# Microscopic cluster models I

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2. Important concepts: isospin, antisymmetrization
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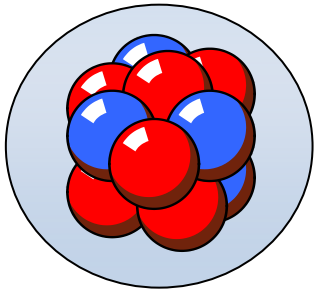
# 1. Introduction

## Definition of a microscopic model



- **Wave functions**
  - fully antisymmetric
  - Depend on all nucleon coordinates → complicated many-body problem!
  - Exchange of particles i and j
    Pauli principle

$$P_{ij}\Psi(1,2,\dots i,\dots j,\dots A) = -\Psi(1,2,\dots j,\dots i,\dots A)$$

- **Hamiltonian**
  - given by

$$H = \sum_i T_i + \sum_{j>i} V_{ij} + \sum_{k>j>i} V_{ijk} + \cdots$$

with
$T_i$ = kinetic energy of nucleon *i*
$V_{ij}$ = two-body nucleon-nucleon interaction
- Contains a nuclear part $V_{ij}^N$: short range
- Contains a coulomb part $V_{ij}^C$: long range $\sim e^2/r$

$V_{ijk}$=three-body interaction (often neglected)

# 1. Introduction

**Main advantages**

- Predictive power: in principle there is no parameter
- Coherent description of different processes:
  - spectroscopy (energies, radii, electromagnetic transitions, etc.)
  - scattering (elastic, transfer, radiative capture, etc. )

**Main problems**

- $V_{ij}^{N}$ is not exactly known
  → approximations, **effective** NN interaxctions (adapted to the model)
- The Schrödinger equation may involve many terms (A(A-1)/2)
  → cannot be solved exactly
- Difficult to apply to scattering states

→ **various models**

- Shell model (and extensions: No-core shell model)
- Fermionic Molecular Dynamics
- Cluster models: Resonating Group Method (RGM), Generator Coordinate Method (GCM)

Important concepts for (all) microscopic models:

2. Antisymmetrization, isospin formalism
3. Nucleon-nucleon interactions

# 2. Isospin, Antisymmetrization

## A. Isospin formalism

- The wave functions depend on all nucleon coordinates:
  - Space $\boldsymbol{r}$
  - Spin $\boldsymbol{s}$
  - Isospin $\boldsymbol{t}$

- Isospin formalism
  masses of neutron and proton very similar: $m_n$=939.57 MeV, $m_p$=938.27 MeV
  difference: 0.14%
  Charge symmetry : $V_N^{pp} \approx V_N^{nn}$ for the nuclear interaction
  but: $V_C^{pp} \neq V_C^{nn}$ for the Coulomb interaction

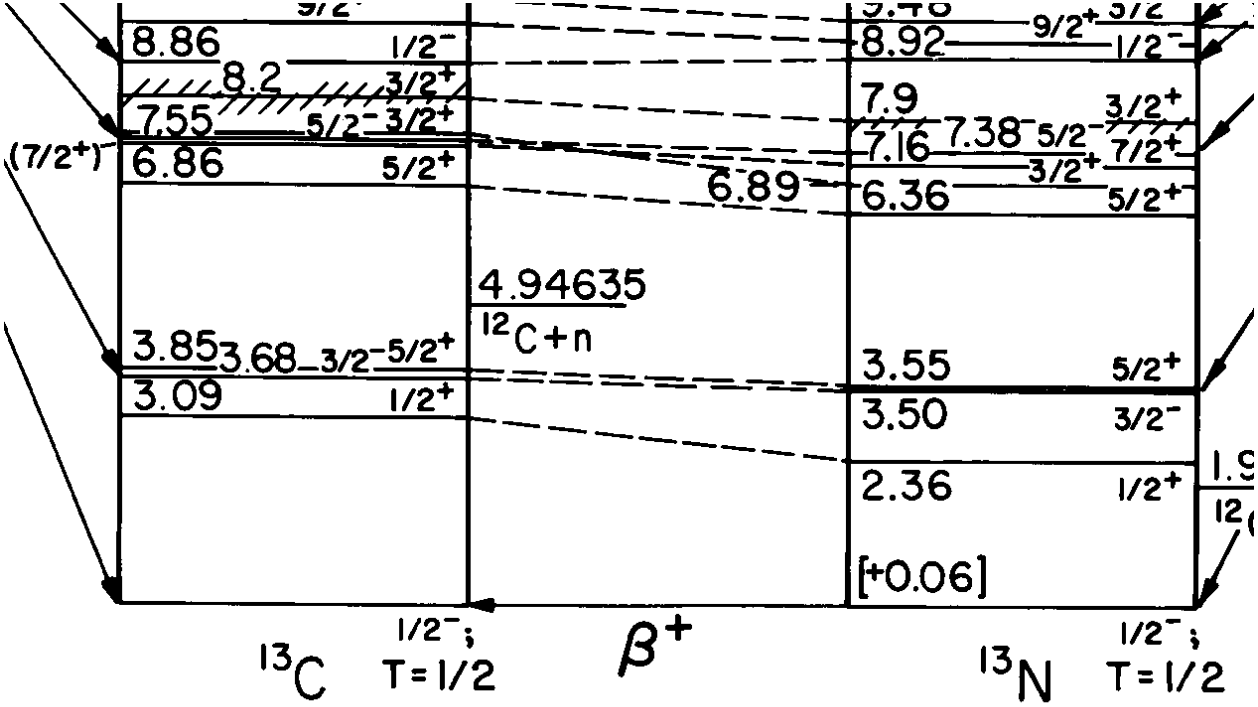
- neutron and proton are two states of a single particle: the nucleon
  nucleon= particle with isospin $t = 1/2$
  neutron $t_z = +1/2$
  proton $t_z = -1/2$
  → for the nucleus $T_z = \frac{N-Z}{2}, T \geq |T_z|\ , T = |T_Z|, |T_Z| + 1, \ldots$

- For two nucleons $T = t_1 + t_2$
  → $T = 0, T_z = 0$ (deuteron)
  → $T = 1, T_z = -1,0,1$ (diproton, dineutron, deuteron excited: unbound)

# 2. Isospin, Antisymmetrization

Nuclei: $^{13}$C (Z=6, N=7)– $^{13}$N (Z=7, N=6) :

$T_z = +1/2, -1/2$: mirror nuclei, similar spectra

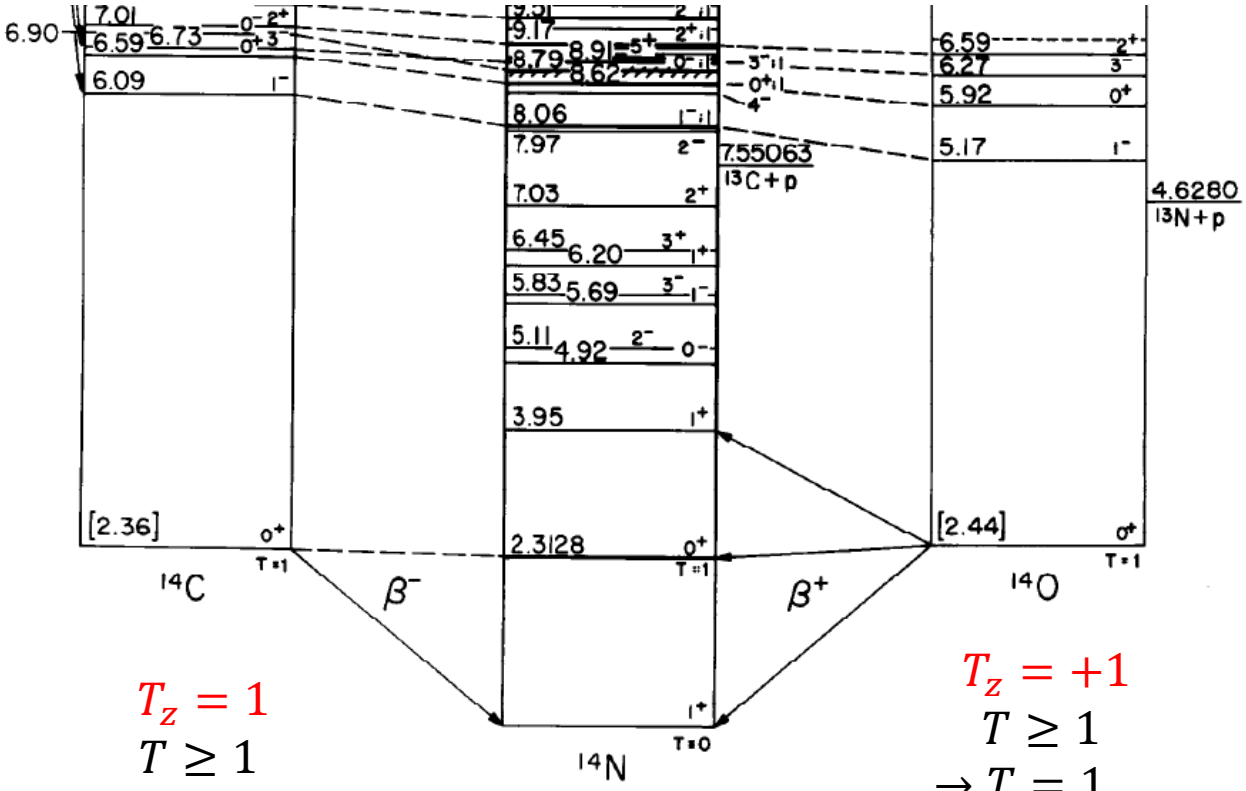



$T_z = 1/2$
$T \geq 1/2$

$T_z = -1/2$
$T \geq 1/2$

# 2. Isospin, Antisymmetrization

Other example: $^{14}C$ ($T_z$=1), $^{14}N$ ($T_z$=0), $^{14}O$ ($T_z$=-1)




$T_z = 1$

$T \geq 1$

$\rightarrow T = 1, \ldots$

$T_z = 0$

$T \geq 0$

$\rightarrow T = 0,1, \ldots$

$T_z = +1$

$T \geq 1$

$\rightarrow T = 1, \ldots$

## B. Antisymmerization

- Each nucleon has an individual wave function

$$\phi_{m_s m_t}(\boldsymbol{r}) = \phi(r)|\frac{1}{2}m_s> |\frac{1}{2}m_t>$$

| Space | Spin | Isospin |
|---|---|---|
| Example: gaussian | $m_s = \pm\frac{1}{2}$ | $m_t = \pm\frac{1}{2}$ |

- Total wave function of the system: $\Psi(1,2,\dots,A) = \phi_1(\boldsymbol{r_1})\phi_2(\boldsymbol{r_2})\dots\phi_A(\boldsymbol{r_A})$
  The spin and isospin coordinates are implied

- Pauli principle $P_{ij}\Psi(1,2,\dots i,\dots j,\dots A) = -\Psi(1,2,\dots j,\dots i,\dots A)$
  $P_{ij}$: exchanges particles i and j
  → the total wave function must be: $\Psi(\boldsymbol{r_1},\boldsymbol{r_2},\dots\boldsymbol{r_A}) = \mathcal{A}\phi_1(\boldsymbol{r_1})\phi_2(\boldsymbol{r_2})\dots\phi_A(\boldsymbol{r_A})$

  Operator $\mathcal{A}$: defines all possible permutations between A elements (A!)

$$\mathcal{A} = \sum_{p=1}^{A!} \epsilon_p P_p$$

where $P_p$ = permutation of the A elements
$\epsilon_p$ = sign of the permutation

# 2. Isospin, Antisymmetrization

- Antisymmetrization operator

$$\mathcal{A} = \sum_{p=1}^{A!} \epsilon_p P_p$$

- Examples
  - 2 particles: $\mathcal{A} = 1 - P_{12}$ (2 terms : 2!)
  - 3 particles: $\mathcal{A} = 1 + P_{231} + P_{312} - P_{132} - P_{213} - P_{321}$ (6 terms: 3!=6)
  - 4 particles: 24 terms (4!)

- Important property : $\mathcal{A}^2 = A!\,\mathcal{A}$
  Example for 2 particles:

$$\mathcal{A}^2 = (1 - P_{12})(1 - P_{12}) = 1 - 2P_{12} + (P_{12})^2 = 2 - 2P_{12} = 2\mathcal{A}$$

- Slater determinant

$$\Psi(\boldsymbol{r_1},\dots,\boldsymbol{r_A}) = \mathcal{A}\phi_1(\boldsymbol{r_1})\phi_2(\boldsymbol{r_2})\dots\phi_A(\boldsymbol{r_A}) = \begin{bmatrix} \phi_1(\boldsymbol{r_1}) & \cdots & \phi_A(\boldsymbol{r_1}) \\ \vdots & \ddots & \vdots \\ \phi_1(\boldsymbol{r_A}) & \cdots & \phi_A(\boldsymbol{r_A}) \end{bmatrix}$$
$$= \det|\phi_1 \dots \phi_A|$$

vanishes if two rows or two columns are identical (fermions)

- 2 particles $\Psi(\boldsymbol{r_1},\boldsymbol{r_2}) = \mathcal{A}\phi_1(\boldsymbol{r_1})\phi_2(\boldsymbol{r_2})$
$$= \det|\phi_1\phi_2|$$
$$= \phi_1(\boldsymbol{r_1})\phi_2(\boldsymbol{r_2}) - \phi_1(\boldsymbol{r_2})\phi_2(\boldsymbol{r_1})$$
$$= \begin{vmatrix} \phi_1(\boldsymbol{r_1}) & \phi_2(\boldsymbol{r_1}) \\ \phi_1(\boldsymbol{r_2}) & \phi_2(\boldsymbol{r_2}) \end{vmatrix}$$

- Example: $\alpha$ particle: 4x4 determinant
  - Common radial part (shell model: gaussian function) $\phi_0(r) = \exp(-r^2/2b^2)$
  - 2 possibilities for the isospin (neutron, proton)
  - 2 possibilities for the spin (up, down)
  - $\Psi = \det|\phi_0 n\uparrow \;\; \phi_0 n\downarrow \;\; \phi_0 p\uparrow \;\; \phi_0 n\downarrow|$

- Matrix elements between Slater determinants

2 Slater determinants

$\Psi = \mathcal{A}\psi_1\psi_2 \ldots \psi_A = \det|\psi_1 \ldots \psi_A|$
$\Phi = \mathcal{A}\phi_1\phi_2 \ldots \phi_A = \det|\phi_1 \ldots \phi_A|$

Quantities needed

- Overlap $< \Psi|\Phi >$

- One-body matrix elements $< \Psi|O_1|\Phi >$ , with $O_1 = \sum_{i=1}^{A} o(r_i)$
  example: kinetic energy

- Two-body matrix elements $< \Psi|O_2|\Phi >$ , with $O_2 = \sum_{i,j=1}^{A} o(r_i, r_j)$
  example: nucleon-nucleon interaction

**a) Overlap**

$$< \Psi|\Phi > = < \psi_1\psi_2 \dots \psi_A\mathcal{A}|\mathcal{A}\phi_1\phi_2 \dots \phi_A >$$

$$= A! < \psi_1\psi_2 \dots \psi_A|\mathcal{A}|\phi_1\phi_2 \dots \phi_A > \text{ (since } \mathcal{A}^2 = A!\,\mathcal{A})$$

$$= A! \begin{bmatrix} < \psi_1|\phi_1 > & \cdots & < \psi_1|\phi_A > \\ \vdots & \ddots & \vdots \\ < \psi_A|\phi_1 > & \cdots & < \psi_A|\phi_A > \end{bmatrix}$$

➔ Simple determinant with the invividual overlaps

➔ Factor $A!$ can be introduced in the wave function $\Psi \rightarrow (A!)^{-1/2}\Psi$

**b) One-body matrix elements**

One-body operator $O = \sum_{I=1}^{A} o(r_i)$

Example: kinetic energy: $T = \sum_i \left(-\frac{\hbar^2}{2m}\right) \Delta_i$

rms radius $< r^2 > = \frac{1}{A} \sum_i r_i^2$

Then $\langle \Psi | O | \Phi \rangle = \langle \psi_1 \cdots \psi_A | \mathcal{A} O \mathcal{A} | \varphi_1 \cdots \varphi_A \rangle$

$= \langle \psi_1 \cdots \psi_A | O \mathcal{A}^2 | \varphi_1 \cdots \varphi_A \rangle$

$= A! \langle \psi_1 \cdots \psi_A | O \mathcal{A} | \varphi_1 \cdots \varphi_A \rangle$

$= \sum_{ij} \langle \psi_i | o | \varphi_j \rangle M_{ij}$

with $M_{ij}$ = order one minor of the overlap matrix B

$$B = \begin{pmatrix} \langle \psi_1 | \varphi_1 \rangle & \cdots & \langle \psi_1 | \varphi_N \rangle \\ \vdots & & \vdots \\ \langle \psi_N | \varphi_1 \rangle & \cdots & \langle \psi_N | \varphi_N \rangle \end{pmatrix} \quad i \rightarrow M_{ij}, \quad j$$

**c) Two-body matrix elements**

2-body operator (NN interaction): $V = \sum_{i,j} v(r_i, r_j)$

$$\langle \Psi | V | \Phi \rangle = \sum_{ijkl} M_{ij,kl} \times \left[ \underbrace{\langle \psi_i \psi_j | v | \varphi_k \varphi_l \rangle}_{\text{Direct term}} - \underbrace{\langle \psi_i \psi_j | v | \varphi_l \varphi_k \rangle}_{\text{exchange term}} \right]$$

$M_{ij,kl}$ = order-two minor of the overlap matrix B

➔ **systematic calculations, well adapted to numerical calculations**

# 3. The nucleon-nucleon interaction

**A. 2-nucleon system:** wave function $\Psi(\boldsymbol{r_1}, \boldsymbol{r_2}, m_{s1}, m_{s2}, m_{t1}, m_{t2})$

Wave function antisymmetric : $P_{12}\Psi$=-$\Psi$

where $P_{12}$ exchanges the space, spin, and isospin coordinates

$\Psi_{LST}(\boldsymbol{r}) = \Phi_L(\boldsymbol{r})|SM_S > |TM_T >$ : factorization of space, spin, isospin

Relative orbital momentum $\boldsymbol{L}$, total spin $\boldsymbol{S} = \boldsymbol{S_1} + \boldsymbol{S_2}$, total isospin $\boldsymbol{T} = \boldsymbol{T_1} + \boldsymbol{T_2}$

For S=1

$$|11> = |\frac{1}{2}\frac{1}{2}> |\frac{1}{2}\frac{1}{2}>$$

$$|10> = \frac{1}{\sqrt{2}}(|\frac{1}{2}\frac{1}{2}> |\frac{1}{2}-\frac{1}{2}> + |\frac{1}{2}-\frac{1}{2}> |\frac{1}{2}\frac{1}{2}>)$$

$$|1-1> = |\frac{1}{2}-\frac{1}{2}> |\frac{1}{2}-\frac{1}{2}>$$

➔ symmetric (triplet, S=1)

For S=0

$$|00> = \frac{1}{\sqrt{2}}(|\frac{1}{2}\frac{1}{2}> |\frac{1}{2}-\frac{1}{2}> - |\frac{1}{2}-\frac{1}{2}> |\frac{1}{2}\frac{1}{2}>)$$

➔ antisymmetric (singlet, S=0)

$S = 0$: antisymmetric $\rightarrow P^{\sigma}|S = 0> = -|S = 0>$

$S = 1$: symmetric $\rightarrow P^{\sigma}|S = 1> = +|S = 1>$

Spin-exchange operator $P^{\sigma}$: eigenvalues $(-1)^{S+1}$

spin $P^{\sigma} = \frac{1+\boldsymbol{\sigma_1}.\boldsymbol{\sigma_2}}{2}$

Same properties for the isospin

isospin $P^{\tau} = \frac{1+\boldsymbol{\tau_1}.\boldsymbol{\tau_2}}{2}$

➔ $\boldsymbol{P_{12} = P^r P^{\sigma} P^{\tau}}$ exchanges all coordinates of both nucleons (space, spin, isospin)

**B. Generalized Pauli principle**

Nucleons are fermions → two-nucleon wave function must be antisymmetric

$P_{12} = P^r\, P^\sigma P^\tau = -1$ → Generalized Pauli principles

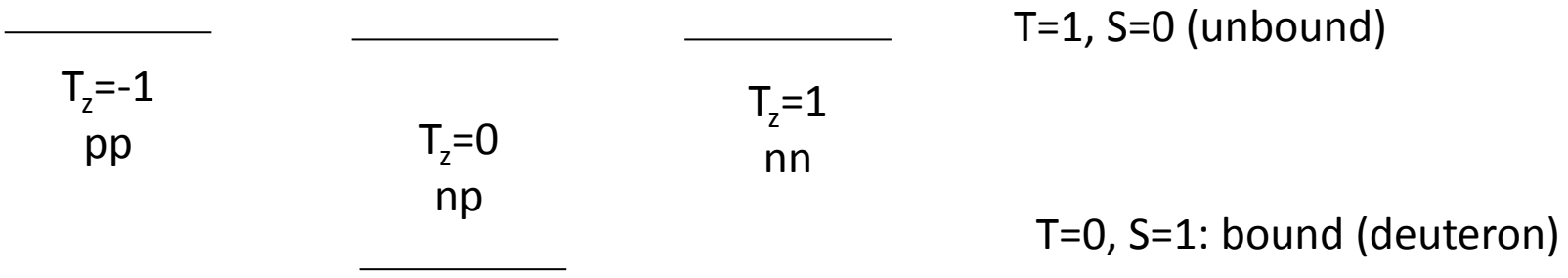
Space: $P^r$ → phase $(-1)^L$

Spin: $P^\sigma$ → phase $(-1)^{S+1}$

Isospin: $P^\tau$ → phase $(-1)^{T+1}$

➔ Selection rule: $(-1)^{L+S+T} = -1$ for the nucleon-nucleon system

- parity+ (L even): 4 states: S=0, T=1 (3 values for $T_z$), S=1, T=0




- Parity – (L odd): 4 states: (S=0,T=0), (S=1,T=1): unbound

# 3. The nucleon-nucleon (NN) interaction

Total NN interaction $V(i,j) = V_N(i,j) + V_C(i,j)$

Indices $i$ and $j$ include $(r, s_s, t_z)$

- Coulomb interaction (isospin formalism): $V_C(i,j) = \frac{e^2}{|r_i - r_j|}\left(\frac{1}{2} - t_{iz}\right)\left(\frac{1}{2} - t_{jz}\right)$
- Nuclear interaction: $V_N(i,j)$ not known exactly

General form of the nuclear interaction $V_N = V_N^{central} + V_N^{spin-orbit} + V_N^{tensor}$

$\Delta L = 0,$
$\Delta S = 0$
Dominant term

$\Delta L = 1$
$\Delta S = 1$

$\Delta L = 2$
$\Delta S = 2$

**C. How to deduce the general form of $V_N^{central}$ ?**

The NN wave function satisfies 2 eigenvalue problems:

- $P_{12}\Psi_{LST}(\boldsymbol{r}) = -\Psi_{LST}(\boldsymbol{r})$ with $P_{12} = P^r P^\sigma P^\tau$

- $H\Psi_{LST}(\boldsymbol{r}) = \left(t_1 + t_2 + V_N^{central}(1,2)\right)\Psi_{LST}(\boldsymbol{r}) = E\Psi_{LST}(\boldsymbol{r})$

2 operators with the same eigenfunctions

$\rightarrow [H, P_{12}] = 0$

$\rightarrow \left[V_N^{central}, P_{12}\right] = 0$

Most general form for $V_N^{central}$

$V_N^{central}(r) = w(r) + m(r)P^r + b(r)P^\sigma + h(r)P^\tau$

with *w(r)*=Wigner term

*m(r)*=Majorana term

*b(r)*=Bartlett term

*h(r)*=Heisenberg term

Functions w(r),m(r),b(r),h(r) are adjusted to experiment (B, Q, μ, phase shiftss, etc.)

- Gaussian
- Woods-Saxon

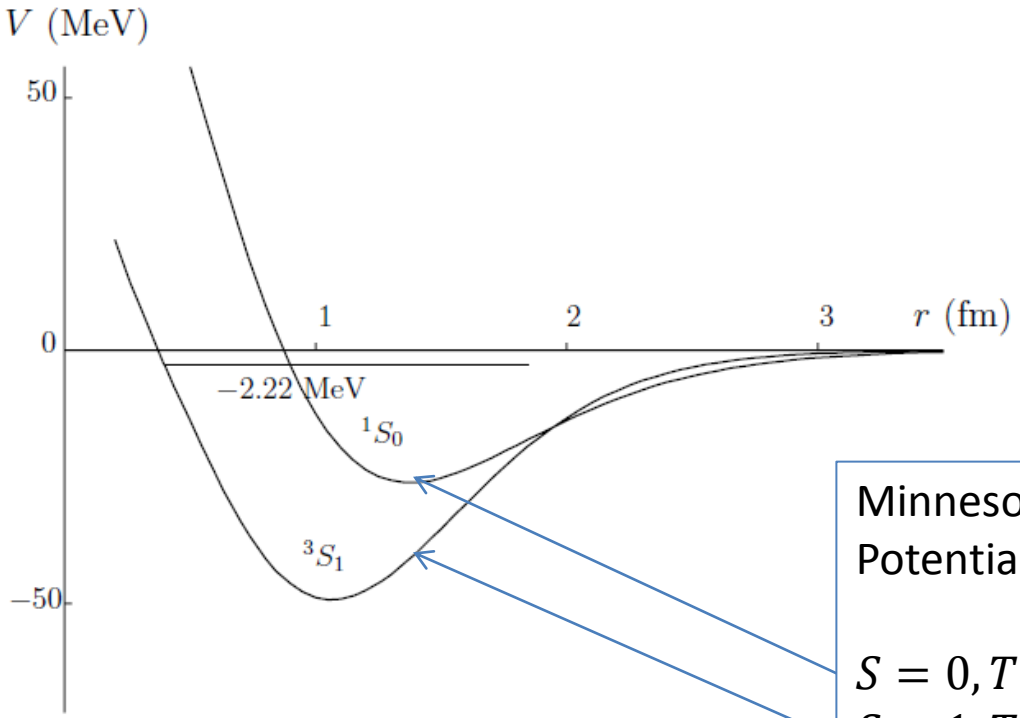
# 3. The nucleon-nucleon (NN) interaction

- General expression : $V(r) = w(r) + m(r)P^r + b(r)P^\sigma + h(r)P^\tau$
- System n+p ($T_z$=0), L even ➔ 2 possibilities

$< T = 0, S = 1 | V | T = 0, S = 1 > = w(r) + m(r) + b(r) - h(r)$

$< T = 1, S = 0 | V | T = 1, S = 0 > = w(r) + m(r) - b(r) + h(r)$

➔ different potentials for S=0 (singlet) and S=1 (triplet)




Minnesota potential (gaussians)
Potentials n-p for S=0 et S=1

$S = 0, T = 1$: no bound state
$S = 1, T = 0$: one bound state: deuteron

# 3. The nucleon-nucleon (NN) interaction

« Non central » terms : $V = V_{cent}(r) + V_{LS}(r)\boldsymbol{L}.\boldsymbol{S} + V_T(r)\boldsymbol{S_{12}}$

- Spin-orbit: $V_{LS}(r)\boldsymbol{L}.\boldsymbol{S}$ **:** $\Delta S = 0, \pm 1, \Delta L = 0$
- Tensor: $V_T(r)\boldsymbol{S_{12}}$, with $\boldsymbol{S_{12}} = \left[[\boldsymbol{s_1} \otimes \boldsymbol{s_2}]^2 \otimes [\boldsymbol{r_1} \otimes \boldsymbol{r_2}]^2\right]^0$
  - $\Delta S = 0, \pm 1, \pm 2, \Delta L = 0, \pm 2$
  - $\Psi = \alpha\Psi_{010} + \beta\Psi_{210}$ (with $\beta^2 \approx 5\%$ : amplitude of the L=2 component)
  - Tensor responsible : of $L = 0$ and $L = 2$ mixing in the deuteron
    of the deuteron quadrupole moment
- Possible additional terms $\boldsymbol{(L.S)^2}, \boldsymbol{L^2}, \boldsymbol{etc}$ …

**Interaction obtained from field theory**

OPEP (One Pion-Exchange Potential)

$$V_{OPEP} = V_\pi \boldsymbol{t_1} \cdot \boldsymbol{t_2}$$

With $$V_\pi = \frac{4}{3} f_\pi^2 \hbar c \left[ 4\, \boldsymbol{s_1} \cdot \boldsymbol{s_2} + \left(1 + \frac{3\lambda_\pi}{r} + \frac{3\lambda_\pi^2}{r^2}\right) \boldsymbol{S_{12}} \right] \frac{\mathrm{e}^{-\mathrm{r}/\lambda_\pi}}{r}$$

$\lambda_\pi = \frac{\hbar}{mc}$ associated with the exchanged particle (here: pion)

$f_\pi^2 \approx 0.075, \lambda_\pi \approx 1.43$ fm

**Realistic potentials**

- Fitted on NN properties (p+p, p+n, analyzing power, deuteron, etc)
- Examples: Reid, Paris, Bonn, Argonne (Yukawa functions)
- Very complicated
- Problems to apply to many-nucleon systems (3-body forces?)

**Effective potentials**

- Adapted to the model (shell model), include some NN properties
- Used in cluster models
- Examples: Volkov (optimizes $\alpha$, $^{16}$O), Minnesota ($\alpha$+$\alpha$ scattering, deuteron)

# 4. The shell model

# 4. The shell model

Exact Hamiltonian

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

replaced by

$$H = \sum_{i=1}^{A} T_i + \sum_{i=1}^{A} U_i(r_i) + H_{res}$$

where $H_{res}$ is the residual Hamiltonian (small, neglected)

→ mean field: (A-1) nucleons generate a « mean » potential acting on the last nucleon

Single-particle potential: $U(r) = \frac{1}{2} m\omega^2 r^2$ , oscillator parameter $b = \left(\frac{\hbar}{m\omega}\right)^{1/2}$

If we neglect $H_{res}$ :

$$H = \sum_{i=1}^{A} h_i$$

- independent-particle model: the A-body problem is replaced by A one-body problems

$$h_i \phi_i = e_i \phi_1$$

- Total energy of the nucleus $E = \sum_{i=1}^{A} e_i$
- Total wave fuinction of the nucleus $\Psi = \phi_1 \ldots \phi_A$ + antisymmetrization

## Single-particle hamiltonian

1. **Spin neglected :** $h\phi(r) = \left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2\right)\phi(r) = e\phi(r)$

$e_{n_r,\ell} = \hbar\omega(2n_r + \ell + \frac{3}{2})$ only depends on $n = 2n_r + \ell$

$\phi_{n_r,\ell,m}(r,\theta,\phi) = R_{n_r\ell}(r)Y_\ell^m(\theta,\phi)$

$n_r$ = radial quantum number

$\ell$ = orbital momentum

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

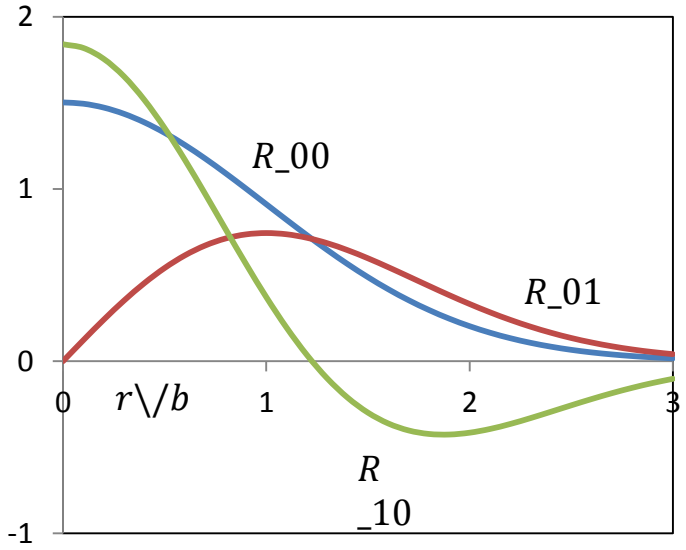
$R_{n_r\ell}(r)$ = radial functions : Laguerre × $\exp(-r^2/2b^2)$

Examples:

$$R_{00}(r) = 2\pi^{-1/4}\exp\left(-\frac{r^2}{2b^2}\right)$$

$$R_{01}(r) = 2\sqrt{\frac{2}{3}}\pi^{-1/4}\,\mathrm{r}\exp\left(-\frac{r^2}{2b^2}\right)$$

$$R_{10}(r) = \sqrt{6}\pi^{-1/4}\left(1 - \frac{2r^2}{3b^2}\right)\exp\left(-\frac{r^2}{2b^2}\right)$$



Degeneracy $N_n = (n+1)(n+2)/2$



$n = 3\ (1p, 0f), N_n = 10$



$n = 2\ (1s, 0d), N_n = 6$



$n = 1\ (0p), N_n = 3$



$n = 0\ (0s), N_n = 1$



N=Z=40 nucleons



N=Z=20: $^{40}$Ca

N=Z=8: $^{16}$O

N=Z=2: $^{4}$He

| n | $n_r, \ell$ | Degeneracy |
|---|---|---|
| 0 | (0,0)=0s | 1 |
| 1 | (0,1)=0p | 3 |
| 2 | (1,0)=1s<br>(0,2)=0d | 6=1+5 |
| 3 | (1 1)=1p<br>(0,3)=0f | 10=3+7 |

Magic numbers:

- SM: **2,8,20,40,70,112, etc.**
- Exp: **2,8,20,28,50, 82, 126**

→ Necessity of a spin-orbit force

2. **Spin included**

$$h\phi(r) = \left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2 + \ell \cdot s\, V_{SO}(r)\right)\phi(r) = e\phi(r)$$

- Good quantum number: $j = \ell + s$
- Individual wave functions

$$\phi_{n_r,\ell,j,m} = |n_r \ell j m> = \sum_{m_s} < \ell m_\ell \frac{1}{2} m_s | j m > \phi_{n_r,\ell,m_\ell} \times \chi_{m_s} \quad (\text{with } j = \ell$$

- Notation: $n_r \ell_j$ examples: $0s_{1/2}$, $0p_{1/2}$, $0p_{3/2}$, $1s_{1/2}$, etc.
- Matrix element of $\ell \cdot \boldsymbol{s}$

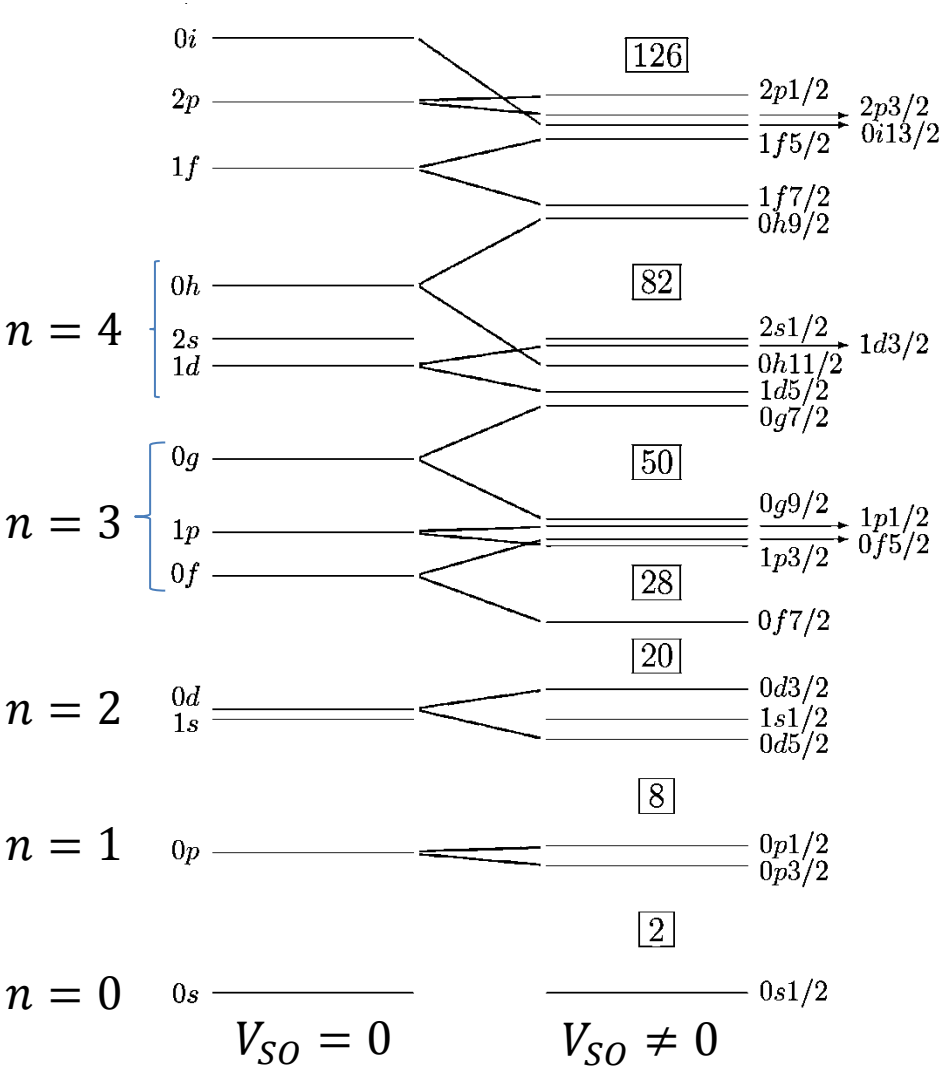
$$< j\ell m\, |\ell \cdot \boldsymbol{s}| j'\ell' m' > = \frac{1}{2}[j(j+1) - \ell(\ell+1) - s(s+1)]\delta_{jj'}\, \delta_{\ell\ell'}\, \delta_{mm'}$$

$$= \frac{1}{2}\ell \text{ for } j = \ell + \frac{1}{2}$$

$$= -\frac{1}{2}(\ell+1) \text{ for } j = \ell - \frac{1}{2}$$

Then

- Orbital $j = \ell + \frac{1}{2}$ is lower if $V_{SO}(r) < 0$
- Splitting proportional to $2\ell + 1$ → increases with $\ell$




Magic numbers: **2,8,20,28,50,82,126**
In agreement with experiment

For a closd shell: $J = 0$

Magic nuclei with N=Z: $^{4}$He, $^{16}$O, $^{40}$Ca
Other examples:

- $^{48}$Ca (Z=20, N=28)
- $^{132}$Sn (Z=50, N=82)
- $^{208}$Pb (Z=82, N=126)
- etc…

## Shell model for several nucleons

$$H = \sum_i^A h_i$$

Then $E = \sum_i e_i$

$$\Psi(\boldsymbol{r_1}, \dots, \boldsymbol{r_A}) = \mathcal{A}\phi_1(\boldsymbol{r_1})\phi_2(\boldsymbol{r_2}) \dots \phi_A(\boldsymbol{r_A}) = \det|\phi_1 \dots \phi_A|$$

Each orbital is charachterized by the quantum numbers $n_r \ell j m$

- For a given shell there are in general several basis states $\Psi_\lambda$ (combination of angular momenta $JM$).
  Example: 2 particles in the p shell: $\frac{6\times5}{2} = 15$ combinations

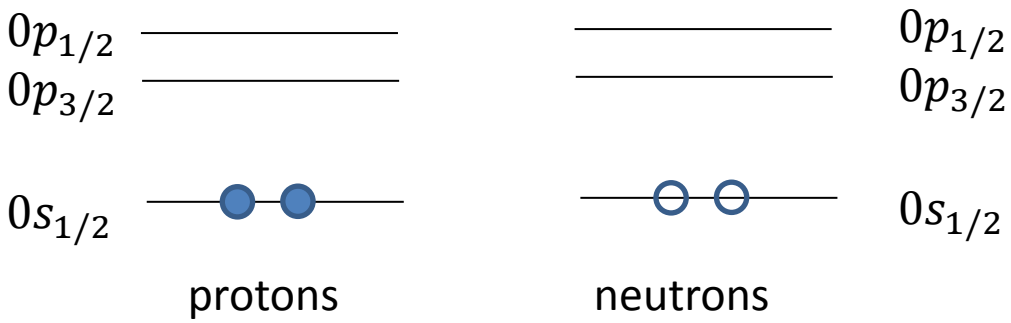
- One computes the matrix elements $< \Psi_\lambda | J^2 | \Psi_{\lambda'} >$ eigenvalues $J(J+1)$
  $< \Psi_\lambda | J_z | \Psi_{\lambda'} >$ eigenvalues $M$

- From the diagonalization, one gets shell-model wave functions with definite values of $J$ and $M$.

$$\Psi^{JM\pi} = \sum_\lambda c_\lambda^{JM\pi} \Psi_\lambda$$

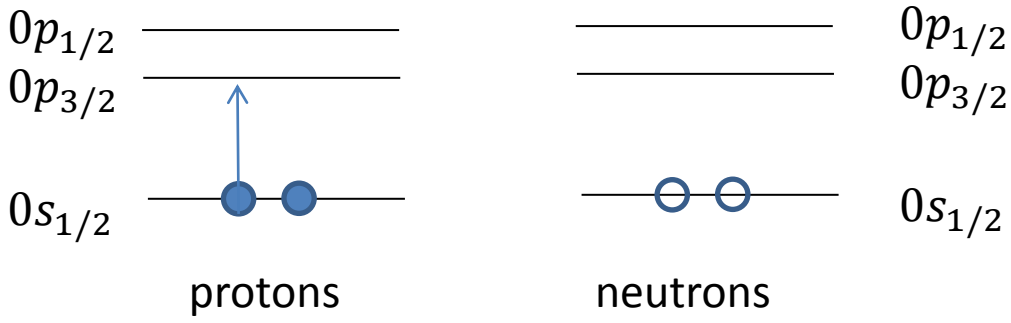
Examples

**1. The α particle (N=0)**




One function
J=0, M=0

**2. The α particle (N=1)**




Number of functions
2*6=12 for protons

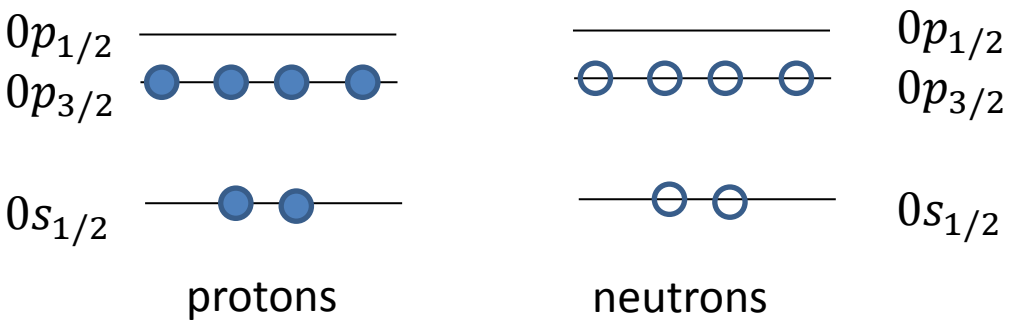
→ 24 possibilities

→ negative-parity states

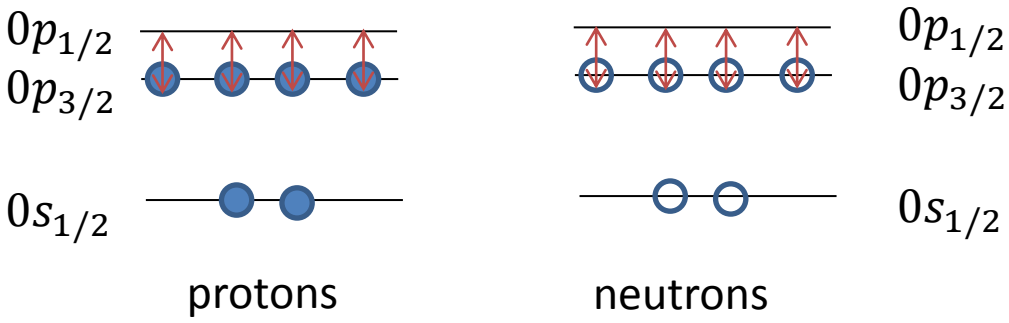
The number of basis functions strongly increases with
- The nucleon numbers
- The maximum $N$ value

➔ No Core Shell Model

**Example 2: $^{12}$C**

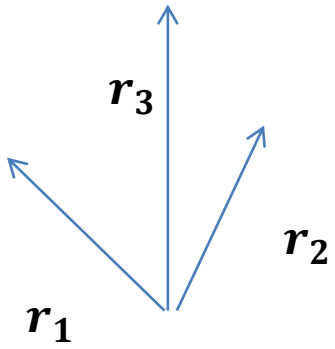



Lowest configuration
$J = 0^+$, 1 function




Excitations in the $0p_{1/2}$ shell
6 orbitals, 4 particles
→ 15 possibilities for n,p
→ 225 Slater determinants
→ $J = 0^+, 1^+, 2^+, 3^+, 4^+$

**Removal of the center-of-mass**




- Absolute coordinates $\boldsymbol{r}_i$
- c.m. coordinate: $\boldsymbol{R_{cm}} = \frac{1}{A}\sum_i \boldsymbol{r_i}$
- Relative coordinates: $\boldsymbol{\xi_i} = \boldsymbol{r}_i - \boldsymbol{R}_{cm}$

$\Psi(\boldsymbol{r_1} \ldots \boldsymbol{r_A}) = \det|\phi_1(\boldsymbol{r_1})\phi_2(\boldsymbol{r_2}) \ldots \phi_A(\boldsymbol{r_A})|$ , if $r_i \to r_i + S$ : $\Psi$ changes
→ not translation invariant (not physical)

Translation: $\Psi(\boldsymbol{r_1} \ldots \boldsymbol{r_A}) = \exp\left(-\frac{AR_{cm}^2}{2b^2}\right)\tilde{\Psi}\,(\boldsymbol{\xi_1}, \ldots \boldsymbol{\xi_A})$ = Bethe and Rose theorem

Depends on origin

Does NOT depend on origin

➔ Exact factorization of the c.m. wave function

Factorization: $\Psi(\boldsymbol{r_1} \ldots \boldsymbol{r_A}) = \exp\left(-\frac{AR_{cm}^2}{2b^2}\right) \widetilde{\Psi}(\boldsymbol{\xi_1}, \ldots \boldsymbol{\xi_A})$

Consequences

| | | |
|---|---|---|
| $\Psi(\boldsymbol{r_1} \ldots \boldsymbol{r_A})$ | is a Slater determinant | is not translation invariant |
| $\widetilde{\Psi}(\boldsymbol{\xi_1}, \ldots \boldsymbol{\xi_A})$ | is not a Slater determinant | is translation invariant |

→ calculations are performed with SD $\Psi(\boldsymbol{r_1} \ldots \boldsymbol{r_A})$
+ correction for the c.m. motion

**Gartenhaus and Schwartz theorem:**
Matrix elements with $\Psi(\boldsymbol{r_1} \ldots \boldsymbol{r_A})$ and with $\widetilde{\Psi}(\boldsymbol{\xi_1}, \ldots \boldsymbol{\xi_A})$ are equivalent provided that, in the operators:

$$r_i \to r_i - R_{cm}$$
$$p_i \to p_i - \frac{1}{A} P_{cm}$$

Example: kinetic energy $T \to T - T_{cm}$
→ simple treatment of the c.m.

# 5. Overview of microscopic models

**1. No-Core Shell Model**

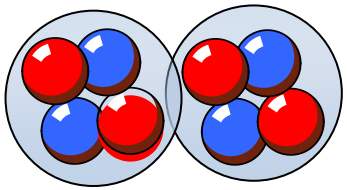
- Extensions of the traditional shell model
- All orbitals centred at the same origin
- Very large bases (up to $10^9$ functions) → specific diagonalization techniques

**2. Fermionic Molecular Dynamics (FMD)**
**Antisymmetrized Molecular Dynamics (AMD)**

- A single Slater determinant
- Orbitals centred at different origins
  → c.m. problems
- Each orbital contains several parameters (origin, oscillator parameter, etc.)
  → minimization over a **large set of parameters**

# 5. Overview of microscopic models

- **Cluster models**
  the A nuclei form « clusters » inside the nucleus
  origin: the $\alpha$ particle is strongly bound → keeps its own identity in the nucleus
  typical clusters: strongly bound nuclei (**alpha particle**)
  example : $^{8}$Be=$\alpha$+$\alpha$ - formed of 4 neutrons and 4 protons grouped in 2 $\alpha$



**Cluster** approximation $\Psi = \mathcal{A}\phi_1\phi_2 g(\rho)$

with

$\phi_1, \phi_2$ = internal wave functions (**input, shell-model**)

$g(\rho)$ =relative wave function (**output**)

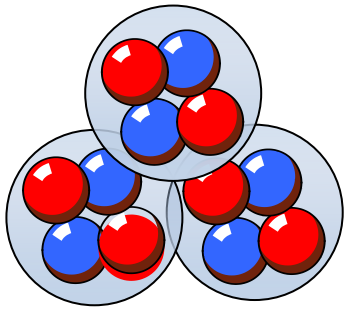
$\mathcal{A}$ = antisymmetrization operator

=Resonating Group Method (RGM)

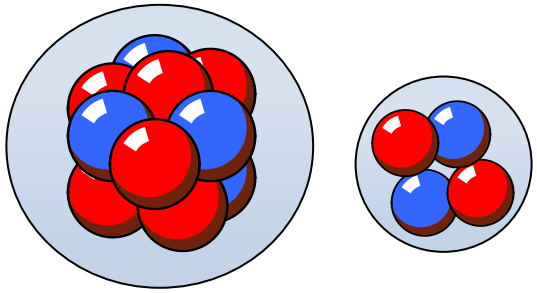
Describes spectroscopy and reactions

RGM: non systematic calculations → GCM

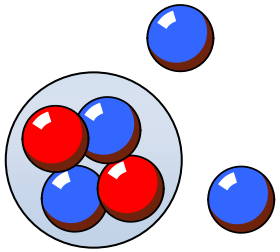
# 5. Overview of microscopic models



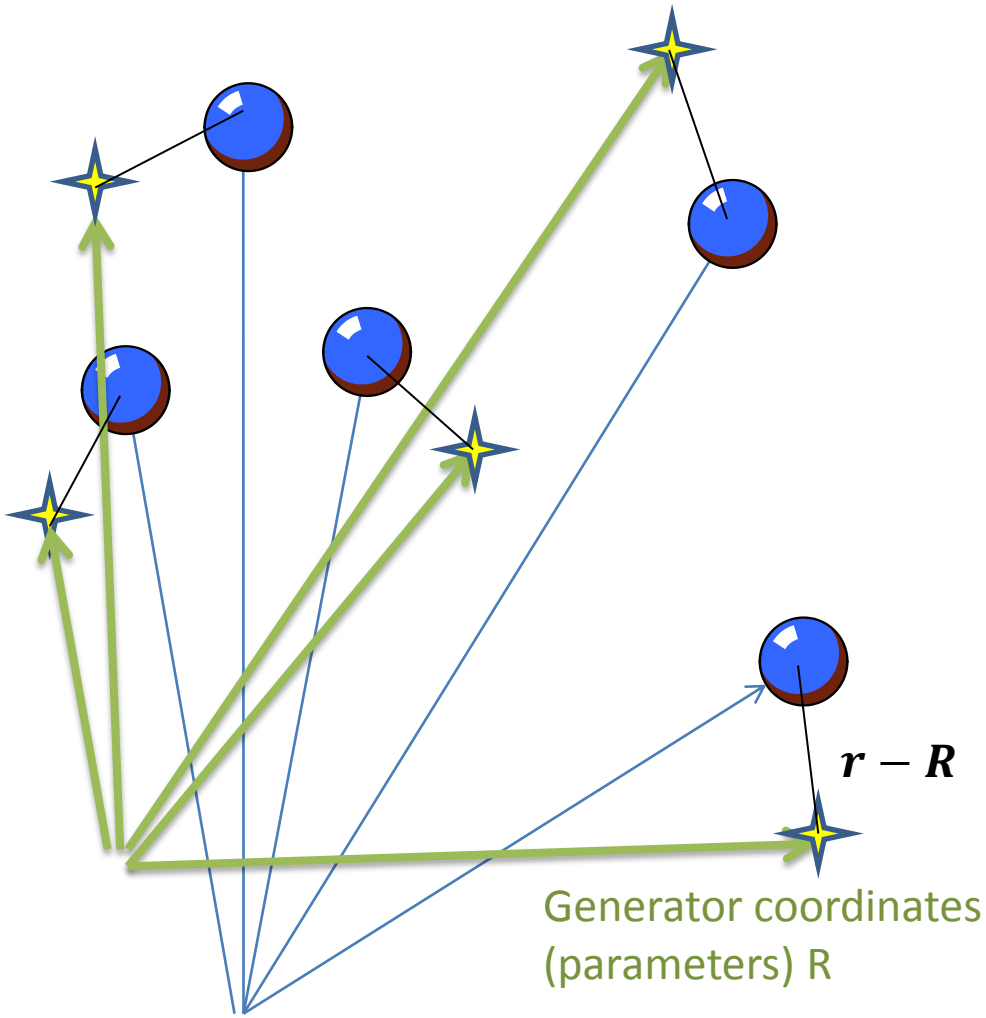
$^{12}$C described by 3 alphas



$^{20}$Ne described by $^{16}$O+$\alpha$



$^{6}$He described by $\alpha$+n+n
nucleon=« particular » cluster, numerical techniques identical




## FMD, AMD

each orbital has its own center

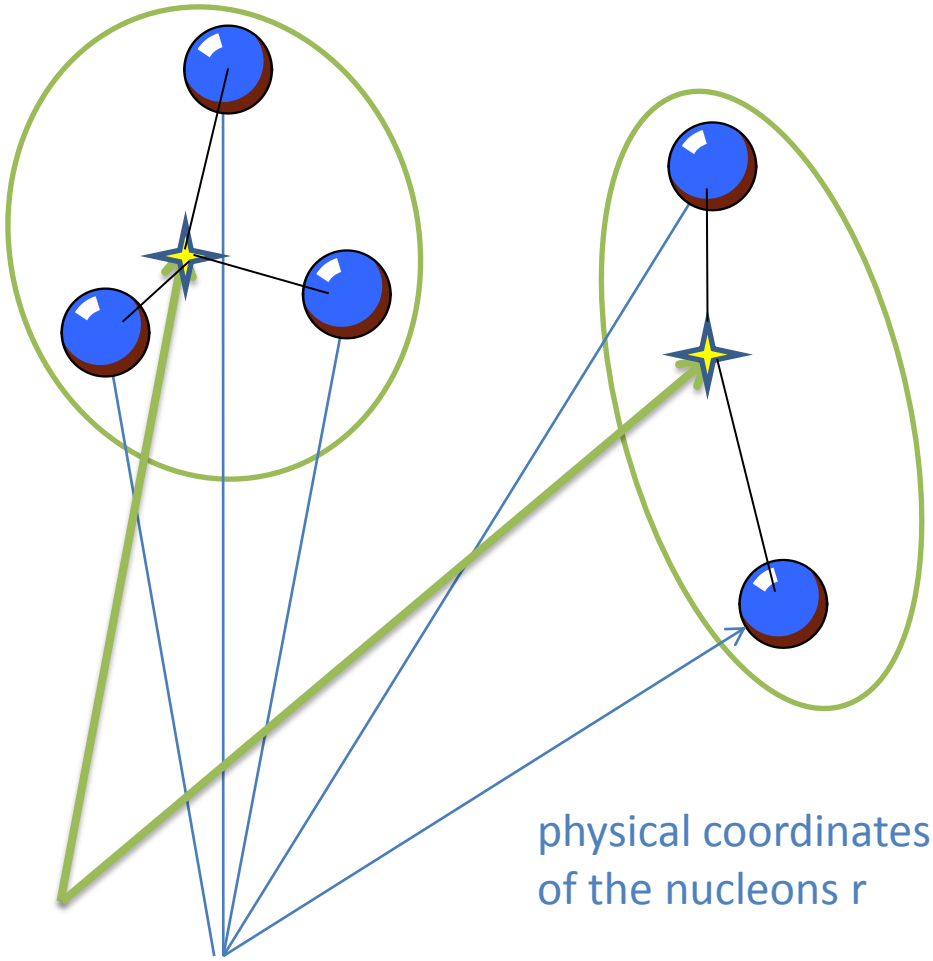
gaussians depending on $\boldsymbol{r} - \boldsymbol{R}$

$$\phi(r_i) = \exp(-(r_i - R_i)^2 / 2b_i^2)$$

→ minimization over

- all $R_i$
- all oscillator parameters $b_i$

Only one Slater determinant

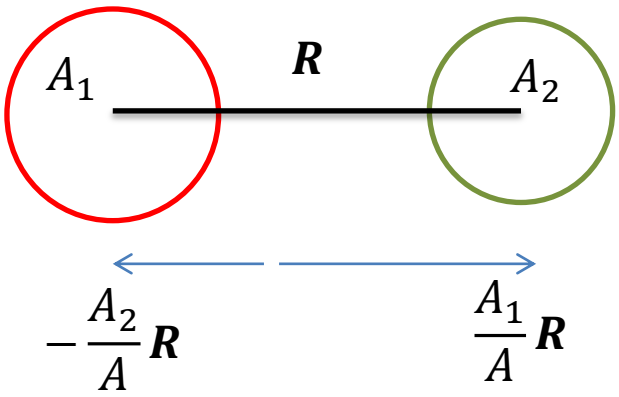



## Cluster models

- Orbitals of a cluster are centred at the same point
  =cluster approximation
- oscillator parameters identical
  (→ no c.m. problems)
- Combination of several Slater determinants

# 6. The Generator Coordinate Method (GCM)

## 1. Wave functions




Two clusters with shell-model orbitals $\Phi_1$ and $\Phi_2$

- Cluster 1: $\Phi_1 = \det\left|\varphi_1\left(-\frac{A_2}{A}\boldsymbol{R}\right)\ldots\varphi_{A_1}\left(-\frac{A_2}{A}\boldsymbol{R}\right)\right|$
- Cluster 2: $\Phi_2 = \det\left|\Psi_1\left(\frac{A_1}{A}\boldsymbol{R}\right)\ldots\Psi_{A_2}\left(\frac{A_1}{A}\boldsymbol{R}\right)\right|$
- Same oscillator parameters for all orbitals → c.m. problems are easily solved

- Two-cluster basis state

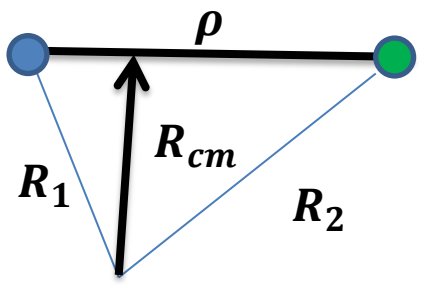
$$\Phi(R) = \det\left|\varphi_1\left(-\frac{A_2}{A}\boldsymbol{R}\right)\ldots\varphi_{A_1}\left(-\frac{A_2}{A}\boldsymbol{R}\right)\Psi_1\left(\frac{A_1}{A}\boldsymbol{R}\right)\ldots\Psi_{A_2}\left(\frac{A_1}{A}\boldsymbol{R}\right)\right|$$
$$= \mathcal{A}\Phi_1\left(-\frac{A_2}{A}\boldsymbol{R}\right)\Phi_2\left(\frac{A_1}{A}\boldsymbol{R}\right)$$

2. Equivalence between the GCM and RGM

- Factorization of the c.m. function for one cluster

$$\Phi(S) = \exp\left(-A\frac{(S-S_{cm})^2}{2b^2}\right)\Phi(0)$$

- For two clusters:




$$\boldsymbol{\rho} = \boldsymbol{R}_1 - \boldsymbol{R}_2$$
$$A\boldsymbol{R}_{cm} = A_1\boldsymbol{R}_1 + A_2\boldsymbol{R}_2$$

Then $\Phi(\boldsymbol{R}) = \mathcal{A}\Phi_1\left(-\frac{A_2}{A}\boldsymbol{R}\right)\Phi_2\left(\frac{A_1}{A}\boldsymbol{R}\right)$

$$= \exp\left(-A\frac{R_{cm}^2}{2b^2}\right)\mathcal{A}\Phi_1(0)\Phi_2(0)\exp\left(-\mu\frac{(\boldsymbol{\rho}-\boldsymbol{R})^2}{2b^2}\right)$$

→ exact factorization of the c.m. motion

# 6. The Generator Coordinate Method (GCM)

Equivalence between the RGM and GCM

- GCM:

basis state: $\Phi(\boldsymbol{R}) = \mathcal{A}\Phi_1(0)\Phi_2(0)\exp\left(-\mu\frac{(\boldsymbol{\rho}-\boldsymbol{R})^2}{2b^2}\right) = \mathcal{A}\phi_1\phi_2\exp\left(-\mu\frac{(\boldsymbol{\rho}-\boldsymbol{R})^2}{2b^2}\right)$

→ combination of basis states

$\Psi = \int f(R)\Phi(R)dR = \mathcal{A}\phi_1\phi_2\int f(\boldsymbol{R})\exp\left(-\mu\frac{(\rho-R)^2}{2b^2}\right)dR$

- RGM: $\Psi = \mathcal{A}\phi_1\phi_2 g(\boldsymbol{\rho})$

➔ GCM and RGM are equivalent with $g(\boldsymbol{\rho}) = \int f(\boldsymbol{R})\exp\left(-\mu\frac{(\boldsymbol{\rho}-\boldsymbol{R})^2}{2b^2}\right)d\boldsymbol{R}$

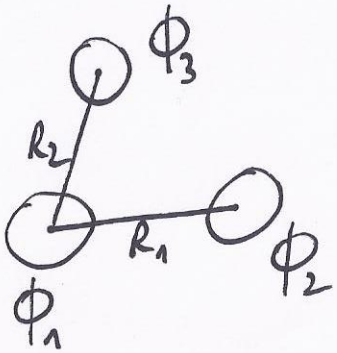
$f(\boldsymbol{R})$= generator function

GCM method

- gaussian expansion of the radial wave functions (R=generator coordinate)
- basis functions are expressed as Slater determinants → appropriate to numerical calculations (systematic)
- other expansion possible $g(\rho) = \int F(b)\exp\left(-\mu\frac{\rho^2}{2b^2}\right)db$

=gaussians centred at $\rho = 0$, with different widths

3. Extension to multicluster systems




more than 1 generator coordinate

ex: $^{12}C = \alpha + \alpha + \alpha$

$^{6}He = \alpha + n + n$

GCM basis

- $\Phi(\bar{R}_1, \bar{R}_2) = \mathcal{A}\, \Phi_1(\bar{S}_1)\, \Phi_2(\bar{S}_2)\, \Phi_3(\bar{S}_3)$

  where $\bar{S}_1, \bar{S}_2, \bar{S}_3$ are determined from $\bar{R}_1, \bar{R}_2$

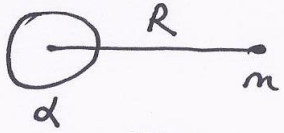
- Same c.m. factorization

## 4. Matrix elements between GCM basis functions

- $\phi(R)$ = A x A Slater determinant

- factorization spin - isospin

**Simple example 1: $\alpha + n$**




$$\phi(\vec{R}) = \det \left| \underbrace{\varphi(-\tfrac{\vec{R}}{5}) n\downarrow \quad \varphi(-\tfrac{\vec{R}}{5}) n\uparrow \quad \varphi(-\tfrac{\vec{R}}{5}) p\downarrow \quad \varphi(-\tfrac{\vec{R}}{5} p\uparrow)}_{\alpha \text{ particle}} \quad \underbrace{\varphi(\tfrac{4\vec{R}}{5} n\downarrow)}_{\text{neutron}} \right|$$

with $\varphi(\vec{s}) = n_0 \exp\left(-\frac{(\vec{r}-\vec{s})^2}{2b^2}\right)$ = os orbital

$$\langle \varphi(s) | \varphi(s') \rangle = \exp\left(-\frac{(\vec{s}-\vec{s}')^2}{4b^2}\right)$$

# 6. The Generator Coordinate Method (GCM)

Overlap between 2 SD

$$\langle \phi(\bar{R}) \mid \phi(\bar{R}') \rangle = \begin{vmatrix} a & d & & \\ c & b & & \\ & & a & \\ & & & a \end{vmatrix} = a^3 (ab - cd)$$

$n\downarrow$ $n\uparrow$ $p\downarrow$ $p\uparrow$

with $a = \langle \varphi(-\frac{R}{5}) \mid \varphi(-\frac{R'}{5}) \rangle$

$b = \langle \varphi(\frac{4R}{5}) \mid \varphi(\frac{4R'}{5}) \rangle$

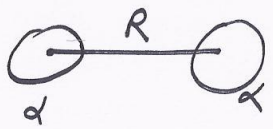
$c = \langle \varphi(\frac{4R}{5}) \mid \varphi(-\frac{R'}{5}) \rangle$

$d = \langle \varphi(-\frac{R}{5}) \mid \varphi(\frac{4R'}{5}) \rangle$

Kinetic energy, NN interaction: same principle

# 6. The Generator Coordinate Method (GCM)

**Simple example 2 : $\alpha + \alpha$**




$$\phi(R) = \det \Big| \underbrace{\varphi(-\tfrac{R}{2})\, n\downarrow \;\; \varphi(-\tfrac{R}{2})\, n\uparrow \;\; \varphi(-\tfrac{R}{2})\, p\downarrow \;\; \varphi(-\tfrac{R}{2})\, p\uparrow}_{\alpha} \;\; \underbrace{\varphi(\tfrac{R}{2})\, n\downarrow \cdots}_{\alpha} \Big|$$

Overlap

$$\langle \phi(R) \mid \phi(R') \rangle = \begin{vmatrix} a & d & & & \\ c & b & & & \\ & & a & d & \\ & & c & b & \\ & & & & a \; d \\ & & & & c \; b \end{vmatrix} = (ab - cd)^4$$

$$a = \langle \varphi(-\tfrac{\bar{R}}{2}) \mid \varphi(-\tfrac{\bar{R}'}{2}) \rangle = \exp\left(-\frac{(\bar{R}-\bar{R}')^2}{16 b^2}\right)$$

$$\Rightarrow \boxed{\langle \phi(\bar{R}) \mid \phi(\bar{R}') \rangle = N(\bar{R}, \bar{R}') = \left\{ \exp\left[-\frac{(R-R')^2}{8b^2}\right] - \exp\left[-\frac{(R+R')^2}{8b^2}\right] \right\}^4}$$

Remark : $N(R, R') \to 0$ if $R \to 0$ or $R' \to 0$ (S.D. vanishes)

# 6. The Generator Coordinate Method (GCM)

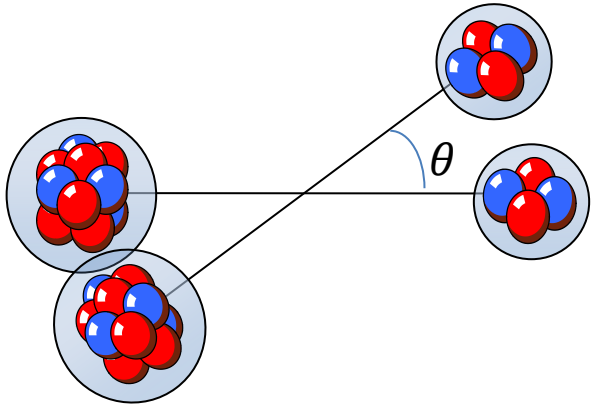
5. Angular-momentum projection

The GCM basis functions must be projected on spin $J$ (rotation invariance)

From $\Phi(\boldsymbol{R}) \rightarrow \Phi^{JM}(R) = \int Y_J^M(\Omega_R)\Phi(\boldsymbol{R})\mathrm{d}\Omega_R$

Projected matrix elements in the GCM (overlap, spins zero)

$$< \Phi^J\ (R)|\Phi^J(R') > = \int d\sin\theta\ \ P_J(\cos\theta) < \Phi(R\ )|\Phi(R',\theta) >$$




Always 2 steps:

1) non-projected matrix elements $< \Phi(R\ )|\Phi(R',\theta) >$: involve Slater determinants

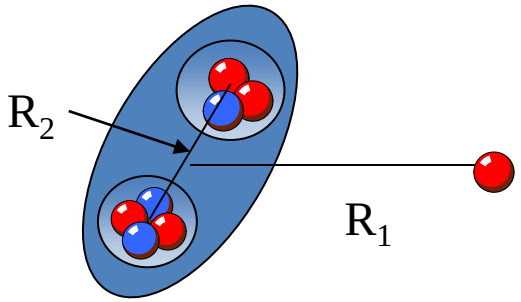
2) **projected matrix elements** $< \Phi^J\ (R)|\Phi^J(R') >$

- For 2 clusters systems: one dimensional integrals (in general: numerical integration)
- For 3 clusters systems: more dimensions (5-7 according to the projection method)

6. Extensions

- $\alpha+\alpha$ and $\alpha$+n very simple: 2 clusters
  0s orbitals
  1 Slater determinant
  no excited state
  → analytical calculations are simple

- Possible generalizations
  - 3 clusters (or more)
    projection more complicated (multidimension)




  - p, sd orbitals: many Slater determinants
    → analytical calculations not possible

  - Multichannel calculations: $\Psi = \mathcal{A}\phi_1\phi_2 g(\rho) + \mathcal{A}\phi_1^*\phi_2^* g^*(\rho) + \cdots$
    → better wave functions
    → inelastic scattering, transfer

# 7. Reactions with the GCM

# 7. Reactions with the GCM

Hamiltonian of the system $H = \sum_i T_i + \sum_{j>i} V_{ij}$

At large distances:

$$H \to H_1 + H_2 + T_\rho + \frac{Z_1 Z_2 e^2}{\rho}$$

$$\Psi \to \phi_1 \phi_2 g(\rho)$$

- In cluster models the wave function is written as $\Psi = \mathcal{A}\phi_1\phi_2 g(\rho)$
  → natural expression at large distances ($\mathcal{A}$ negligible)
  → important advantage with respect to other microscopic theories

- GCM basis state

Before projection: $\Phi(R) = \mathcal{A}\phi_1\phi_2 \exp\left(-\frac{\mu(\rho-R)^2}{2b^2}\right)$ → gaussian at large distances

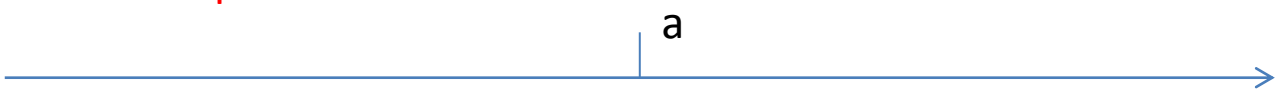
After projection: $\Phi^{\ell m}(R) = \int Y_\ell^m(\Omega_R)\Phi(R)d\Omega_R = \mathcal{A}\phi_1\phi_2\Gamma_\ell(\rho, R)$

with $\Gamma_\ell(\rho, R) = \exp\left(-\frac{\mu(\rho^2+R^2)}{2b^2}\right) i_\ell\left(\frac{\mu\rho R}{b^2}\right)$, $i_\ell(x)$ = Hankel function

➔ **Can be used in the R-matrix theory**

Microscopic R-matrix: simple generalization with GCM basis functions

## Non-microscopic R-matrix




**internal region**: $r \leq a$

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

**external region**: $r \geq a$

Nuclear potential negligible

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

## Microscopic R-matrix


**internal region**: $r \leq a$

$$\Psi_{\text{int}} = \mathcal{A}\phi_1\phi_2 g_{int}(\rho)$$
$$= \sum_i f(R_i)\Phi(R_i)$$

**external region:** $r \geq a$

- Nuclear potential negligible
- Antisymmetrization negligible

$$\Psi_{\text{ext}} = \phi_1\phi_2 g_{ext}(\rho)$$
$$g_{ext}(r) = I_\ell(r) - U_\ell O_\ell(r)$$

Microscopic R-matrix theory

- Internal region

$$\Psi_{\text{int}} = \mathcal{A}\phi_1\phi_2 g_{int}(\rho) = \sum_i f(R_i)\Phi(R_i)$$

- External region:

$$\Psi_{\text{ext}} = \phi_1\phi_2(I_\ell(r) - U_\ell O_\ell(r))$$

For the R-matrix we need matrix elements computed over the internal region
$< \Phi(R_i)|H - E + \mathcal{L}(L)|\Phi(R_j) >_{int}$

Two steps:

1. Calculation of the matrix elements over the whole space (Slater determinants)
2. Calculation of the correction over the external region

$$< \Phi(R_i)\left|\Phi\left(R_j\right) >_{int} = < \Phi(R_i)\right|\Phi\left(R_j\right) > - < \Phi(R_i)|\Phi(R_j) >_{ext}$$

$$< \Phi(R_i)|\Phi(R_j) >_{int} = < \Phi(R_i)|\Phi(R_j) > - < \Phi(R_i)|\Phi(R_j) >_{ext}$$

$< \Phi(R_i)|\Phi(R_j) >$: matrix element between Slater determinants

$< \Phi(R_i)|\Phi(R_j) >_{ext}$=correction over the external region

In the external region: $\Phi^{\ell m}(R) = \mathcal{A}\phi_1\phi_2\Gamma_\ell(\rho, R) \approx \phi_1\phi_2\Gamma_\ell(\rho, R)$

→ Matrix element

$$< \Phi(R_i)|\Phi(R_j) >_{ext} = \int_a^\infty \Gamma_\ell(\rho, R_i)\, \Gamma_\ell(\rho, R_j)\rho^2 d\rho$$

Similar expressions for

- Kinetic energy
- Coulomb potential

➔ Same R-matrix formalism

➔ Determination of scattering properties (scattering matrix, wave functions, etc.)

Some remarks

- Extension to multichannel calculations
- Extension to bound states: iterative method (as in the non-microcopic R-matrix)
- Access to continuum states: important for resonances (exotic nuclei present resonances or are unbound in their ground state)
- Partial widths: parametrized by the multichannel Breit-Wigner approximation of the scattering matrix.
  Near a resonance:

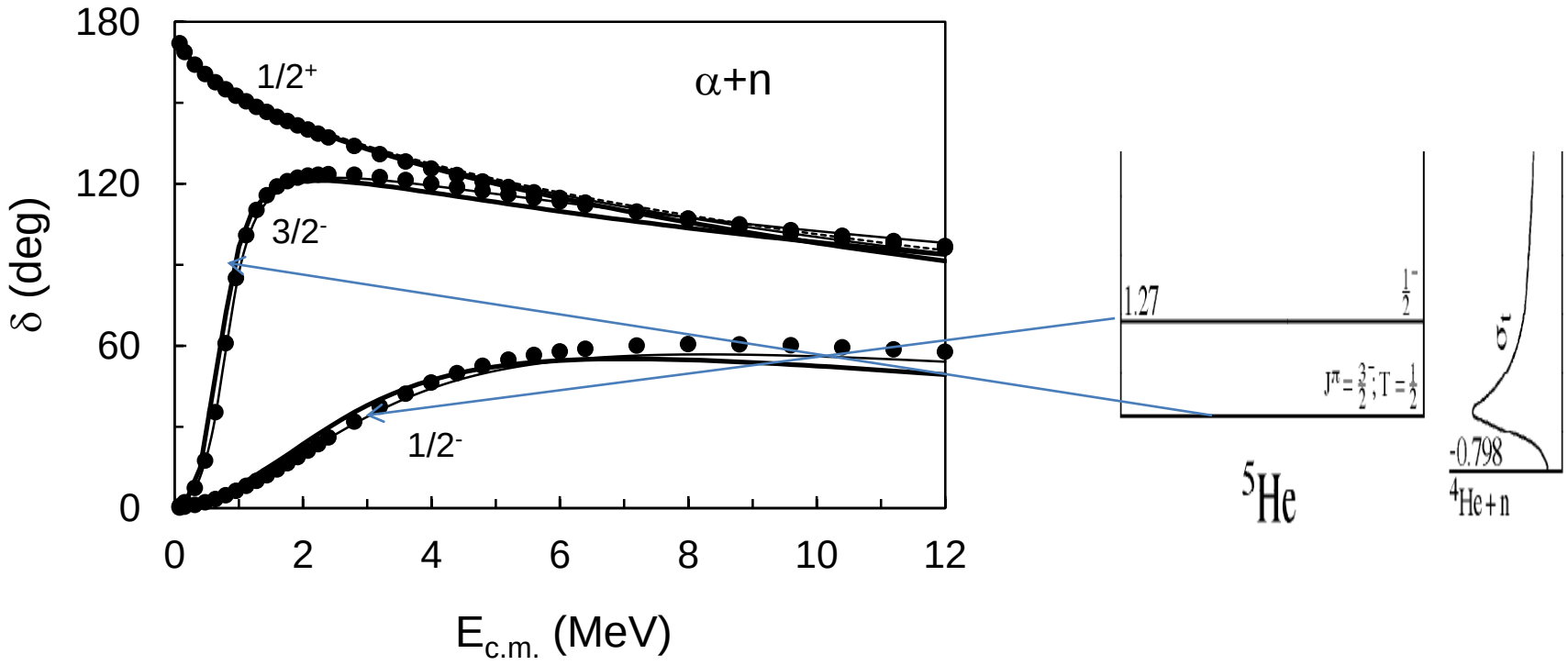
$$U_{ij}(E) \approx \delta_{ij} - i\frac{\Gamma_i \Gamma_j}{E_R - E + i\Gamma/2}$$

Many channels: very difficult!
→ iterative method
  - P. D. and M. Vincke, *Phys. Rev. A 42 (1990) 3835*
  - Provides a direct definition of the partial widths

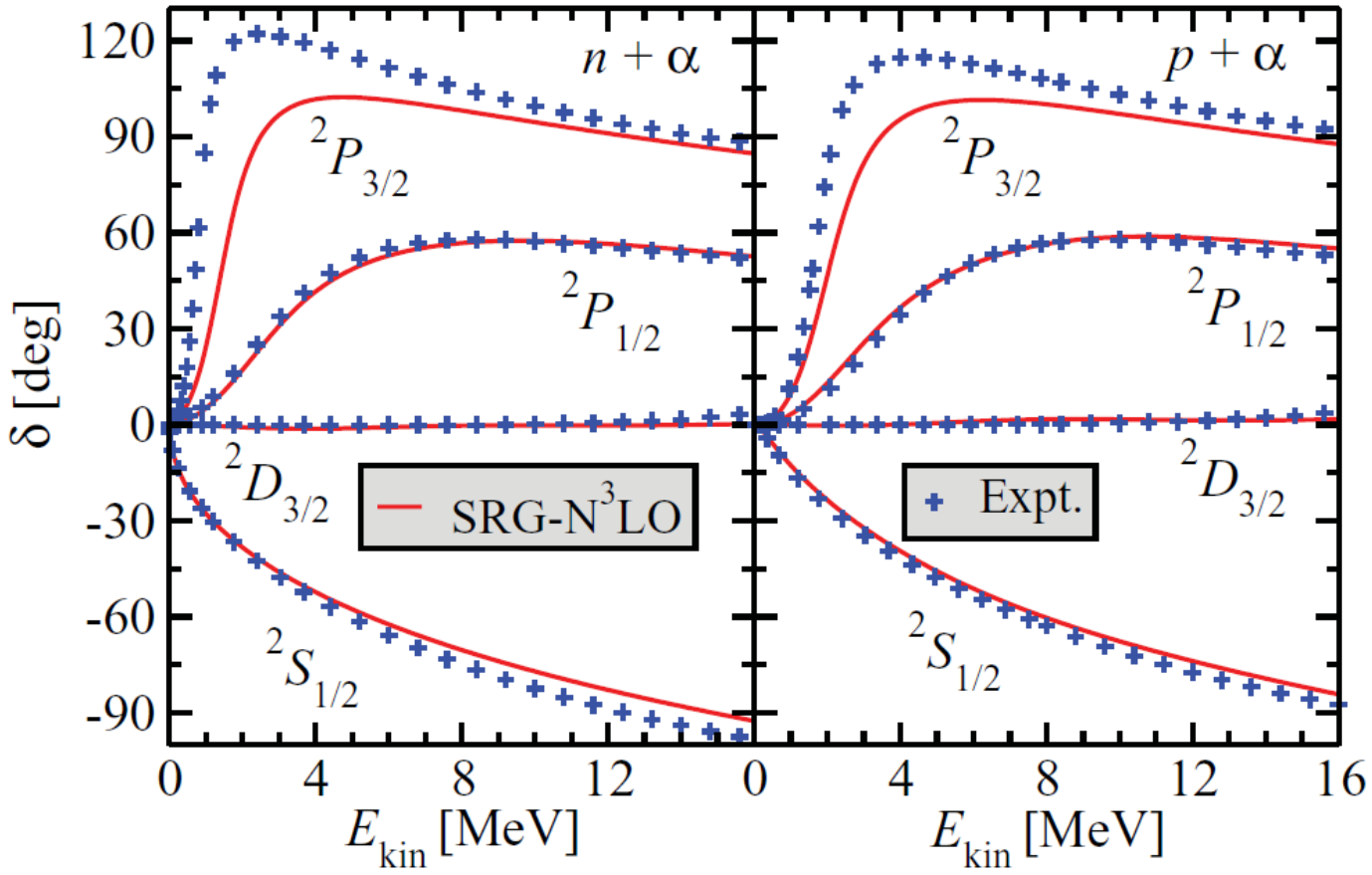
Example 1: α+n phase shifts

2 inputs:

- oscillator parameter for the α cluster. Differents criteria:
  - rms radius
  - minimum binding energy
- NN interactions: Minnesota, Volkov
  Each interaction contains one parameter ($u \approx 1$) for Minnesota, ($M \approx 0.6$) for Volkov

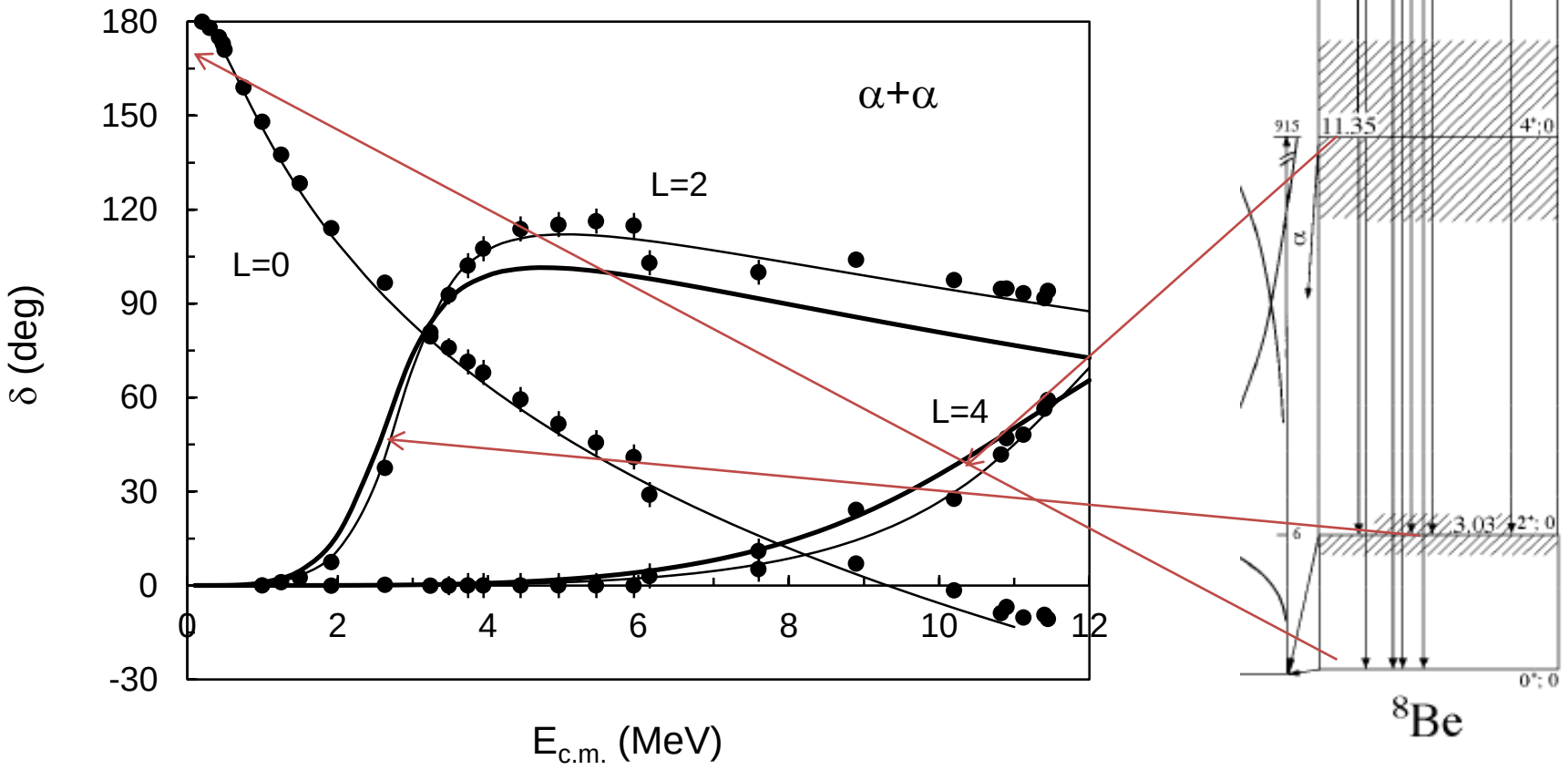


**Ab initio calculation: No Core Shell Model** (Nmax=17)
P. Navratil et al., Phys. Rev. C 82 (2010) 034609
Realistic interaction – missing NNN force?




In general: feasible for nucleus+nucleon scattering

Example 2: α+α


α+α
L=0
L=2
L=4
δ (deg)
E$_{c.m.}$ (MeV)
180
150
120
90
60
30
0
-30
0
2
4
6
8
10
12
915
11.35
4+; 0
3.03
2+; 0
0+; 0
$^{8}$Be