What did we learn from the microscopic model of collisions?

TRIUMF, 18 February 2014

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Outline

- Introduction
- Resonating-Group method (RGM)
- Generator-Coordinate method (GCM)
- Forbidden and almost forbidden states
- A question about No-Core Shell Model
- Conclusion

Introduction

- The microscopic cluster model of collisions known as RGM or GCM is the ancestor of present *ab initio* descriptions

- Main feature:
  Pauli antisymmetrization of scattering states
  Indistinguishable particles ⇒ non-locality

- Can some aspects of its evolution be useful now for the NCSM-RGM ?

- It started in 1937…

Two 1937 papers at the origin of the MCM of collisions

DECEMBER 1, 1937 PHYSICAL REVIEW VOLUME 52

Molecular Viewpoints in Nuclear Structure

JOHN ARCHIBALD WHEELER[1]
University of North Carolina, Chapel Hill, North Carolina

(Received August 17, 1937)

Why 'resonating'?
→ not related to the notion of resonance
= antisymmetric
= microscopic

binding energy of H^3. Application of the same type of approximate wave function to the description of nuclear structure in general, gives rise to the concept of resonating group structure. This picture regards the constituent neutrons and protons as divided into various groups (such as alpha-particles) which are continually being broken and reformed in new ways. Group theory gives information as

⇒ group = cluster

The wave function of the whole system has the proper antisymmetry when written in the form

$$\Psi(1,\cdots\mathbf{N}) = \sum_{\text{dist}} F\left(\frac{1+2+3+4}{4}, \frac{5+6+7+8}{4}, \cdots\right)\Phi(1234)\Phi(5678)\cdots \quad (7)$$

⇒ RGM wave function

Here Φ is the wave function for a single alpha-particle, completely antisymmetrical[9] with re-

Non locality in collisions !

DECEMBER 1, 1937 PHYSICAL REVIEW VOLUME 52

On the Mathematical Description of Light Nuclei by the Method of Resonating Group Structure

JOHN A. WHEELER
University of North Carolina, Chapel Hill, North Carolina
(Received August 17, 1937)

The wave function for the composite nucleus is written as a properly antisymmetrized combination of partial wave functions, corresponding to various possible ways of distributing the neutrons and protons into various groups, such as alpha-particles, di-neutrons, etc. The dependence of the total wave function on the intergroup separations is determined by the variation principle. The analysis is carried out in detail for the case that the configurations

we obtain the radial wave equations of the method of resonating group structure:

$$[(\hbar^2/2\mu_i)(d^2/dr^2-L(L+1)/r^2)+E-E_i]f_J(iLSr)$$

$$=\sum_{jL'S'}\int H_J(iLSr;jL'S'\rho)f_J(jL'S'\rho)d\rho$$

$$=g_J(iLSr), \quad (25)$$

RGM equation
(non locality)

ELASTIC SCATTERING

The collision of H^1 and H^3 with energy too small to form n^1+He^3 comes under case B. For every given E, Eqs. (25) will now possess a solution. The wave functions for configurations

Application to collisions

Resonating-group method (RGM)

Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m_N} - T_{\rm CM} + \sum_{i>j=1}^{A} (V_{ij}^N + V_{ij}^C) + \dots$$

Cluster wave functions

ϕ_1, ϕ_2 : frozen functions depending on A_1-1 and A_2-1 internal coordinates (antisymmetric, translation invariant, good angular momentum and parity)

- based in general on the harmonic-oscillator shell model
- often with the simplifying assumption: same oscillator parameters

Relative coordinate

$$\boldsymbol{\rho} = \frac{1}{A_1}(\boldsymbol{r}_1 + \dots + \boldsymbol{r}_{A_1}) - \frac{1}{A_2}(\boldsymbol{r}_{A_1+1} + \dots + \boldsymbol{r}_A)$$

Not a physical observable ! (not fully symmetric)
$\Rightarrow$ at the origin of non locality

Resonating-group wave function (single channel)

$$\Psi = \mathcal{A}\phi_1\phi_2 g(\boldsymbol{\rho}) + \dots$$

g has no physical meaning, except asymptotically (phase shift)

Assumptions of the RGM

Forces
- restricted to effective forces by the cluster assumption
- exchange terms of Coulomb interaction often neglected

Example: in α+p with a simple $(0s)^4$ harmonic-oscillator α cluster
- matrix elements of the tensor interaction vanish
- very slow convergence if repulsive core

Channels
- few channels
- possibility of additional shell-model terms

Main initial difficulty of the RGM
- painful treatment of antysymmetrization

Example: d + n $\quad \boldsymbol{\rho} = \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2) - \boldsymbol{r}_3 \qquad \boldsymbol{\xi} = \boldsymbol{r}_1 - \boldsymbol{r}_2$

$$P_{13}\,\boldsymbol{\rho} = \frac{1}{2}(\boldsymbol{r}_3 + \boldsymbol{r}_2) - \boldsymbol{r}_1 = -\frac{1}{2}\boldsymbol{\rho} - \frac{3}{4}\boldsymbol{\xi} \qquad P_{13}\,\boldsymbol{\xi} = \boldsymbol{r}_3 - \boldsymbol{r}_2 = -\boldsymbol{\rho} + \frac{1}{2}\boldsymbol{\xi}$$

Resonating-group equation

$$\left[-\frac{\hbar^2}{2\mu}\Delta + V_D(\rho)\right] g(\boldsymbol{\rho}) + \int_0^\infty \left[K^H(\boldsymbol{\rho},\boldsymbol{\rho}') + EK^N(\boldsymbol{\rho},\boldsymbol{\rho}')\right] g(\boldsymbol{\rho}')d\boldsymbol{\rho}' = Eg(\boldsymbol{\rho})$$

Problems:

- Determination of Hamiltonian K^H and norm K^N kernels
  Calculations were non systematic
  Early calculations of α + α scattering contained errors
  Solution: generator coordinates

- Coulomb term
  The Coulomb interaction was approximated by its direct term
  Solution: Gaussian expansion

- Numerical resolution of integro-differential equation
  Finite differences inaccurate
  Solution: computational *R*-matrix method on a Lagrange mesh
  M. Hesse, J. Roland, DB, Nucl. Phys. A 709 (2002) 184

- Forbidden states → ill-conditioned, instability of solutions
  Many tests of numerical tricks (weak imaginary term, …)
  Solution: elimination of poles of *R* matrix

Accurate RGM calculations for collisions

- Wildermuth and Tang 1977 (no generator coordinates)

- Tang 1981 (use of complex generator coordinates)

- Multichannel RGM (Y.C. Tang, Y. Fujiwara, …)

Conclusion:
An important step is the introduction of the generator coordinate method (GCM):
Calculations became systematic and heavier systems became accessible.

Questions:
- Is something like the GCM possible in *ab initio* calculations?
- Are (almost) forbidden states a problem?

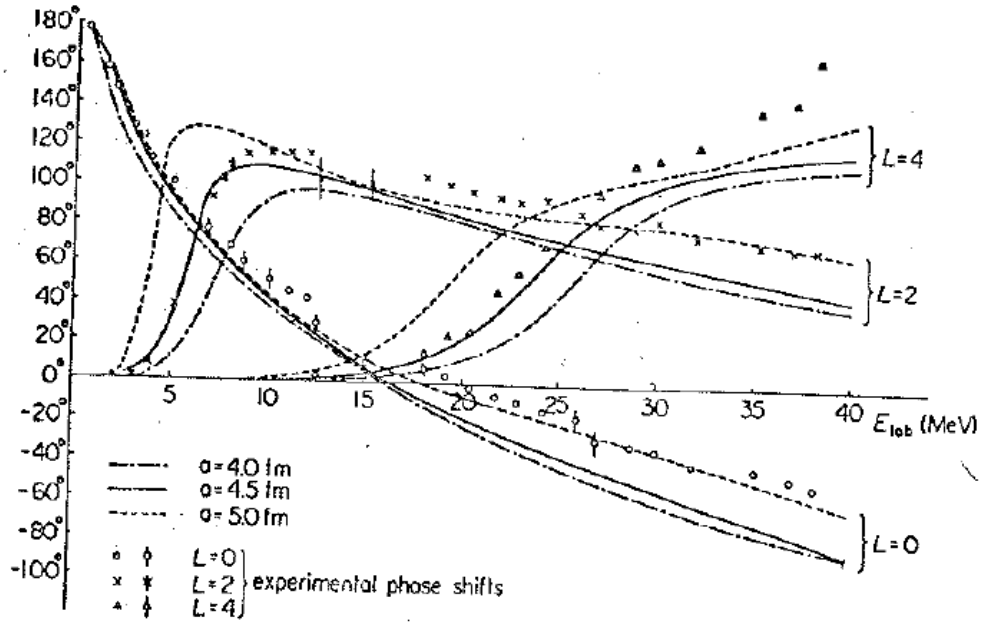
⇒ would the advantages of the GCM still be useful?

Generator-coordinate method (GCM)

1970: H. Horiuchi, B. Giraud

α + α scattering

H. Horiuchi, Prog. Theor. Phys. 43 (1970) 375



- Qualitatively nice results with only 5 values of the generator coordinate
- But instability with respect to channel radius
- Corrected in the Microscopic *R*-matrix method ⇒ more economical than RGM

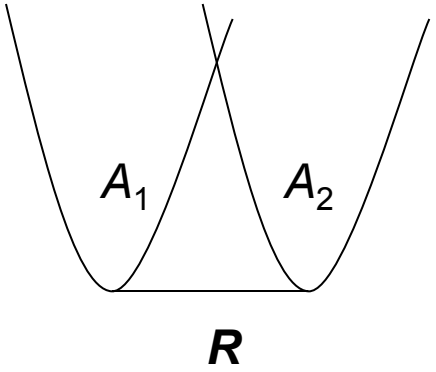
  DB, P.-H. Heenen, Nucl. Phys. A 233 (1974) 304

Generator-coordinate method (GCM)

Slater determinant in the two-centre harmonic-oscillator shell model

$$\Phi(\boldsymbol{R}) = \mathcal{A}\Phi_1\left(-\frac{A_2}{A}\boldsymbol{R}\right)\Phi_2\left(\frac{A_1}{A}\boldsymbol{R}\right)$$
$$= \varphi_{\rm CM}\mathcal{A}\phi_1\phi_2\Gamma(\boldsymbol{\rho}-\boldsymbol{R})$$

shifted Gaussian



Relation with RGM

$$\Psi = \mathcal{A}\phi_1\phi_2 g(\boldsymbol{\rho})$$
$$\varphi_{\rm CM}\Psi = \int d\boldsymbol{R} f(\boldsymbol{R})\Phi(\boldsymbol{R})$$
$$g(\boldsymbol{\rho}) = \int d\boldsymbol{R} f(\boldsymbol{R})\Gamma(\boldsymbol{\rho}-\boldsymbol{R})$$

Hill-Wheeler equation (formal presentation : never used !)

$$\int [H(\boldsymbol{R},\boldsymbol{R}') - EN(\boldsymbol{R},\boldsymbol{R}')] f(\boldsymbol{R}')d\boldsymbol{R}' = 0$$

Systematic calculation of kernels !

In practice:

- Projection on angular momentum
- Finite expansion

$$\varphi_{\rm CM}\Psi_{lm} = \sum_{j=1}^{N} f_{lj}\Phi_{lm}(R_j)$$

(freedom of choice of generator coordinates R_j)

- Variational equations

$$\sum_{j=1}^{N}[H_l(R_i,R_j) - EN_l(R_i,R_j)]f_{lj} = 0$$

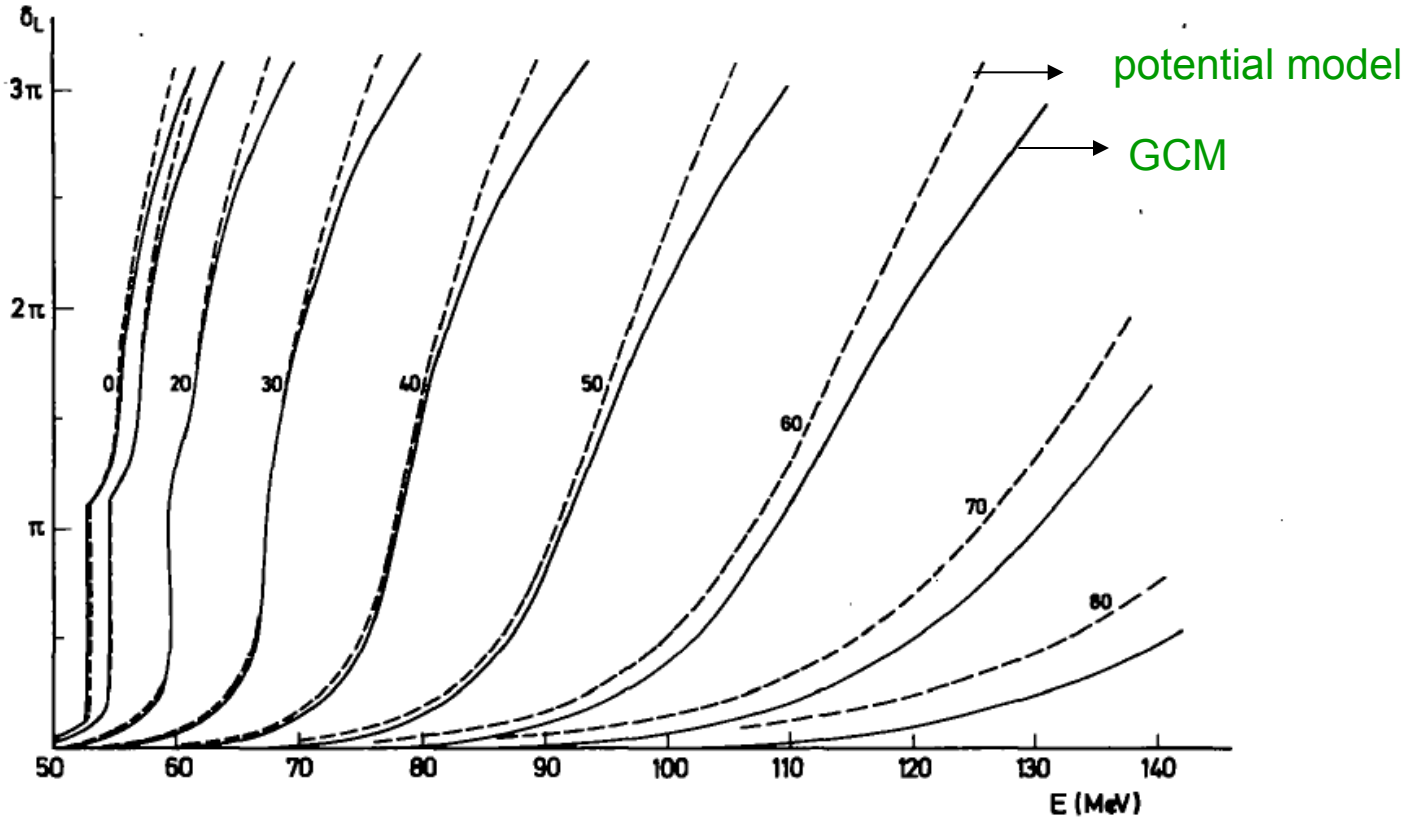
- *R*-matrix technique or similar for the continuum
  (GCM expansion in the internal region and connection with correct asymptotics: microscopic R-matrix method)

Advantages of the GCM

- Systematic calculations with Slater determinants (analytical and/or numerical)
- No more problem with Coulomb (exact calculation possible)
- No problem with forbidden states (automatically eliminated) or almost forbidden states
- Heavier clusters accessible
- Multichannel

Collisions between p- and sd-shell nuclei possible with GCM

L = 0 - 80 phase shifts of single-channel
^{40}Ca + ^{40}Ca elastic scattering



DB, Y. Salmon, Nucl. Phys. A 323 (1979) 521

Main advantage of the GCM

- equivalent to RGM but more economical
  to derive and easier to solve

Difficulty

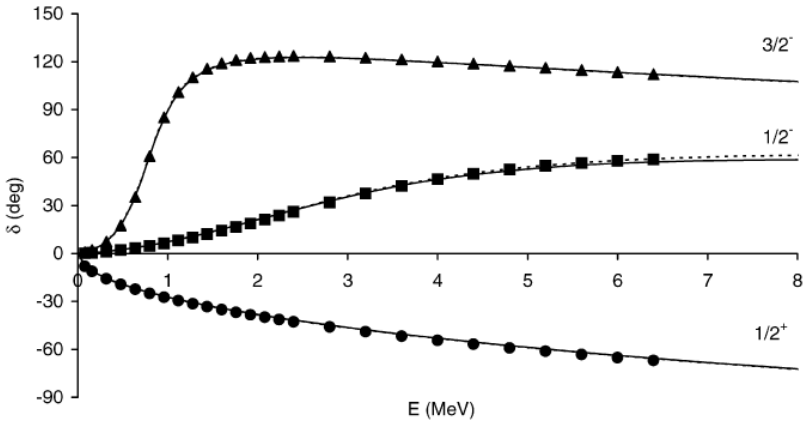
- wrong asymptotics (Gaussian)
- corrected with microscopic R-matrix method

Main applications

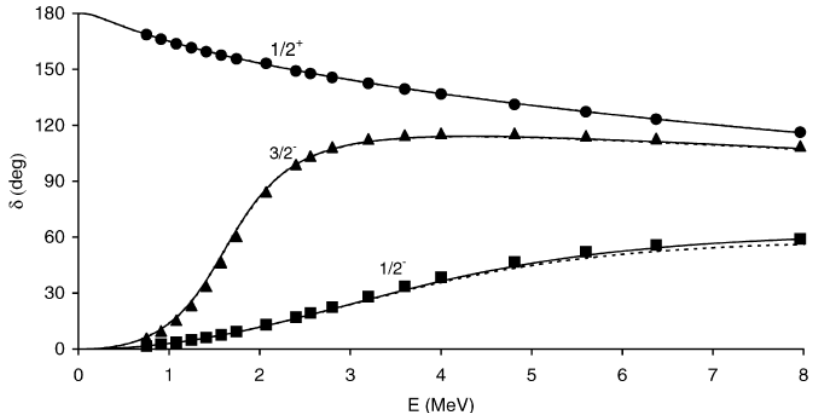
- elastic scattering
- radiative capture
- beta decay with cluster emission
- …

Simple example of GCM

α + n scattering



α + p scattering

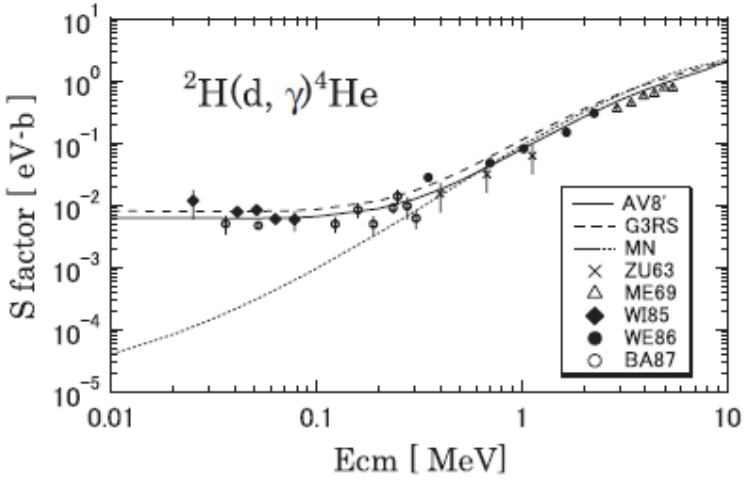


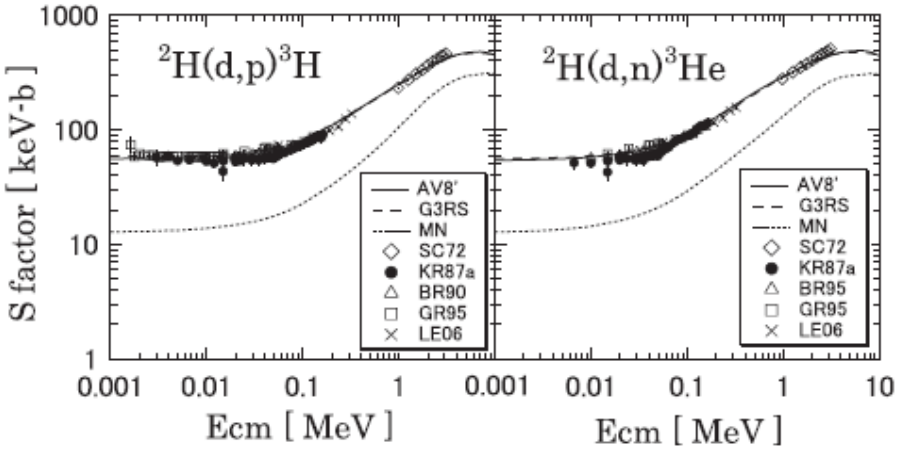
Minnesota
effective force
u = 0.96
+
zero-range spin-orbit
S_0 = 35.6/35.5

R. Kamouni, DB, Nucl. Phys. A 791 (2007) 68

GCM without cluster assumption: d + d reactions

Multichannel:
physical states
+ pseudostates





AV8'
+ effective
3-body force
+ Coulomb

no parameters

K. Arai, S. Aoyama, Y. Suzuki, P. Descouvemont, DB, Phys. Rev. Lett. 107 (2011) 132502

Forbidden and almost forbidden states

Non-zero relative functions may exist for which the antisymmetric RGM wave functions vanish

$$\mathcal{A}\phi_1\phi_2 g^{FS}(\boldsymbol{\rho}) = 0$$

- Solutions of the RGM equation at all energies

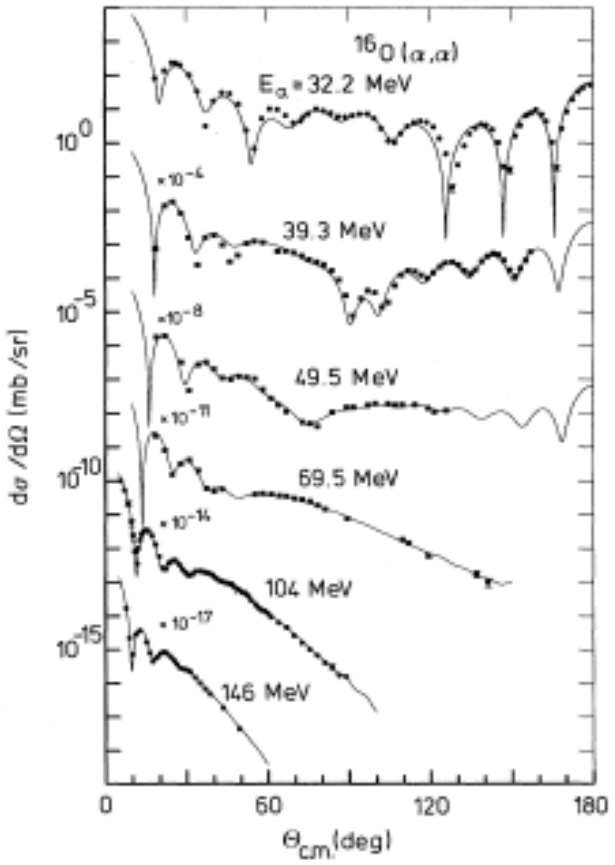
- « Pollute » the (non-physical) RGM relative functions *g* but not the fully antisymmetric (physical) wave functions

- Only exist:

- for the two-centre harmonic-oscillator model
- with equal size parameters

- Then, do they have a physical importance? Surprisingly, the answer is yes

Global potential for α + ^{16}O scattering:
deep potential simulating the forbidden states

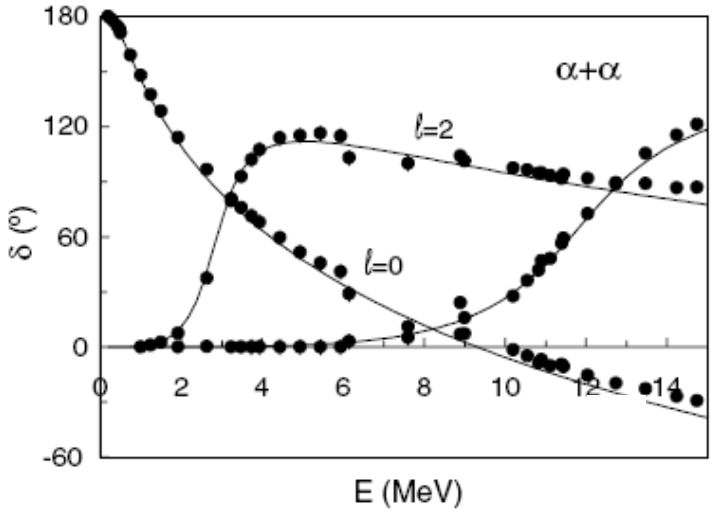


F. Michel et al, Phys. Rev. C 28 (1983) 1904

Role of forbidden states in α + α scattering

GCM with equal oscillator parameters

m_l forbidden states
(m_0 = 2, m_2 = 1, m_4 = 0)



Levinson-Swan theorem

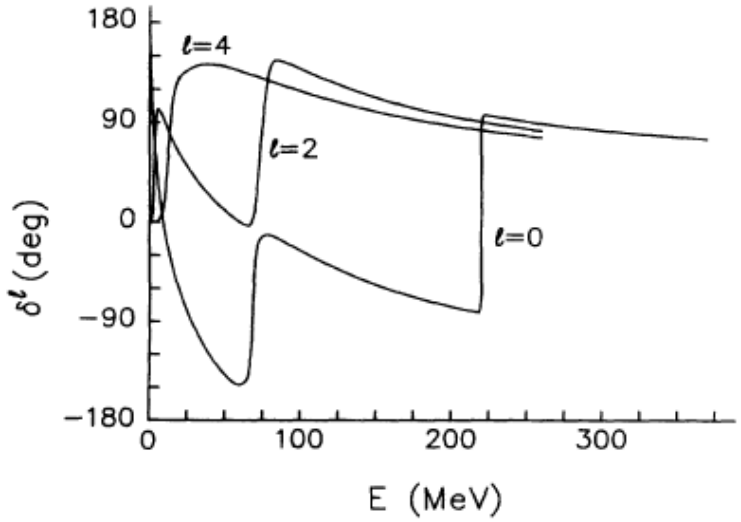
$$\delta_l(0) - \delta_l(\infty) = (n_l + m_l)\pi$$

P. Descouvemont, DB, Rep. Prog. Phys. 73 (2010) 036301

The accuracy of the low-energy behaviour is strongly related to the physical behaviour of the Levinson theorem

α+α scattering
GCM with non-harmonic monopolar distortion

No forbidden states… but almost forbidden states (AFS)



Different Levinson theorem

$$\delta_l(0) - \delta_l(\infty) = n_l \pi$$

but same behavior at low energies

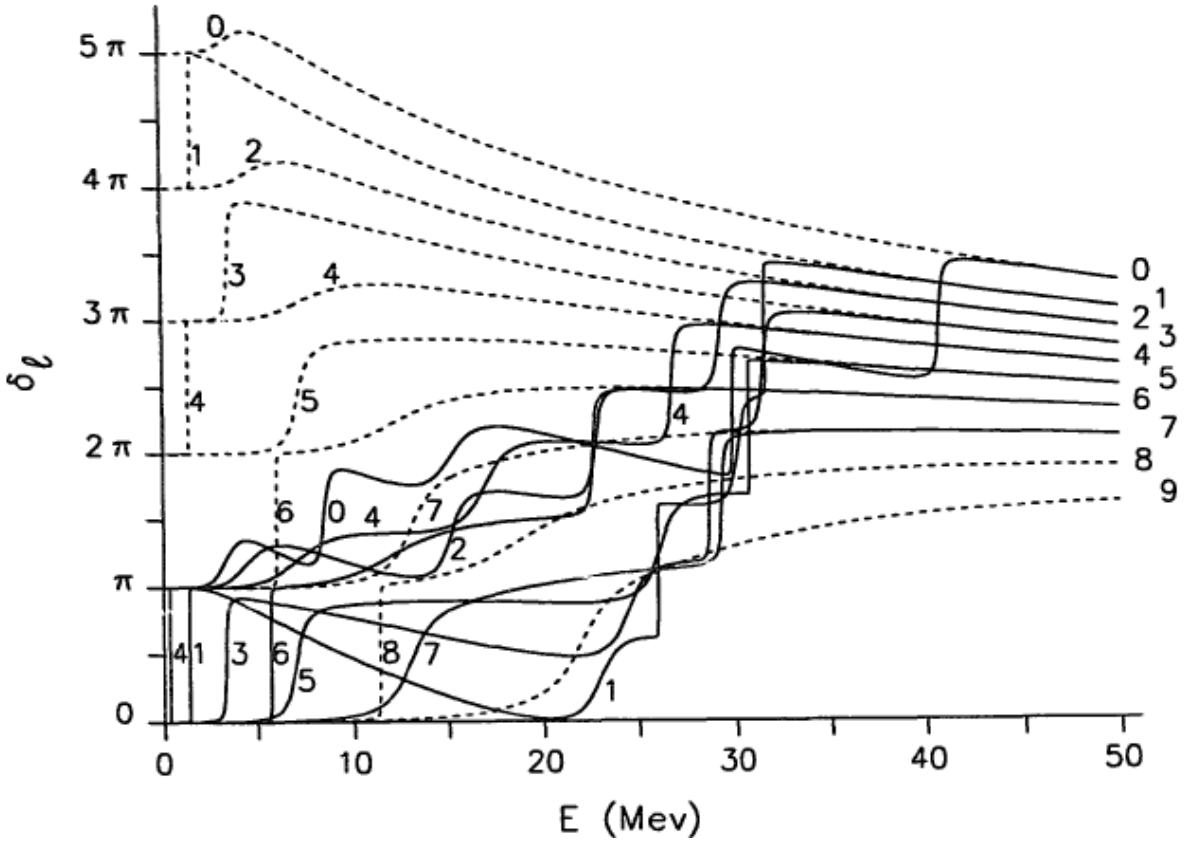
DB, M. Kruglanski, Phys. Rev. C 45 (1992) 1321

- AFS easily identified at high energies

- If AFS at low energies: 'Pauli resonances'
  (can be mixed up with physical resonances ⇒ α + ^{16}O example)

GCM calculation of α + ^{16}O scattering with $b_\alpha \neq b_O$

22 generator coordinates



Full lines: with Pauli resonances
Dashed lines: after elimination of AFS

M. Kruglanski, DB, Nucl. Phys. A548 (1992) 39

Elimination of Pauli resonances in GCM

Eigenvalues of norm kernel

$$\sum_j [N_l(R_i, R_j) - \mu_{ln} n_l(R_i, R_j)] C_{lnj} = 0$$

$$N_l(R', R) = \langle \Phi_{lm}(R') | \Phi_{lm}(R) \rangle = \langle \varphi_{\rm CM} \mathcal{A} \phi_1 \phi_2 \Gamma_l(\rho, R') | \varphi_{\rm CM} \mathcal{A} \phi_1 \phi_2 \Gamma_l(\rho, R) \rangle$$

$$n_l(R', R) = \langle \Gamma_l(\rho, R') | \Gamma_l(\rho, R) \rangle$$

K. Varga, R.G. Lovas, Phys. Rev. C 37 (1988) 2906

New GCM basis

$$\tilde{\Phi}_{nlm} = (\mu_{ln})^{-1/2} \sum_j C_{lnj} \Phi_{lm}(R_j)$$

- m_l basis states corresponding to small eigenvalues are dropped
  $\Rightarrow$ elimination of Pauli resonances

Is there an equivalent of the RGM to GCM transition
for the No-Core Shell Model description of collisions?

$$g(\boldsymbol{\rho}) = \int g(\boldsymbol{R})\delta(\boldsymbol{\rho} - \boldsymbol{R})d\boldsymbol{R} \quad \longrightarrow \quad g(\boldsymbol{\rho}) = \int f(\boldsymbol{R})e^{-(\boldsymbol{\rho}-\boldsymbol{R})^2/b^2}d\boldsymbol{R}$$

- Can it simplify the calculations?
  - no need to transform the RGM equation

$$\mathcal{H}g = E\mathcal{N}g$$

into a Schrödinger-like equation

$$\mathcal{N}^{-1/2}H\mathcal{N}^{-1/2}\hat{g} = E\hat{g}$$

- no need for RGM wave function $\hat{g} = \mathcal{N}^{1/2}g$
  (calculations performed with Slater determinants)

- Can it reduce computer times?
  - possibly smaller number of generator coordinates
    (freedom of choice)

- Are there (almost) forbidden states? (elimination possible)

Conclusion

- Many successes of the microscopic cluster model of collisions with few parameters in an effective force
- Model specially useful for applications involving bound and scattering states simultaneously
- Forbidden states explain deep potentials

- Is a GCM-like extension possible for NCSM-RGM calculations?
- Would it be useful?