\eta_{\ell} \exp(2i\delta_{\ell}) - 1)P_{\ell}(\cos\theta) \right|^{2}$ Reaction cross section: $\sigma = \frac{\pi}{k^{2}} \sum_{\ell} (2\ell + 1)(1 - \eta_{\ell}^{2})$

4. The R-matrix Method

Goals:

- 1. To solve the Schrödinger equation (E>0 or E<0)
 - 1. Potential model
 - 2. 3-body scattering
 - 3. Microscopic models
 - 4. Many applications in nuclear and atomic physics

2. To fit cross sections

- 1. Elastic, inelastic \rightarrow spectroscopic information on resonances
- 2. Capture, transfer \rightarrow astrophysics

References:

- A.M. Lane and R.G. Thomas, Rev. Mod. Phys. 30 (1958) 257
- F.C. Barker, many papers

Principles of the R-matrix theory

Standard variational calculations

- Hamiltonian $H\Psi = E\Psi$
- Set of *N* basis functions $u_i(r)$ with $\Psi(r) = \sum c_i u_i(r)$

→Calculation of $H_{ij} = \langle u_i | H | u_j \rangle$ over the full space $N_{ij} = \langle u_i | u_j \rangle$

(example: gaussians: $u_i(r)=exp(-(r/a_i)^2)$)

$$N_{ij} = \int_{0}^{\infty} u_i(r)u_j(r)dr$$
$$H_{ij} = \int_{0}^{\infty} u_i(T+V)u_jdr$$

- Eigenvalue problem : $\sum (H_{ij} EN_{ij})c_i = 0 \rightarrow \text{upper bound on the energy}$
- But: Functions $u_i(r)$ tend to zero \rightarrow not directly adapted to scattering states

Principles of the R-matrix theory

Extension to the R-matrix: includes boundary conditions

a. Hamiltonian

$$H\Psi = E\Psi$$
, with $H \to T + \frac{Z_1 Z_2 e^2}{r}$

b. Wave functions Set of N basis functions $u_i(r) \Psi(r) = \sum_i c_i u_i(r)$ valid in a limited range with $\Psi \rightarrow (I_i(kr) - U_i * O_i(kr)) Y_i^m(\Omega)$

 \rightarrow correct asymptotic behaviour (E>0 and E<0)

- Spectroscopy: short distances only Collisions : short *and* large distances
- R matrix: deals with collisions
- Main idea: to divide the space into 2 regions (radius *a*)
 - Internal: $r \le a$: Nuclear + coulomb interactions
 - External: *r* > *a* : Coulomb only

Exit channels



Here: elastic cross sections



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Plan of the lecture:

- The *R*-matrix method: two applications
 Solving the Schrödinger equation (essentially E>0)
 Phenomenological *R*-matrix (fit of data)
- Applications
- Other reactions: capture, transfer, etc.

c. R matrix

N basis functions u_i(r) are valid in a *limited range* (r ≤ a)
 ⇒ in the internal region:

$$\Psi_{int}(r) = \sum_{i=1}^{N} c_i u_i(r), \text{ for } r \le a \qquad (c_i = \text{coefficients})$$

At large distances the wave function is Coulomb
 ⇒ in the external region:

$$\Psi_{ext}(r) = A(I_{l}(kr) - U_{l} * O_{l}(kr)), \text{ for } r > a$$

 Idea: to solve with

$$\sum_{i} (H_{ij} - EN_{ij})c_{i} = 0$$

$$H_{ij} = \langle u_{i} | H | u_{j} \rangle_{int} \quad \text{defi}$$

$$N_{ij} = \langle u_{i} | u_{j} \rangle_{int}$$

defined in the internal region

• But T is not hermitian over a finite domain,

$$< u_i | T | u_j >_{int} \neq < u_j | T | u_i >_{int}$$

$$\int_0^a u_i \frac{d^2}{dr^2} u_j dr \neq \int_0^a u_j \frac{d^2}{dr^2} u_i dr, \text{ if } a \neq \infty$$
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• Bloch-Schrödinger equation:

$$(H - E + \mathcal{L}(L_0)) \Psi^{\ell m} = \mathcal{L}(L_0) \Psi^{\ell m},$$

• With $\mathcal{L}(L_0)$ =Bloch operator (surface operator) – constant L_0 arbitrary

$$\mathcal{L}(L_0) = \frac{\hbar^2}{2\mu m_N a} \delta(\rho - a) \begin{pmatrix} d \\ d\rho \end{pmatrix} \rho,$$

• Now we have $T + \mathcal{L}(L_0)$ hermitian:

$$< u_i | T + \mathcal{L}(L_0) | u_j >_{int} = < u_j | T + \mathcal{L}(L_0) | u_i >_{int}$$

• Since the Bloch operator acts at *r*=*a* only:

$$(H - E + \mathcal{L}(L_0)) \Psi_{int}^{\ell m} = \mathcal{L}(L_0) \Psi_{ext}^{\ell m},$$

• Here L₀=0 (boundary-condition parameter)
• Summary: $(H - E + \mathcal{L}(0)) \Psi_{int}^{\ell m} = \mathcal{L}(0) \Psi_{ext}^{\ell m}$, (1)

$$\Psi_{int}^{\ell m} = \sum_{i} c_i^{\ell} u_i^{\ell}(r) \tag{2}$$

$$\Psi_{ext}^{\ell m} = (I_{\ell}(kr) - U^{\ell}(E)O_{\ell}(kr))$$
(3)

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

$$\sum_{i} c_{i}^{\ell} < u_{j}^{\ell} | H + \mathcal{L}(0) - E | u_{i}^{\ell} >_{int} = < u_{j}^{\ell} | \mathcal{L}(0) | \Psi_{ext}^{\ell} >, \quad \longrightarrow \text{Provides } c_{i}$$
(inversion of D)
$$\bigcup_{i}(E)$$

$$\sum_{i} c_{i}^{\ell} u_{i}^{\ell}(a) = (I_{\ell}(ka) - U^{\ell}(E)O_{\ell}(ka)) \quad \text{Continuity at } r=a$$

$$U^{\ell} = \frac{I_{\ell}(ka) - kaI'_{\ell}(ka)R^{\ell}}{O_{\ell}(ka) - kaO'_{\ell}(ka)R^{\ell}}$$

$$U^{\ell} = \frac{I_{\ell}(ka) - kaI'_{\ell}(ka)R^{\ell}}{O_{\ell}(ka) - kaO'_{\ell}(ka)R^{\ell}} = \frac{I_{\ell}(ka)}{O_{\ell}(ka)} \frac{1 - L^{*}R^{\ell}}{1 - LR^{\ell}} = \exp(2i\delta^{\ell}) \qquad L = ka \frac{O'_{\ell}(ka)}{O_{\ell}(ka)}$$

With the R-matrix defined as

$$R^{\ell}(E) = \frac{\hbar^2 a}{2\mu} \sum_{ij} u_i^{\ell}(a) (D^{\ell}(E))_{ij}^{-1} u_j^{\ell}(a)$$

If the potential is real:

R real, $|U|=1, \delta$ real

Procedure (for a given l):

- 1. Compute matrix elements $D_{ij}^{\ell}(E) = \langle u_i^{\ell} | H + \mathcal{L}(0) E | u_j^{\ell} \rangle_{int}$
- 2. Invert matrix D
- 3. Compute R matrix
- 4. Compute the collision matrix U

$$L = ka \frac{O'_{\ell}(ka)}{O_{\ell}(ka)} = S(E) + iP(E)$$

S(E)=shift factor P(E)=penetration factor



E (MeV)

Interpretation of the R matrix

$$\begin{split} \Psi_{ext}^{\ell}(r) &= A(I_{\ell}(kr) - U^{\ell}(E)O_{\ell}(kr)) \qquad (1) \\ U^{\ell} &= \frac{I_{\ell}(ka) - kaI_{\ell}'(ka)R^{\ell}}{O_{\ell}(ka) - kaO_{\ell}'(ka)R^{\ell}} \to R^{\ell} = \frac{I_{\ell}(ka) - U^{\ell}O_{\ell}(ka)}{ka(I_{\ell}'(ka) - U^{\ell}O_{\ell}'(ka))} \\ \\ \text{From (1):} \qquad \frac{\Psi'^{\ell}(a)}{\Psi^{\ell}(a)} &= k \frac{I_{\ell}'(ka) - U^{\ell}O_{\ell}'(ka)}{I_{\ell}(ka) - U^{\ell}O_{\ell}(ka)} = \frac{1}{aR^{\ell}} \end{split}$$

Then:
$$R^{\ell} = rac{1}{a(\log \Psi^{\ell}(a))'}$$

=inverse of the logarithmic derivative at a



Example
$$u_i^\ell(r) = r^\ell \exp(-(r/a_i)^2)$$

Gaussians with different widths

$$N_{ij} = \langle u_i^{\ell} | u_j^{\ell} \rangle_{inl} \\ = \int_0^a r^{2\ell} \exp(-(r/a_i)^2 - (r/a_j)^2) dr$$

Can be done exactly (incomplete γ function)

Matrix elements of H can be calculated analytically for gaussian potentials Other potentials: numerical integration

Input data

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

Requirements

- a large enough : $V_N(a) \sim 0$
- *n* large enough (to reproduce the internal wave functions)
- *n* as small as possible (computer time)
 - \rightarrow compromise

Tests

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

Results for $\alpha + \alpha$

- potential : V(r)=-126*exp(-(r/2.13)²) (Buck potential)
- Basis functions: u_i(r)=r^ℓ*exp(-(r/a_i)²) with a_i=x₀*a₀⁽ⁱ⁻¹⁾ (geometric progression) typically x₀=0.6 fm, a₀=1.4



Elastic phase shifts



- 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

Wave functions at 5 MeV, a= 7 fm



Other example : sine functions

$$u_i^\ell(r) = \sin\frac{\pi r}{a}(n - \frac{1}{2})$$

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



→ Not a good basis (no flexibility)

Example of resonant reaction: ¹²C+p



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



2.5 ng=7 2 E=0.8 MeV 1.5 Phase shifts a=7 fm 1 0.5 0 180 5 10 15 -0.5 -160 140 -1 - exact w f 120 - internal -1.5 delta (deg.) external 100 -2 exact 80 r (fm) ng=10 60 ng=8 40 2.5 ng=10 ng=7 20 2 E=0.8 MeV 0 1.5 2.5 0.5 1.5 -20 0 exact wf 1 E (MeV) internal 0.5 external 0 10 5 15 -0.5 -1 -1.5 -2 r (fm)

Wave functions

Resonance energies

$$U^{\ell} = \frac{I_{\ell}(ka)}{O_{\ell}(ka)} \frac{1 - L^{\star}R^{\ell}}{1 - LR^{\ell}}, \text{ with } L(E) = S(E) + iP(E)$$

= $\exp(2i\delta^{\ell}) = \exp(2i(\delta^{\ell}_{HS} + \delta^{\ell}_{R}))$

with

$$\exp(2i\delta_{HS}^{\ell}) = \frac{I_{\ell}(ka)}{O_{\ell}(ka)} \to \delta_{HS}^{\ell} = -\arctan\frac{F_{\ell}(ka)}{G_{\ell}(ka)} \quad \text{Hard-sphere phase shift}$$
$$\exp(2i\delta_{R}^{\ell}) = \frac{1 - L^{\star}R^{\ell}}{1 - LR^{\ell}} \to \delta_{R}^{\ell} = \arctan\frac{PR}{1 - SR} \quad \text{R-matrix phase shift}$$

- Resonance energy E_r defined by $1 S(E_r)$. In general: must be solved numerically \widehat{b}_{T}^{i} 100
- Resonance width Γ defined by $\tan \delta_R(E) \approx$



Application of the R-matrix to bound states

Positive energies:

Negative energies:

$$u_{l}'' - \frac{l(l+1)}{r^{2}}u_{l}(r) + (k^{2} - 2k\eta)u_{l}(r) = 0$$
$$u_{l}'' - \frac{l(l+1)}{r^{2}}u_{l}(r) + (-k^{2} - 2k\eta)u_{l}(r) = 0$$

Coulomb functions F_{ℓ} G_{ℓ} Whittaker functions $W_{-\eta,\ell+1/2}(2x)$

Asymptotic behaviour:

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

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

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

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

Starting point of the R matrix:

$$H\Psi = E\Psi$$

$$H \to T + \frac{Z_1 Z_2 e^2}{r}$$

$$\Psi \to W_{-\eta, l+1/2} (2kr) Y_l^m (\Omega)$$

• R matrix equations $(H - E + \mathcal{L}(L)) \Psi_{int}^{\ell m} = \mathcal{L}(L) \Psi_{ext}^{\ell m}$, (1)

$$\Psi_{int}^{\ell m} = \sum_{i} c_i^{\ell} u_i^{\ell}(r) \tag{2}$$

$$\Psi_{ext}^{\ell m} = CW_{-\eta,\ell+1/2}(2kr) \tag{3}$$

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

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

$$\sum_{i} c_{i}^{\ell} < \underbrace{u_{i}^{\ell} | H + \mathcal{L}(L) - E | u_{j}^{\ell} >_{int} = \langle u_{j}^{\ell} | \mathcal{L}(L) | \Psi_{ext}^{\ell} > = 0,}_{\mathsf{D}_{ij}(\mathsf{E})}$$
if $L = 2ka \frac{W'(2ka)}{W(2ka)}$

• But: L depends on the energy, which is not known \rightarrow iterative procedure

Application to the ground state of ¹³N=¹²C+p



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

Calculation with a=7 fm

•ng=6 (poor results)

•ng=10 (good results)

Iteration	ng=6	ng=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

Wave functions (a=7 fm)









5. Phenomenological R matrix

Goal: fit of experimental data

• Basis functions
$$\Psi_{int}^{\ell}(r) = \sum_{i} c_i^{\ell} u_i^{\ell}(r)$$

• R matrix equations

$$R(E) = \frac{\hbar^2 a}{2\mu} \sum_{ij} u_i^{\ell}(a) (D^{\ell}(E))_{ij}^{-1} u_j^{\ell}(a)$$

with
$$D_{ij}^{\ell}(E) = \langle u_i^{\ell} | H + \mathcal{L}(0) - E | u_j^{\ell} \rangle_{int}$$

The choice of the basis functions is arbitrary

BUT must be consistent in R(E) and D(E)

Change of basis

- Eigenstates of $(H + \mathcal{L}(0))\Psi_{\lambda} = E_{\lambda}\Psi_{\lambda}$ over the internal region
- Ψ_λ expanded over the same basis: $\Psi_\lambda(r) = \sum_i d_i^\lambda u_i(r)$
- \rightarrow standard diagonalization problem

$$\sum_{i} d_i^{\lambda} < u_i | H + \mathcal{L}(0) - E_{\lambda} | u_j >_{int} = 0$$

Instead of using $u_i(r)$, one uses $\Psi_i(r)$

$$R(E) = \frac{\hbar^2 a}{2\mu} \sum_{\lambda\lambda'} \Psi_{\lambda}(a) \left(D^{\ell}(E) \right)_{\lambda\lambda'}^{-1} \Psi_{\lambda'}(a)$$

$$D_{\lambda\lambda'}^{\ell}(E) = \langle \Psi_{\lambda} | H + \mathcal{L}(0) - E | \Psi_{\lambda'} \rangle_{int}$$

= $(E_{\lambda} - E) \delta_{\lambda\lambda'}$

$$R(E) = \frac{\hbar^2 a}{2\mu} \sum_{\lambda} \frac{|\Psi_{\lambda}(a)|^2}{E_{\lambda} - E} = \sum_{\lambda} \frac{\gamma_{\lambda}^2}{E_{\lambda} - E}$$

$$R(E) = \frac{\hbar^2 a}{2\mu} \sum_{\lambda} \frac{|\Psi_{\lambda}(a)|^2}{E_{\lambda} - E} = \sum_{\lambda} \frac{\gamma_{\lambda}^2}{E_{\lambda} - E}$$

Completely equivalent

With
$$\gamma_{\lambda} = \sqrt{\frac{\hbar^2 a}{2\mu}} \Psi_{\lambda}(a)$$
 = reduced width

→2 steps: computation of eigen-energies E_{λ} (=poles) and eigenfunctions computation of reduced widths from eigenfunctions

Remarks: • E_{λ} =pole energy: different from the resonance energy depend on the channel radius • γ_{λ} proportional to the wave function at $a \rightarrow$ measurement of clustering (depend on a!) large $\gamma_{\lambda} \rightarrow$ strong clustering • dimensionless reduced width $\theta_{\lambda}^{2} = \frac{\gamma_{\lambda}^{2}}{\gamma_{W}^{2}}$, with $\gamma_{W}^{2} = \frac{3\hbar^{2}}{2\mu a^{2}}$ = Wigner limit • <u>http://pntpm.ulb.ac.be/Nacre/Programs/coulomb.htm</u>: web page to compute reduced widths

Example : ¹²C+p

- potential : V=-70.5*exp(-(r/2.70)²)
- Basis functions: $u_i(r)=r^{\ell}\exp(-(r/a_i)^2)$ with $a_i=x_0^*a_0^{(i-1)}$





$$R(E) = \sum_{\lambda} \frac{\gamma_{\lambda}^2}{E_{\lambda} - E}$$



Link between "standard" and "phenomenological" R-matrix:

- Standard R-matrix: parameters are calculated from basis functions
- Phenomenological R-matrix: parameters are fitted to data



→ In phenomenological approaches (one resonance): $R(E) \approx \frac{\gamma_0^2}{E_0 - E} + R_0$

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Approximations: $R_0(E)=R_0=$ constant (background) $R_0(E)=0$: Breit-Wigner approximation: one term in the R matrix **<u>Remark</u>**: the R matrix method is NOT limited to resonances ($R=R_0$)

¹²C+p

Summary

Solving the Schrödinger equation in a basis with *N* functions provides:

$$R(E) = \sum_{\lambda=1}^{N} \frac{\gamma_{\lambda}^2}{E_{\lambda} - E}$$

where E_{λ} , γ_{λ} are calculated from matrix elements between the basis functions



Other approach: consider E_{λ} , γ_{λ} as free parameters (no basis)

 \rightarrow Phenomenological R matrix

Question: how to relate R-matrix parameters with experimental information?

Resonance energies



with

$$\exp(2i\delta_{IIS}^{\ell}) = \frac{I_{\ell}(ka)}{O_{\ell}(ka)} \rightarrow \delta_{IIS}^{\ell} = -\arctan\frac{F_{\ell}(ka)}{G_{\ell}(ka)}$$
$$\exp(2i\delta_{R}^{\ell}) = \frac{1 - L^{\star}R^{\ell}}{1 - LR^{\ell}} \rightarrow \delta_{R}^{\ell} = \arctan\frac{PR}{1 - SR}$$

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$$\delta_R^{\ell}(E) = \arctan \frac{P(E)R(E)}{\mathbf{1} - S(E)R(E)}$$

Resonance energy E_r defined by $1 - S(E_r)R(E_r) = 0 \rightarrow \delta_R = 90^\circ$ In general: must be solved numerically



The Breit-Wigner approximation

Single pole in the R matrix expansion $R(E) \approx \frac{\gamma_0^2}{E_0 - E}$ Phase shift: $\delta_R(E) = \arctan \frac{P(E)R(E)}{1 - S(E)R(E)} \approx \arctan \frac{\gamma_0^2 P(E)}{E_0 - E - \gamma_0^2 S(E)}$

Resonance energy E_r, defined by: $E_0 - E_r - \gamma_0^2 S(E_r) = 0$ Not solvable analytically

Thomas approximation: $S(E_r) \approx S(E_0) + S'(E_0)(E_r - E_0)$

Then:
$$E_r \approx E_0 - \frac{\gamma_0^2 S(E_0)}{1 + \gamma_0^2 S'(E_0)}$$

Near the resonance energy E_r:

$$\tan \delta_R(E) \approx \frac{\gamma_0^2 P(E)}{E_0 - E - \gamma_0^2 S(E)} \approx \frac{\gamma_0^2 P(E)}{E_r - E + \gamma_0^2 (S(E_r) - S(E))}$$

$$\approx \frac{\gamma_0^2 P(E)}{E_r - E + \gamma_0^2 (E_r - E) S'(E_r)}$$

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$$\tan \delta_R(E) \approx \frac{\gamma_0^2 P(E)}{E_r - E + \gamma_0^2 (E_r - E) S'(E_r)} \approx \frac{\Gamma(E)}{2(E_r - E)}$$

with
$$\Gamma(E) = 2 \frac{\gamma_0^2}{1 + \gamma_0^2 S'(E_r)} P(E) = 2 \gamma_{obs}^2 P(E)$$

Remarks:

- γ₀, E₀ = "R-matrix", "calculated", "formal" parameters, needed in the R matrix
 •depend on the channel radius *a*
 - •Defined for resonances and bound states (Er<0)
- γ_{obs} , E_r = "observed" parameters
 - model independent, to be compared with experiment
 - should not depend on a
- The total width Γ depends on energy through the penetration factor P
 fast variation with E

 → low energy: narrow resonances (but the reduced width can be large)

Summary



Non-resonant calculations are possible: only a background pole

Link between "calculated" and "observed" parameters

One pole (N=1) $E_{R} = E_{0} - \frac{S(E_{0})\gamma_{0}^{2}}{1 + S'(E_{0})\gamma_{0}^{2}}$ $\gamma_{obs}^{2} = \frac{\gamma_{0}^{2}}{1 + S'(E_{0})\gamma_{0}^{2}}$



Several poles (N>1)

 $1 - S(E_r)R(E_r) = 0$ Must be solved numerically

Generalization of the Breit-Wigner formalism: link between observed and formal parameters when *N*>1

C. Angulo, P.D., Phys. Rev. C **61**, 064611 (2000) – single channel C. Brune, Phys. Rev. C **66**, 044611 (2002) – multi channel

Examples: ¹²C+p and ¹²C+ α

Narrow resonance: ¹²C+p

¹² C+p ($E^r = 0.42$ MeV, $\Gamma = 32$ keV, $J = 1/2^+, \ell = 0$)					
	$a = 4 \mathrm{fm}$	a = 5 fm	$a = 6 \mathrm{fm}$	$a = 7 \mathrm{fm}$	
γ_{obs}^2 (MeV)	1.09	0.59	0.35	0.23	
E_0 (MeV)	-2.15	-0.61	-0.11	0.11	
γ_0^2 (MeV)	3.09	1.16	0.57	0.32	



Broad resonance: ${}^{12}C+\alpha$

	a = 5 fm	a = 6 fm	a = 7 fm
γ_{obs}^2 (MeV)	0.57	0.28	0.16
E_0 (MeV)	0.49	1.92	2.22
γ_0^2 (MeV)	1.17	0.37	0.19

 $^{12}\mathrm{C}{+}\alpha$ ($E^r=2.42$ MeV, $\Gamma=0.42$ MeV, $J=1^-,\ell=1$)



¹⁸Ne+p elastic scattering: C. Angulo et al, Phys. Rev. C67 (2003) 014308

• Experiment at Louvain-la-Neuve: ¹⁸Ne+p elastic

 \rightarrow search for the mirror state of ¹⁹O(1/2⁺)



$$\frac{d\sigma}{d\Omega} = \frac{1}{4k^2} \left| \sum_{l} (2l+1)(\exp(2i\delta_l - 1)P_l(\cos\theta)) \right|^2$$

- Phase shifts d_I defined in the Rmatrix (in principle from *ℓ*=0 to ∞)
- *ℓ*=0: one pole with 2 parameters: energy E₀ reduced width γ₀
- *ℓ*=1, no resonance expected
 →hard-sphere phase shift
- ℓ=2 (J=3/2⁺,5/2⁺): very narrow resonances expected
 →weak influence
- *l*>2: hard sphere
- → The cross section is fitted with 2 parameters








Data analysis: general procedure for elastic scattering

$$\frac{d\sigma}{d\Omega} = \sum_{K_1, K_2, K'_1, K'_2} |f_{K_1 K_2, K'_1 K'_2}(\theta)|^2$$

$$f_{K_1 K_2, K'_1 K'_2}(\theta) = \sum_{J, \pi} \sum_{lI, l'I'} ... U_{lI, l'I'}^{J, \pi} Y_{l'}(\theta, 0)$$

•Only unknown quantity

•To be obtained from models

Problem: how to determine the collision matrix U?

Consider each partial wave Jp



Simple case: ¹⁸Ne+p: spins $I_1=0^+$ and $I_2=1/2^+$ collision matrix 1x1

J	l	
1/2+	0	R matrix: one pole (2 parameters) <i>but could be 3 (background)</i>
1/2-	1	No resonance →Hard sphere
3/2+	2	Very narrow resonance → Hard sphere
3/2-	1	No resonance \rightarrow Hard sphere
≥5/2	≥2	Neglected

More complicated : ⁷Be+p: spins $I_1=3/2^-$ and $I_2=1/2^+$ collision matrix: size larger that one (depends on J)



	J	I, l	
	0+	1,1	No resonance→hard sphere
	0-	2,2	No resonance \rightarrow hard sphere
	1+	1,1 2,1 2,3	 •Res. at 0.63 MeV → Rmatrix I=1 OR I=2 •Channel mixing neglected (U_{ij}=0 for i≠j)
	1-	1,0 1,2 2,2	 Channel mixing neglected <i>l</i>=0: scattering length formalism <i>l</i>=2: hard sphere
	2+	1,1 1,3 2,1 2,3	Channel mixing neglectedHard sphere
	2-	1,2 2,0 2,2 2,4	 Channel mixing neglected <i>l</i>=0: scattering length formalism <i>l</i>=2,4: hard sphere

Finally, 4 parameters: E_R and Γ for the 1⁺ resonance, 2 scattering lengths 75

Other processes: capture, transfer, inelastic scattering, etc.





Example of transfer reaction: ⁶Li(p,a)³He (Nucl. Phys. A639 (1998) 733)

$$R = \begin{pmatrix} R_{pp} & R_{p\alpha} \\ R_{\alpha p} & R_{\alpha \alpha} \end{pmatrix}, \text{ with } R_{\alpha p} = R_{p\alpha}$$

Non-resonant reaction: R matrix=constant

Collision matrix
$$U = \begin{pmatrix} U_{pp} & U_{p\alpha} \\ U_{\alpha p} & U_{\alpha \alpha} \end{pmatrix}$$
, deduced from the R matrix

Cross section:
$$\sigma \sim |U_{pa}|^2$$



Radiative capture



Capture reaction=transition between an initial state at energy E to bound states Cross section ~ $|\langle \Psi_{f}|H_{\gamma}|\Psi_{i}(E)\rangle|^{2}$ Additional pole parameter: gamma width $\langle \Psi_{f}|H_{\gamma}|\Psi_{\iota}(E)\rangle = \langle \Psi_{f}|H_{\gamma}|\Psi_{i}(E)\rangle_{int} + \langle \Psi_{f}|H_{\gamma}|\Psi_{i}(E)\rangle_{ext}$ with $\langle \Psi_{f}|H_{\gamma}|\Psi_{i}(E)\rangle_{int}$ depends on the poles $\langle \Psi_{\phi}|H_{\gamma}|\Psi_{\iota}(E)\rangle_{ext}$ =integral involving the external w.f.

More complicated than elastic scattering! But: many applications in nuclear astrophysics

Microscopic models

• A-body treatment:

$$H = \sum_{i=1}^{A} T_i + \sum_{i< j=1}^{A} V_{ij}$$

with

- $T_{\rm i}$ = kinetic energy of nucleon i
- V_{ii} = nucleon nucleon interaction
- wave function completely antisymmetric (bound and scattering states)
- not solvable when A>3
- Generator Coordinate Method (GCM) basis functions $\Phi_i^{\ell m} = \mathcal{A}\phi_1\phi_2\Gamma_\ell(\rho, R_i)Y_\ell^m(\Omega)$
 - with $\phi_1, \phi_2 =$ internal wave functions $\Gamma_{\ell}(\rho, R) =$ gaussian function R=generator coordinate (variational parameter) $\rho =$ nucleus-nucleus relative coordinate
- At ρ =a, antisymmetrization is negligible \rightarrow the same R-matrix method is applicable

6. Conclusions

- 1. One R-matrix for each partial wave (limited to low energies)
- 2. Consistent description of resonant and non-resonant contributions (not limited to resonances!)
- 3. The R-matrix method can be applied in two ways
 - a) To solve the Schrödinger equation
 - b) To fit experimental data (low energies, low level densities)
- 4. Applications a)
 - Useful to get phase shifts and wave functions of scattering states
 - Application in many fields of nuclear and atomic physics
 - 3-body systems
 - Stability with respect to the radius is an important test
- 5. Applications b)
 - Same idea, but the pole properties are used as free parameters
 - Many applications: elastic scattering, transfer, capture, beta decay, etc.