Mean-field approach to fission and fission cross-section modelling

Universiti Kebangsaan Malaysia – University of Bordeaux

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Part 1:
Going back to quantum mechanics

- Identical particle and many-body problem
- Approximations for stationary states – variational method

The many-body problem

The wave function

The wave-function for *N*-body system → $\Psi(r_1, r_2, r_3 \ldots r_N, t)$.

$|\Psi(r_1, r_2, r_3 \ldots r_N, t)|^2 d^3 r_1 d^3 r_2 d^3 r_3 \ldots d^3 r_N$

➤ gives the probability of finding particles #1 within volume element $d^3 r_1$ centered around r_1 etc.

The normalization condition for the wave function $\displaystyle\int d^3 r_1 \int d^3 r_2 \cdots \int |\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t)|^2 d^3 r_N = 1.$

The Hamiltonian

We can generalize the one-body 3D Schrodinger equation into *N*-body case such that

$$\hat{H} = \sum_{j=1}^{N} \frac{\hat{\vec{P}}_j^2}{2m_j} + \hat{V}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t) = -\sum_{j=1}^{N} \frac{\hbar^2}{2m_j} \nabla_j^2 + \hat{V}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t)$$

Commutation relations

Operators acting on different particles commute, for e.g.

$$[\hat{X}_j, \hat{P}_{x_k}] = i\hbar \delta_{j,k}$$

$$[\hat{P}_{x_j}, \hat{P}_{x_k}] = 0$$

$$[\hat{X}_j, \hat{X}_k] = 0$$

for $j, k = 1,2,3 \ldots N$

The many-body problem – stationary states

When the potential does not dependent on time $\hat{V}(r, t) \rightarrow \hat{V}(r)$, the general Schrodinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t) = \hat{H}\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t)$$

Is written as

$$\left[-\sum_{j=1}^{N} \frac{\hbar^2}{2m_j} \vec{\nabla}_j^2 + V(\vec{r}_1, \ldots, \vec{r}_N) \right] \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = E \, \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$$

With the wave function now given by

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t) = \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \, e^{-iEt/\hbar}.$$

The many-body problem – permutation operator

Let us denote ξ_i to represent coordinates of the particles (position, spin and other internal degrees of freedom).

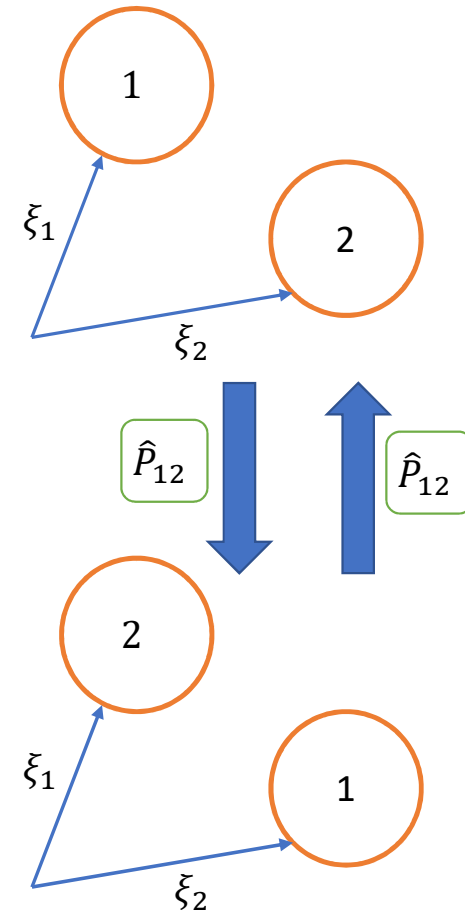We define an operator $\hat{P}_{ij}$ acting to interchange the i_{th} and j_{th} particle such that

$$\hat{P}_{ij}\psi(\xi_1, \dots \xi_i, \dots \xi_j, \dots \xi_N) = \psi(\xi_1, \dots \xi_j, \dots \xi_i, \dots \xi_N)$$

Applying two successive operations of $\hat{P}_{ij}$ on the wave function, we have

$$\hat{P}_{ij}^2\psi(\xi_1, \dots \xi_i, \dots \xi_j, \dots \xi_N) = \hat{P}_{ij}\psi(\xi_1, \dots \xi_j, \dots \xi_i, \dots \xi_N) = \psi(\xi_1, \dots \xi_i, \dots \xi_j, \dots \xi_N)$$

Therefore, $\boxed{\hat{P}_{ij}^2 = 1 \text{ and } \hat{P}_{ij} = \pm 1}$

i.e.
$$\hat{P}_{ij}\psi(\xi_1, \dots \xi_i, \dots \xi_j, \dots \xi_N) = \pm\psi(\xi_1, \dots \xi_i, \dots \xi_j, \dots \xi_N)$$
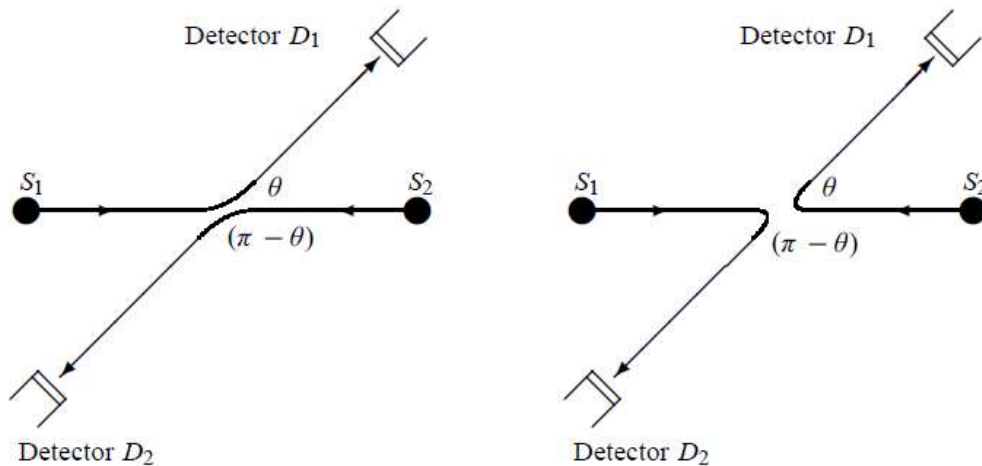
The many-body problem – System of indistinguishable particles

Unlike macroscopic objects, identical particles cannot be distinguished. Why?

Physicists are only able to specify a **complete set of commuting observables** to identify a particle. Nothing more!

The **uncertainty principle** limits the exact information on the location of the particle.

Detector D_1

S_1 θ S_2
$(\pi - \theta)$

Detector D_2

Detector D_1

S_1 θ S_2
$(\pi - \theta)$

Detector D_2

The **probability** must remain the same with interchange of particles.

$$\left|\psi(\xi_1, \dots \xi_i, \dots \xi_j, \dots \xi_N)\right|^2 = \left|\psi(\xi_1, \dots \xi_j, \dots \xi_i, \dots \xi_N)\right|^2$$

Consequence:
Symmetrization postulate says that system with N number of particles is <u>either totally symmetric or antisymmetric</u> under interchange of particles.

The symmetric w.f. for two-particle system is

$$\psi_s(\xi_1, \xi_2) = \frac{1}{\sqrt{2}}\left[\psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2) + \psi_{n_1}(\xi_2)\psi_{n_2}(\xi_1)\right]$$

While the antisymmetric part is

$$\psi_a(\xi_1, \xi_2) = \frac{1}{\sqrt{2}}\left[\psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2) - \psi_{n_1}(\xi_2)\psi_{n_2}(\xi_1)\right]$$

The many-body problem – System of identical non-interacting particles

For a system where all particles have <u>equal mass</u> and experience the <u>same potential</u> i.e. $\hat{V}_i(\xi_i) = \hat{V}(\xi_i)$, the Schrodinger equation for the whole system can be reduced into **N identical <u>one-particle equations</u>**:

$$\left[-\frac{\hbar^2}{2m}\nabla_i^2 + \hat{V}(\xi_i)\right]\psi_{n_i}(\xi_i) = \varepsilon_{n_i}\psi_{n_i}(\xi_i)$$

With the total energy of the system given by a sum of the single-particle energies ε_{n_i}; $E = \sum_i^N \varepsilon_{n_i}$

How about the total wave function?
Can we write it as:

$$\psi_{n_1,n_2,\ldots,n_N}(\xi_1, \ldots \xi_i, \ldots \xi_j, \ldots \xi_N) = \prod_{i=1}^N \psi_{n_i}(\xi_i)$$

No for two reasons

If the wave function is valid, it means that one can <u>identify particle</u> #1 at ξ_1, #2 at ξ_2 etc.

But there is no way to distinguish identical microscopic particles.

The wave function <u>do not have definite parity</u>. For identical particles, the wave function must either be symmetric or antisymmetric.

The many-body problem – System of identical non-interacting particles

Constructing the total wave function using single-particle wave functions

The symmetric wave function is written as:

Two particles system

$$\psi_s(\xi_1, \xi_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2) + \psi_{n_1}(\xi_2)\psi_{n_2}(\xi_1) \right]$$

$$= \frac{1}{\sqrt{2!}} \sum_P \hat{P} \psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2),$$

while the antisymmetric wave function is:

$$\psi_a(\xi_1, \xi_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2) - \psi_{n_1}(\xi_2)\psi_{n_2}(\xi_1) \right]$$

$$= \frac{1}{\sqrt{2!}} \begin{vmatrix} \psi_{n_1}(\xi_1) & \psi_{n_1}(\xi_2) \\ \psi_{n_2}(\xi_1) & \psi_{n_2}(\xi_2) \end{vmatrix}$$

$$= \frac{1}{\sqrt{2!}} \sum_P (-1)^P \hat{P} \psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2)$$

The many-body problem – System of identical non-interacting particles

Constructing the total wave function using single-particle wave functions

The symmetric wave function is written as:

Three particles system

$$\psi_s(\xi_1, \xi_2, \xi_3) = \frac{1}{\sqrt{3!}}\Big[\psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2)\psi_{n_3}(\xi_3) + \psi_{n_1}(\xi_1)\psi_{n_2}(\xi_3)\psi_{n_3}(\xi_2)$$

$$+ \psi_{n_1}(\xi_2)\psi_{n_2}(\xi_1)\psi_{n_3}(\xi_3) + \psi_{n_1}(\xi_2)\psi_{n_2}(\xi_3)\psi_{n_3}(\xi_1)$$

$$+ \psi_{n_1}(\xi_3)\psi_{n_2}(\xi_1)\psi_{n_3}(\xi_2) + \psi_{n_1}(\xi_3)\psi_{n_2}(\xi_2)\psi_{n_3}(\xi_1)\Big]$$

$$= \frac{1}{\sqrt{3!}}\sum_P \hat{P}\psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2)\psi_{n_3}(\xi_3)$$

while antisymmetric wave function is:

$$\psi_a(\xi_1, \xi_2, \xi_3) = \frac{1}{\sqrt{3!}}\sum_P (-1)^P \hat{P}\psi_{n_1}(\xi_1)\psi_{n_2}(\xi_2)\psi_{n_3}(\xi_3)$$

$$= \frac{1}{\sqrt{3!}}\begin{vmatrix} \psi_{n_1}(\xi_1) & \psi_{n_1}(\xi_2) & \psi_{n_1}(\xi_3) \\ \psi_{n_2}(\xi_1) & \psi_{n_2}(\xi_2) & \psi_{n_2}(\xi_3) \\ \psi_{n_3}(\xi_1) & \psi_{n_3}(\xi_2) & \psi_{n_3}(\xi_3) \end{vmatrix}$$

The many-body problem – System of identical non-interacting particles

The symmetric wave function is written as:

$$\psi_s(\xi_1, \xi_2, \ldots, \xi_N) = \frac{1}{\sqrt{N!}} \sum_P \hat{P} \psi_{n_1}(\xi_1) \psi_{n_2}(\xi_2) \cdots \psi_{n_N}(\xi_N)$$

Generalizing to many-particle system

while antisymmetric wave function is:

$$\psi_a(\xi_1, \xi_2, \ldots, \xi_N) = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \psi_{n_1}(\xi_1) \psi_{n_2}(\xi_2) \cdots \psi_{n_N}(\xi_N)$$

$$\psi_a(\xi_1, \xi_2, \ldots, \xi_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{n_1}(\xi_1) & \psi_{n_1}(\xi_2) & \cdots & \psi_{n_1}(\xi_N) \\ \psi_{n_2}(\xi_1) & \psi_{n_2}(\xi_2) & \cdots & \psi_{n_2}(\xi_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{n_N}(\xi_1) & \psi_{n_N}(\xi_2) & \cdots & \psi_{n_N}(\xi_N) \end{vmatrix}$$

The $N \times N$ determinant is known as **Slater determinant**

Pauli exclusion principle
➤ If $n_1 = n_2$, $\psi_a = 0$.
➤ *No two particles can occupy simultaneously the same quantum state of the same fermionic system.*

The many-body problem – System of identical non-interacting particles

The total wave function involves both spatial and spin part and can be written as:

$$\Psi(\vec{r}_1, \vec{S}_1; \vec{r}_2, \vec{S}_2; \ldots; \vec{r}_N, \vec{S}_N) = \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)\chi(\vec{S}_1, \vec{S}_2, \ldots, \vec{S}_N)$$

Spatial   **Spin**

For bosons, total wave function must be **symmetric**.

$$\Psi_{boson} = \begin{cases} \psi_s(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N)\chi_s(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) \\ \psi_a(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N)\chi_a(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) \end{cases}$$

For fermions, total wave function must be **antisymmetric**.
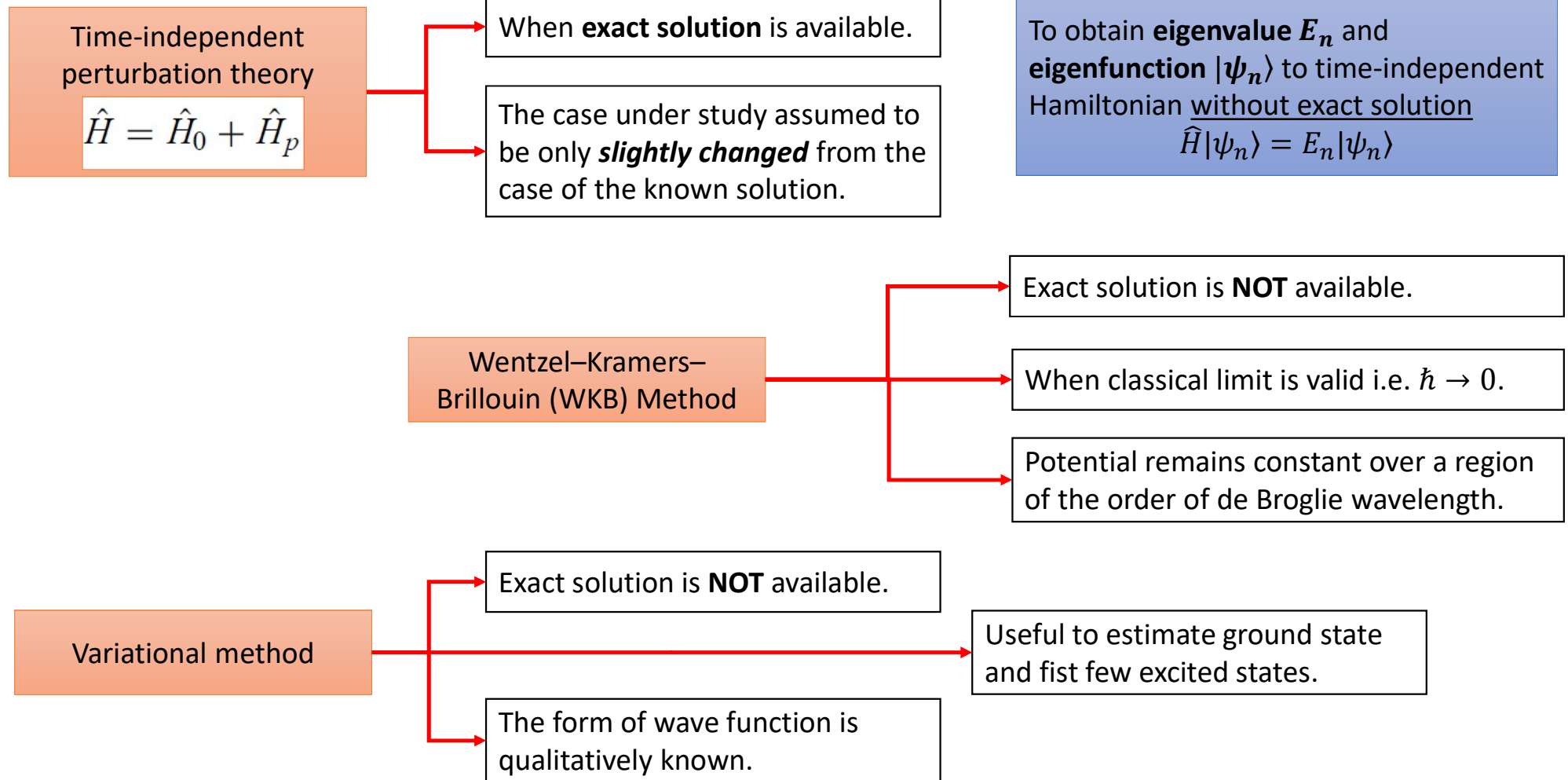
$$\Psi_{boson} = \begin{cases} \psi_a(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N)\chi_s(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) \\ \psi_s(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N)\chi_a(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) \end{cases}$$

Part 1:
Going back to quantum mechanics

- ~~Identical particle and many-body problem~~

- Approximations for stationary states – variational method

Approximations to stationary states – time-independent case

Time-independent perturbation theory

$$\hat{H} = \hat{H}_0 + \hat{H}_p$$

When **exact solution** is available.

The case under study assumed to be only *slightly changed* from the case of the known solution.

To obtain **eigenvalue E_n** and **eigenfunction $|\psi_n\rangle$** to time-independent Hamiltonian <u>without exact solution</u>
$$\widehat{H}|\psi_n\rangle = E_n|\psi_n\rangle$$

Wentzel–Kramers–Brillouin (WKB) Method

Exact solution is **NOT** available.

When classical limit is valid i.e. $\hbar \to 0$.

Potential remains constant over a region of the order of de Broglie wavelength.

Variational method

Exact solution is **NOT** available.

Useful to estimate ground state and fist few excited states.

The form of wave function is qualitatively known.

Approximations to stationary states – Variational method

Variational equation

Instead of solving the eigenvalue equation $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ directly, the aim is to solve variational equation
$$\delta E[\psi] = 0$$
with
$$E[\psi] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$
If $|\psi\rangle$ depends on parameter α, then E also depends on α.

Aim: Vary α to minimize E.

Solving the variational equation;
$$\delta E[\psi] = \delta\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \implies \delta E[\psi] = \delta\langle\psi|\hat{H}|\psi\rangle = 0$$

We then have
$$\delta\langle\psi|\hat{H}|\psi\rangle = \langle\delta\psi|\hat{H}|\psi\rangle + \langle\psi|\hat{H}|\delta\psi\rangle = 0$$

i.e. varying $\langle\delta\psi|\hat{H}|\psi\rangle$ is equivalent to varying its complex conjugate term.

Approximate solution is always higher or equal to the exact solution E_0

Expand the wave function $|\Psi\rangle$ as $|\psi\rangle = \sum_n a_n|\psi_n\rangle$ with $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$

$$E \geq E_0$$

The quantity $E[\psi]$ is then
$$E[\psi] = \frac{\sum_n E_n|a_n|^2}{\sum_n|a_n|^2} \geq \frac{E_0\sum_n|a_n|^2}{\sum_n|a_n|^2} = E_0$$

Full Hilbert space

$E_0 < E' < E''$

E_0

Axial + parity symmetry

E'

Parity symmetry

E''

Approximations to stationary states – Variational method

1 Guess the form of initial wavefunction
Note:
- takes into account all physical properties e.g. symmetries, number of nodes etc.

- adjustable parameters (e.g. $\alpha_1, \alpha_2, ...$) to represent information that we are not sure off.

2 Write the mathematical expression for total energy depending on the various parameters.

$$E(\alpha_1, \alpha_2, ...) = \frac{\langle \psi(\alpha_1, \alpha_2, ...) | \hat{H} | \psi(\alpha_1, \alpha_2, ...) \rangle}{\langle \psi(\alpha_1, \alpha_2, ...) | \psi(\alpha_1, \alpha_2, ...) \rangle}$$

3 Search for the minimum energy by minimizing E with respect to parameters α_i

$$\frac{\partial E(\alpha_1, \alpha_2, ...)}{\partial \alpha_i} = 0$$

To obtain values of $(\alpha_1, \alpha_2, ...)$ that yield minimum E.

4 Insert values of $(\alpha_1, \alpha_2, ...)$ to obtain approximate value of energy

Part 2: Hartree-Fock approach

The Hartree-Fock approach and approximations

Starting from the many-body Hamiltonian operator

$$\widehat{H} = -\sum_{i}^{N} \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i,j=1}^{N}\widehat{V}(r_i, r_j)$$

Kinetic energy operator

Two-body interaction

Assumption:

The wave function of the system can be approximated by a Slater determinant

➢ single-particle (s.p) wave function with s.p. energy e_i obtain after solving the HF equation.

$$\psi(r_1, r_2, \dots r_N) = \frac{1}{\sqrt{N!}}\begin{Vmatrix}\begin{bmatrix}\varphi_1(r_1) & \cdots & \varphi_1(r_N)\\ \vdots & \ddots & \vdots\\ \varphi_N(r_1) & \cdots & \varphi_N(r_N)\end{bmatrix}\end{Vmatrix}$$

The expectation value of the Hamiltonian with respect to the Slater determinant is

$$\langle\psi|\widehat{H}|\psi\rangle = \sum_{i=1}^{N}\langle i|\hat{t}_i|i\rangle + \frac{1}{2}\sum_{i,j=1}^{N}\langle ij|\widehat{V}\{|ij\rangle - |ji\rangle\}$$

$$= \sum_{i=1}^{N}\int \varphi_i^*(r)\left(-\frac{\hbar^2}{2m}\nabla_i^2\right)\varphi_i(r)dr + \frac{1}{2}\sum_{i,j=1}^{N}\int \varphi_i^*(r)\varphi_j^*(r')\hat{v}(r,r')\varphi_i(r)\varphi_j(r')$$

Exchange term

$$-\frac{1}{2}\sum_{i,j=1}^{N}\int \varphi_i^*(r)\varphi_j^*(r')\hat{v}(r,r')\varphi_j(r)\varphi_i(r')$$

The Hartree-Fock approach and approximations

Varying the expectation value of the Hamiltonian operator with respect to all single-particle wave functions

$$\frac{\delta}{\delta\varphi_i^*(x)}\left[\langle\varphi|\widehat{H}|\varphi\rangle - \sum_{i=1}^{N}\varepsilon_i\int\varphi^*(y)\varphi(y)dr\right] = 0$$

Taking variation of one single-particle wave function with respect to another

$$\frac{\delta\varphi_i^*(y)}{\delta\varphi_j^*(x)} = \delta_{ib}\delta(x-y)$$

We have

$$\frac{\delta}{\delta\varphi_b^*(x)}\left\{\sum_{i=1}^{N}\int\varphi_i^*(y)\hat{t}(y)\varphi_i(y)dy + \frac{1}{2}\sum_{i,j=1}^{N}\int\int\varphi_i^*(y)\varphi_j^*(y')\hat{v}(y,y')\varphi_i(y)\varphi_j(y')dy\,dy'\right.$$

$$\left.-\frac{1}{2}\sum_{i,j=1}^{N}\int\int\varphi_i^*(y)\varphi_j^*(y')\hat{v}(y,y')\varphi_j(y)\varphi_i(y')dy\,dy' - \sum_{i=1}^{N}e_i\int\varphi_i^*(y)\varphi_i(y)dr\right\} = 0$$

$$\hat{t}(x)\varphi_i(x) + \frac{1}{2}\sum_{j=1}^{N}\int\varphi_j^*(y')\hat{v}(x,y')\varphi_b(x)\varphi_j(y')dy' + \frac{1}{2}\sum_{i=1}^{N}\int\varphi_i^*(y)\hat{v}(y,x)\varphi_i(y)\varphi_b(x)dy$$

$$-\frac{1}{2}\sum_{j=1}^{N}\int\varphi_j^*(y')\hat{v}(x,y')\varphi_j(x)\varphi_b(y')dy' - \frac{1}{2}\sum_{i=1}^{N}\int\varphi_i^*(y)\hat{v}(y,x)\varphi_b(y)\varphi_i(x)dy - e_b\varphi_b(x) = 0$$

The Hartree-Fock approach and approximations

$$\hat{t}(x)\varphi_i(x) + \frac{1}{2}\sum_{j=1}^{N}\int \varphi_j^*(y')\hat{v}(x,y')\varphi_b(x)\varphi_j(y')dy' + \frac{1}{2}\sum_{i=1}^{N}\int \varphi_i^*(y)\hat{v}(y,x)\varphi_i(y)\varphi_b(x)dy$$

$$-\frac{1}{2}\sum_{j=1}^{N}\int \varphi_j^*(y')\hat{v}(x,y')\varphi_j(x)\varphi_b(y')dy' - \frac{1}{2}\sum_{i=1}^{N}\int \varphi_i^*(y)\hat{v}(y,x)\varphi_b(y)\varphi_i(x)dy - e_b\varphi_b(x) = 0$$

Relabel the index j to i and coordinate representation y' to y.

$$\frac{1}{2}\sum_{i=1}^{N}\int \varphi_j^*(y)\hat{v}(x,y)\varphi_b(x)\varphi_j(y)dy + \frac{1}{2}\sum_{i=1}^{N}\int \varphi_i^*(y)\hat{v}(y,x)\varphi_i(y)\varphi_b(x)dy$$

The force between nucleons
$$\hat{v}(y,x) = \hat{v}(x,y)$$

$$= \left\{\sum_{i=1}^{N}\int \varphi_i^*(y)\hat{v}(x,y)\varphi_j(y)dy\right\}\varphi_b(x)$$

The Hartree-Fock approach and approximations

Applying the same steps to the other terms, we have the Hartree-Fock equations written as:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + \sum_{i=1}^{N}\int \varphi_i^*(y)\hat{v}(x,y)\varphi_j(y)\,dy\right\}\varphi_b(x) - \sum_{i=1}^{N}\int \varphi_i^*(x)\hat{v}(x,y)\varphi_i(y)\varphi_b(y)\,dy = e_b\varphi_b(x)$$

Shorthand notation for one-body density matrix

$$\rho(y) = \sum_{i=1}^{N}\varphi_i^*(y)\varphi_i(y)$$

$$\rho(x,y) = \sum_{i=1}^{N}\varphi_i^*(x)\varphi_i(y)$$

SUMMARY:
Reduction from many-body to one-body problem.

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + \int \rho(y)\hat{v}(x,y)\,dy\right\}\varphi_b(x) - \sum_{i=1}^{N}\int \rho(x,y)\hat{v}(x,y)\varphi_b(y)\,dy = e_b\varphi_b(x)$$

Schrodinger-like equation – to solve for e_b and $\varphi_b(x)$

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + \int \rho(y)\hat{v}(x,y)\,dy\right\}\varphi_b(x) \; \boldsymbol{+} \; \boxed{\text{Non-local term}} = e_b\varphi_b(x)$$

Hartree term

Fock term

Example: Case of density-dependent interaction

Assuming that the potential is written as:
$$\hat{V}(r_1, r_2) = a\delta(r_1 - r_2) + b\rho\left(\frac{r_1 + r_2}{2}\right)\delta(r_1 - r_2)$$

With a and b as parameters to be adjusted.

The expectation value of the potential operator is
$$\langle\hat{V}\rangle = a\int\int \rho(r_1)\rho(r_2)\delta(r_1 - r_2)dr_1 dr_2$$
$$+ba\int\int \rho(r_1)\rho(r_2)\rho\left(\frac{r_1 + r_2}{2}\right)\delta(r_1 - r_2)dr_1 dr_2$$
$$= a\int \rho^2(r)dr + b\int \rho^3(r)dr$$

Variation of $\rho(r)$ with respect to single-particle state$\varphi_b(x)$

$$\frac{\delta}{\delta\varphi_b^*(x)}\rho(r) = \frac{\delta}{\delta\varphi_b^*(x)}\sum_i \varphi_i^*(r)\varphi_i(r)$$
$$= \sum_i \delta_{ib}\delta(r - x)\varphi_i(r)$$
$$= \delta(r - x)\varphi_b(r)$$

The <u>variation</u> of the expectation value of the potential is then
$$\langle\hat{V}\rangle = 2a\int \rho(r)\varphi_b(r)\delta(r - x)dr + 3b\int \rho^2(r)\varphi_b(r)\delta(r - x)dr$$
$$= 2a\rho(x)\varphi_b(x) + 3b\,\rho^2(x)\varphi_b(x)$$
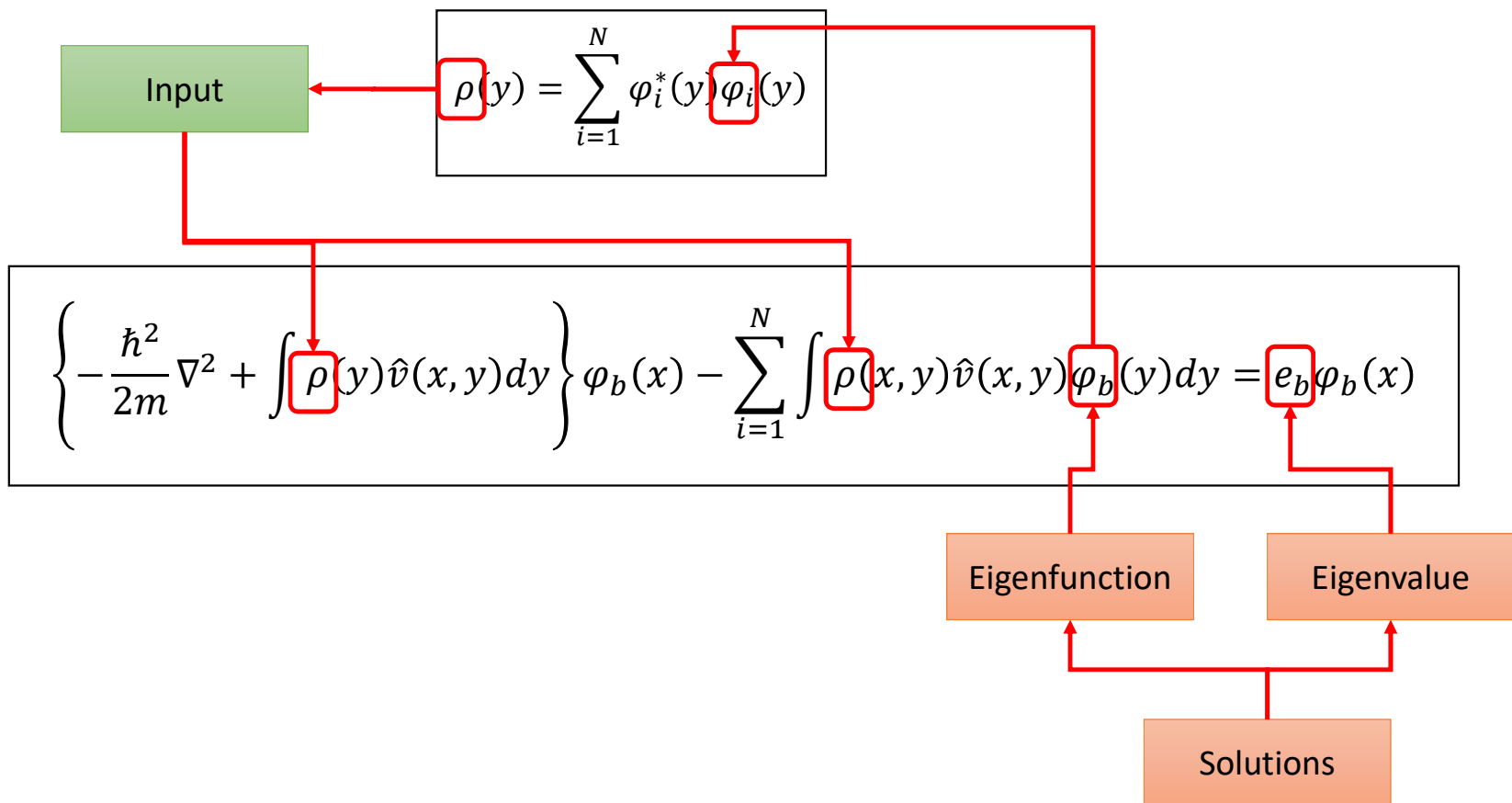
Ignoring the Fock term, the Hamiltonian is then written using the potential obtained previously
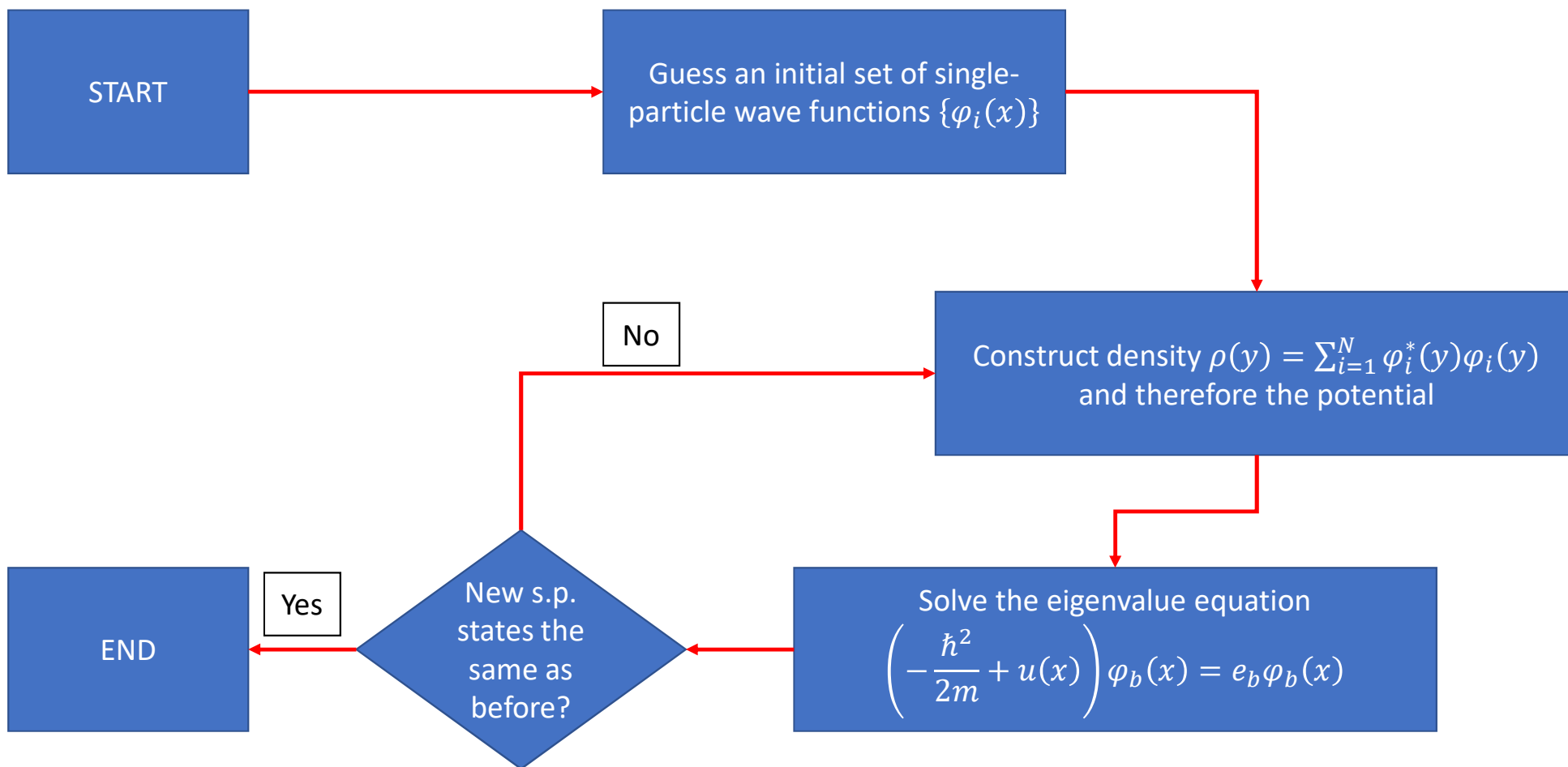$$\langle\hat{V}\rangle = 2a\rho(x)\varphi_b(x) + 3b\,\rho^2(x)\varphi_b(x)$$

The Hartree equation is written as
$$\left(-\frac{\hbar^2}{2m} + [2a\rho(x) + 3b\,\rho^2(x)]\right)\varphi_b(x) = e_b\varphi_b(x)$$

The Hartree-Fock equation: non-linearity

Steps to solving the Hartree-Fock equation

```
┌─────────────┐                  ┌──────────────────────────────┐
│             │                  │  Guess an initial set of single-│
│   START     │ ───────────────► │  particle wave functions $\{\varphi_i(x)\}$│
│             │                  │                              │
└─────────────┘                  └──────────────────────────────┘
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Construct density $\rho(y) = \sum_{i=1}^{N} \varphi_i^*(y)\varphi_i(y)$ and therefore the potential

No

Solve the eigenvalue equation
$$\left(-\frac{\hbar^2}{2m} + u(x)\right)\varphi_b(x) = e_b\varphi_b(x)$$

New s.p. states the same as before?
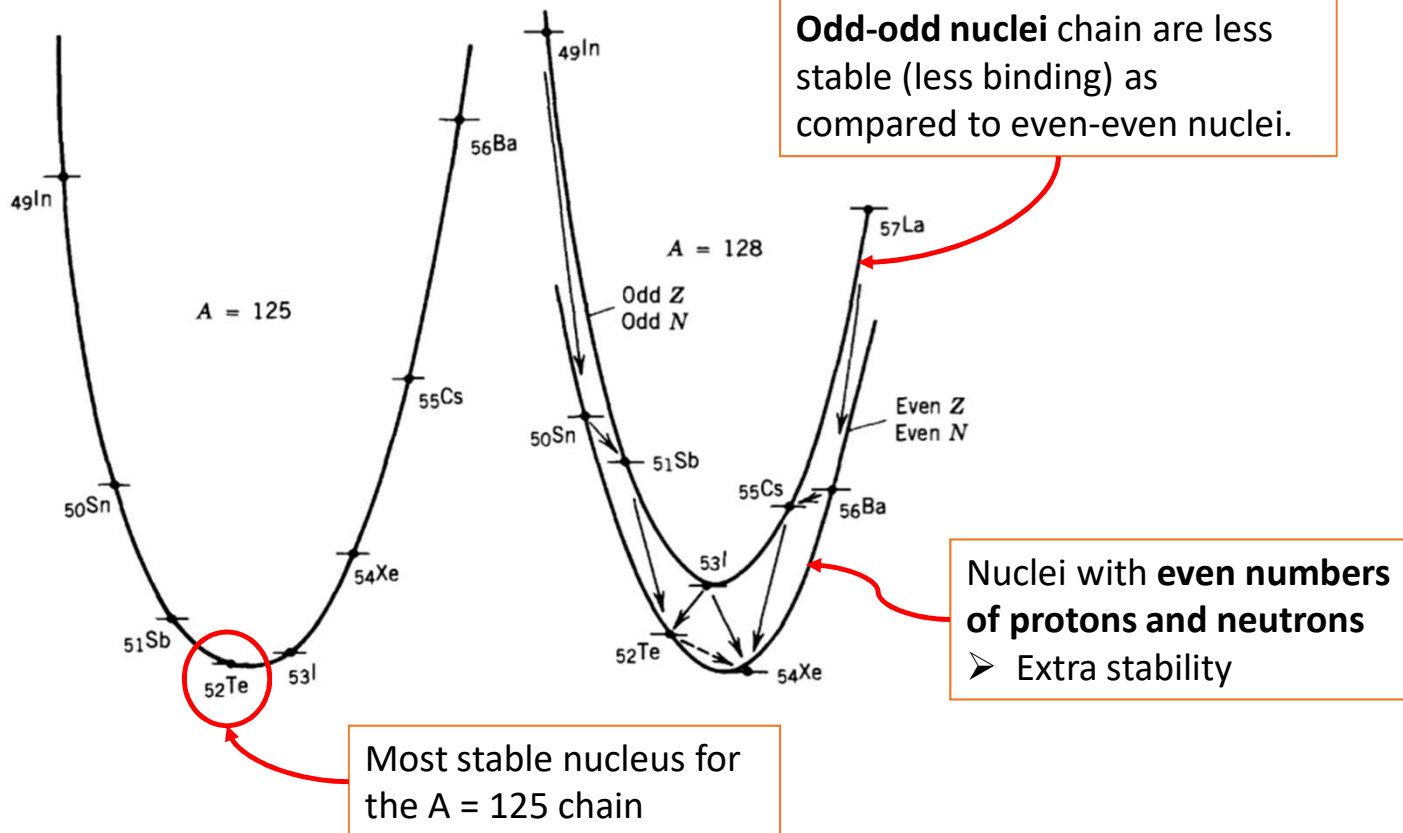
Yes

END

Part 3:
Including pairing correlations

Why pairing is important?

Mass parabola showing the effect of pairing correlations

[taken from Introductory Nuclear Physics by Kenneth Krane]

Odd-odd nuclei chain are less stable (less binding) as compared to even-even nuclei.

Nuclei with **even numbers of protons and neutrons**
➢ Extra stability

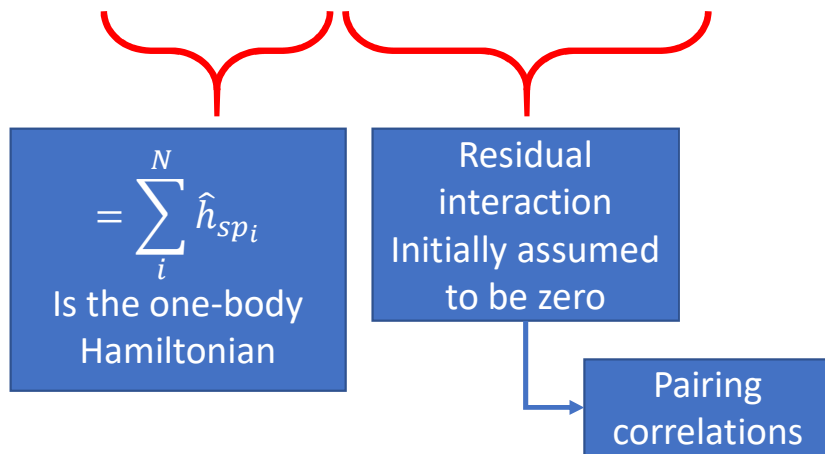Most stable nucleus for the A = 125 chain

How to include pairing into the Hartree-Fock framework?

Starting from the many-body Hamiltonian

$$\hat{H} = \sum_i^N \hat{t}_i + \sum_{i,j=1}^N \hat{V}(r_i, r_j)$$

We introduce an average (mean) potential such that

$$\hat{H} = \sum_i^N (\hat{t}_i + \hat{U}_i) + \sum_{i,j=1}^N (\hat{V}(r_i, r_j) - \hat{U}_i)$$

$$= \sum_i^N \hat{h}_{sp_i}$$

Is the one-body Hamiltonian

Residual interaction
Initially assumed to be zero

Pairing correlations

Within the HF framework, pairing correlations are treated using the BCS approach

Proposed by Bardeen, Cooper, Schrieffer to explain superconductivity in metals

Assumptions:
Condensation of two fermions (called as **Cooper pairs**) into boson-like state.

Attraction between the Cooper pairs is strong enough to overcome Coulomb repulsion between similar charges.

Note:
HF+BCS as an approximation to **Hartree-Fock-Bogoliubov** approach. Found to be equivalent for nuclei near the line of stability.

The BCS wave function

BCS wave function for **ground-state** of an **even-even nucleus** is written:

$$|\text{BCS}\rangle = \prod_{\Omega_k > 0} \left(u_k + v_k \, a_k^+ \, a_{\bar{k}}^+ \right) |0\rangle$$

A vacuum state with no nucleons

The z-component of angular momentum
$$\hat{J}_z |\varphi_k\rangle = \Omega_k |\varphi_k\rangle$$

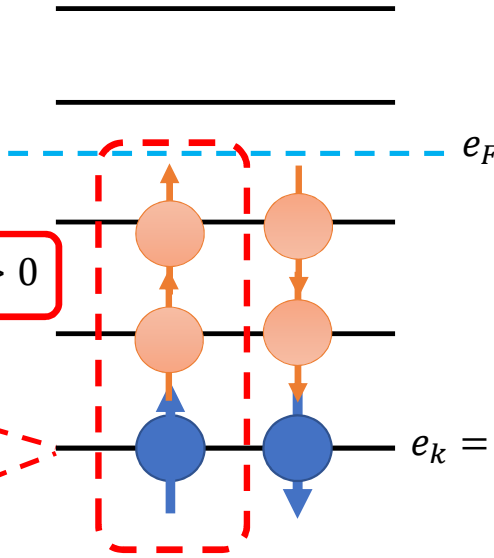Probability for the single-particle state k to be **empty**.

Probability for the single-particle state k to be **filled**.

Creation operator
➤ Remove 1 particle in conjugate state $\bar{k}$

Creation operator
➤ Creating 1 particle in s.p state k.

Simple illustration of BCS wave function
(g.s even-even nucleus)

$\Omega_k > 0$

Normalization of the BCS wave function yields
$$\langle \text{BCS}|\text{BCS}\rangle = \prod_{\Omega_k > 0} \left(u_k^2 + v_k^2 \right)$$

With $u_k^2 + v_k^2 = 1$
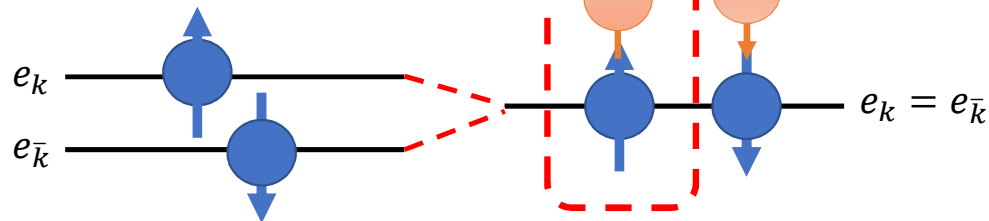
The BCS Hamiltonian & particle number uncertainty

The Hamiltonian to be solved has the form of
$$\hat{H}' = \hat{H} - \boxed{\lambda \hat{N}}$$

A term to constraint the number of particles (nucleons) to a desired value.

Such that
$$\hat{H}' = \sum_{\Omega_k} (e_k - \boxed{\lambda}) a_k^+ a_k + \sum_{\Omega_k, \Omega_k'} \boxed{\langle k\bar{k}|v|k'\bar{k}'\rangle} a_k^+ a_{\bar{k}}^+ \boxed{a_{\bar{k}'} a_{k'}}$$

λ is a **Lagrange multiplier** whose function is that of a chemical energy.

Annihilation operator

The **particle number operator** is defined as
$$\hat{N} = \sum_{\Omega_k} a_k^+ a_k$$
Expectation value of particle number with respect to BCS wave function is
$$\langle \mathrm{BCS}|\hat{N}|\mathrm{BCS}\rangle = 2 \sum_{\Omega_k > 0} v_k^2$$

Residual pairing interaction term acting on nucleon pairs
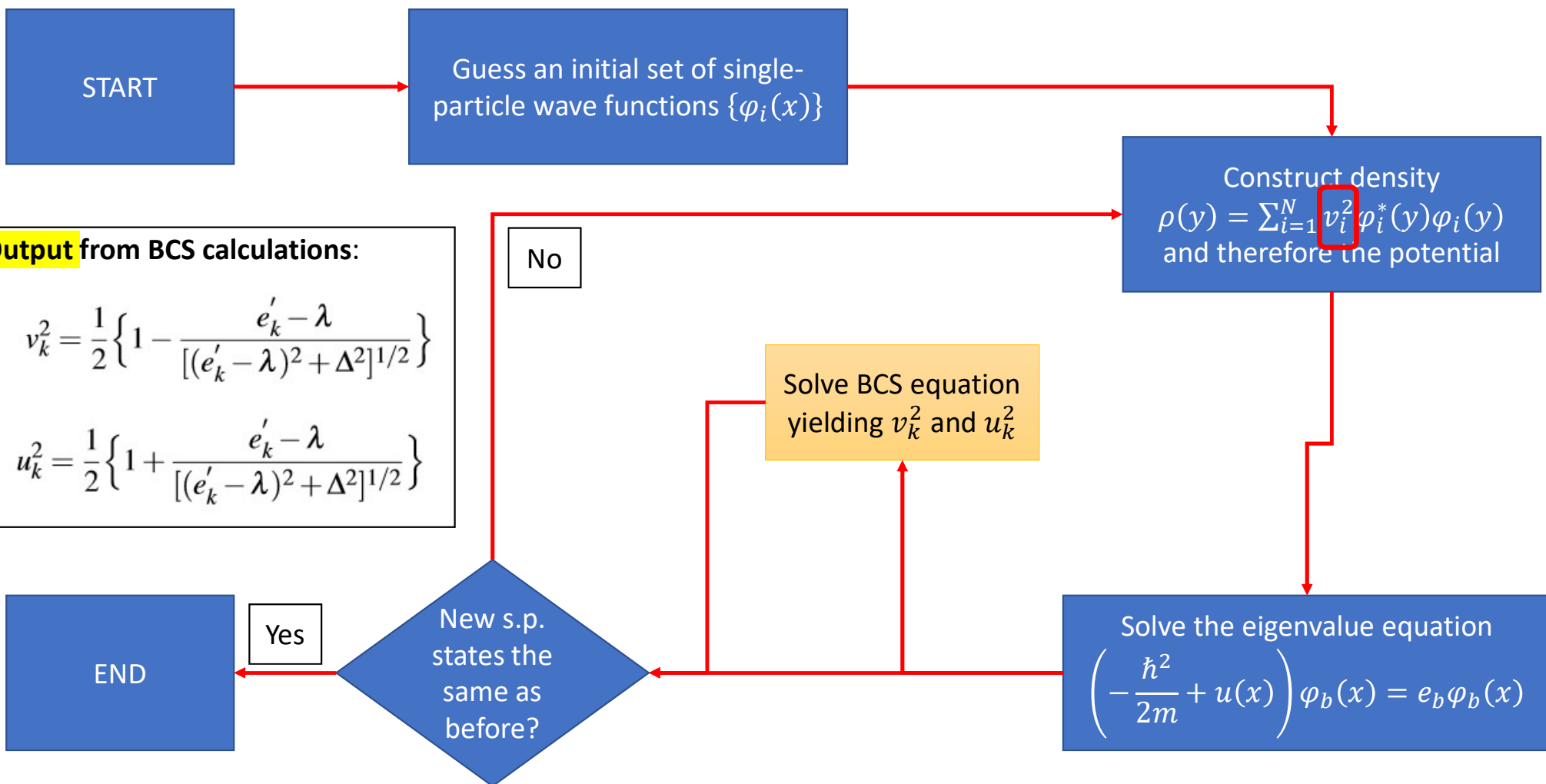
Choice of residual interaction
- Density dependent delta
- Gaussian
- Separable pairing
- **Seniority force**

The uncertainty in the particle number is
$$(\Delta N)^2 = \langle \mathrm{BCS}|\hat{N}^2|\mathrm{BCS}\rangle - \langle \mathrm{BCS}|\hat{N}|\mathrm{BCS}\rangle^2$$
$$= 4 \sum_{\Omega_k > 0} u_k^2 v_k^2$$

Weakness of BCS approach: Number of particle is not conserved!

Consequence of BCS pairing on calculations

```
START ──→ Guess an initial set of single-
          particle wave functions $\{\varphi_i(x)\}$
```

Construct density
$$\rho(y) = \sum_{i=1}^{N} v_i^2 \varphi_i^*(y)\varphi_i(y)$$
and therefore the potential

No

Output from BCS calculations:

$$v_k^2 = \frac{1}{2}\left\{1 - \frac{e_k' - \lambda}{[(e_k' - \lambda)^2 + \Delta^2]^{1/2}}\right\}$$

$$u_k^2 = \frac{1}{2}\left\{1 + \frac{e_k' - \lambda}{[(e_k' - \lambda)^2 + \Delta^2]^{1/2}}\right\}$$

Solve BCS equation
yielding v_k^2 and u_k^2

Solve the eigenvalue equation
$$\left(-\frac{\hbar^2}{2m} + u(x)\right)\varphi_b(x) = e_b\varphi_b(x)$$

New s.p.
states the
same as
before?

Yes

END

Part 4:
Phenomenological nucleon-nucleon interaction

Properties of nucleon-nucleon interaction

Dependence on inter-nucleon distance

Force [10^{-4} N]

repulsive

attractive

0

1   2   3

Nucleon
separation
[fm]
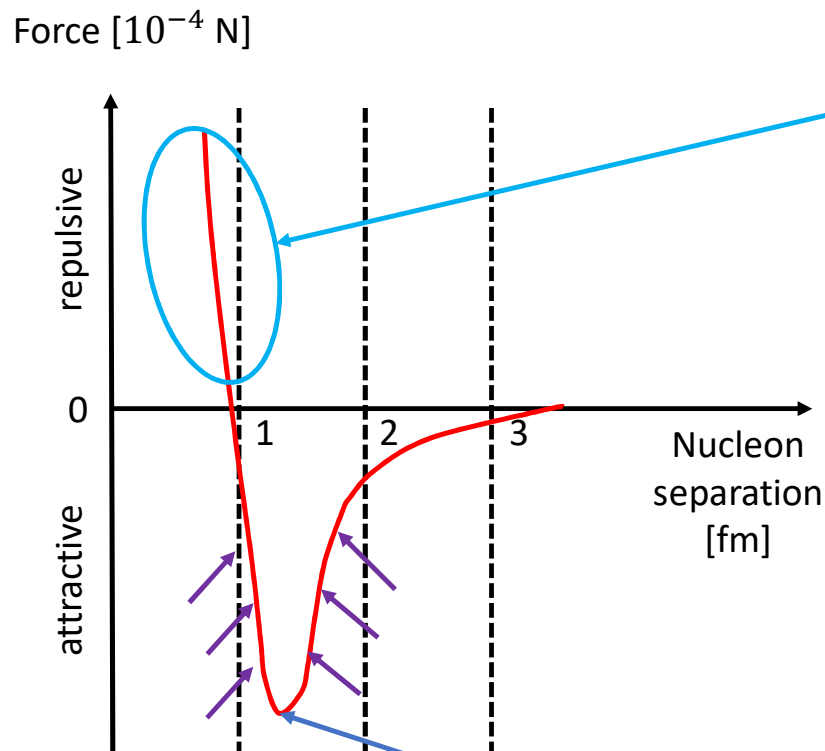
When the nucleon
gets too near, they
repulse one another.

But at short distance, nuclear force
is stronger than Coulomb allowing
it to bind protons together.

Nuclear force is **attractive** when nucleons are
further from their optimal separation distance.

Optimal distance
between two nucleons

Properties of nucleon-nucleon interaction

We begin by identifying the eigenvalue of the spin operator as
$$\hat{S}^2 = S(S+1)\hbar^2$$
where $\hat{S}$ is the total spin of neutron and proton i.e.
$$\hat{S} = \hat{S}_n + \hat{S}_p$$
NB: In this case, the lowest single-particle state has orbital angular momentum $l = 0$.
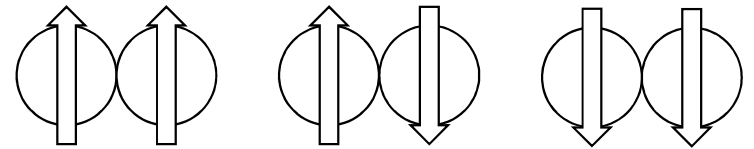
Inserting the equation into the first one, we obtained
$$\hat{S}^2 = \left(\hat{S}_n + \hat{S}_p\right)^2 = \hat{S}_n{}^2 + \hat{S}_p{}^2 + 2\hat{S}_n \cdot \hat{S}_p$$

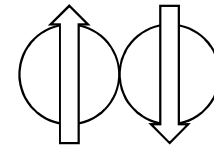$$\hat{S}_n \cdot \hat{S}_p = \frac{1}{2}\left(\hat{S}^2 - \hat{S}_n{}^2 - \hat{S}_p{}^2\right)$$

$$\langle \hat{S}_n \cdot \hat{S}_p \rangle = \frac{\hbar^2}{2}\left(S(S+1) - \frac{3}{2}\right)$$

Spin, S = 1 channel
(Triplet state)

Spin, S = 0 channel
(Singlet state)

$$\langle \hat{S}_n \cdot \hat{S}_p \rangle = \begin{cases} +\dfrac{\hbar^2}{4} \quad ; \ \text{Triplet state} \\[2mm] -\dfrac{3\hbar^2}{4} \quad ; \text{Singlet state} \end{cases}$$

Attractive force
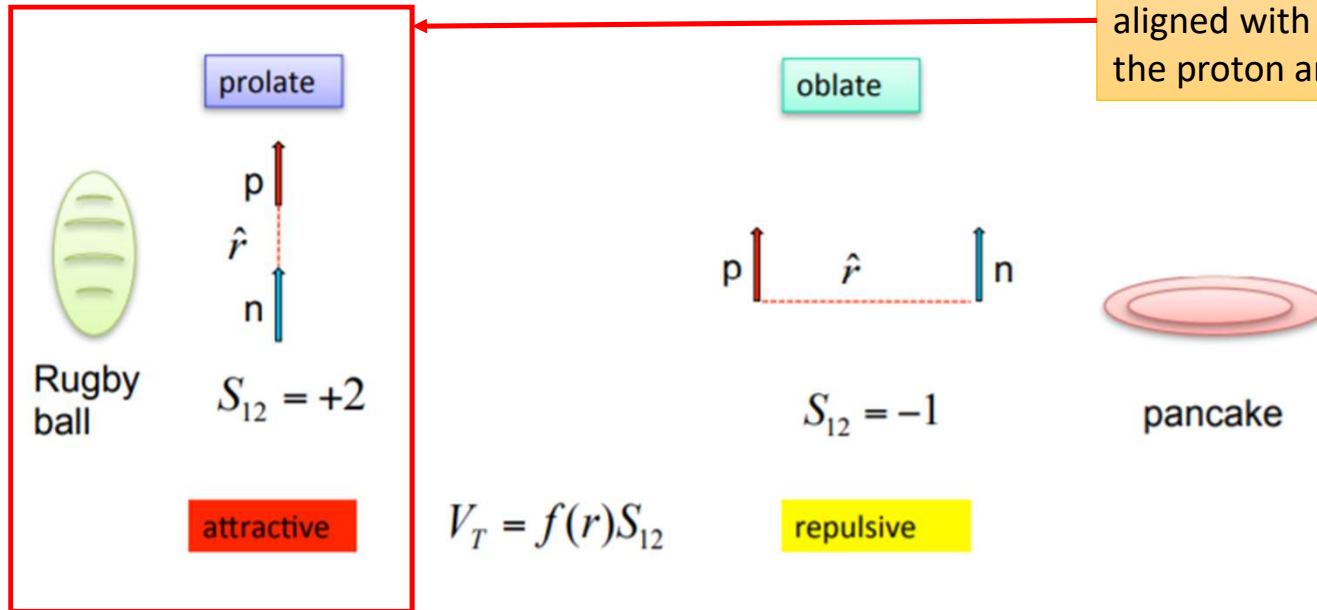
Properties of nucleon-nucleon interaction

Dependence on tensor component

$$S_{12} = [(\vec{\sigma}_1 \times \vec{\sigma}_2)^{(2)} \times Y_2(\hat{r})]^{(0)} \propto 3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

When the orientation of the spins are aligned with the relative distance of the proton and neutron.

prolate

p
$\hat{r}$
n

Rugby ball

$S_{12} = +2$

attractive

$V_T = f(r)S_{12}$

oblate

p $\hat{r}$ n

$S_{12} = -1$

pancake

repulsive

Diagram taken from H. Sagawa and G. Colo [arXiv:1401.6691v2]

Properties of nucleon-nucleon interaction

Dependence on spin-orbit coupling

The expectation value for the spin-orbit coupling is given by:

$$\langle \hat{l} \cdot \hat{s} \rangle = \frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)]$$
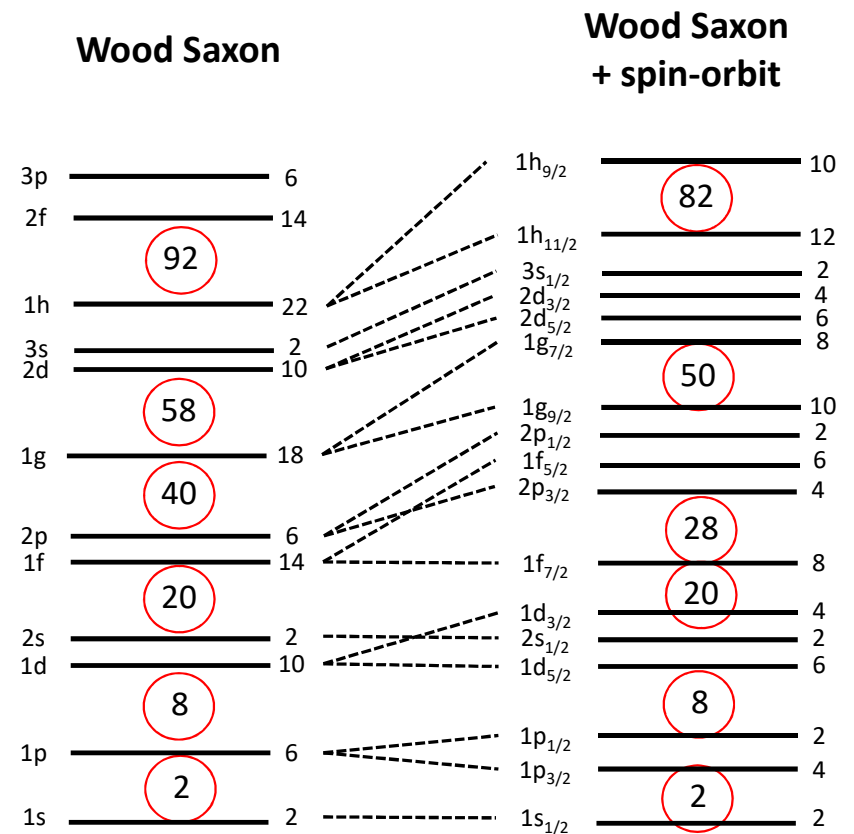
Recall that the total angular momentum

$$j = \begin{cases} l + \frac{1}{2} \\ l - \frac{1}{2} \end{cases}$$
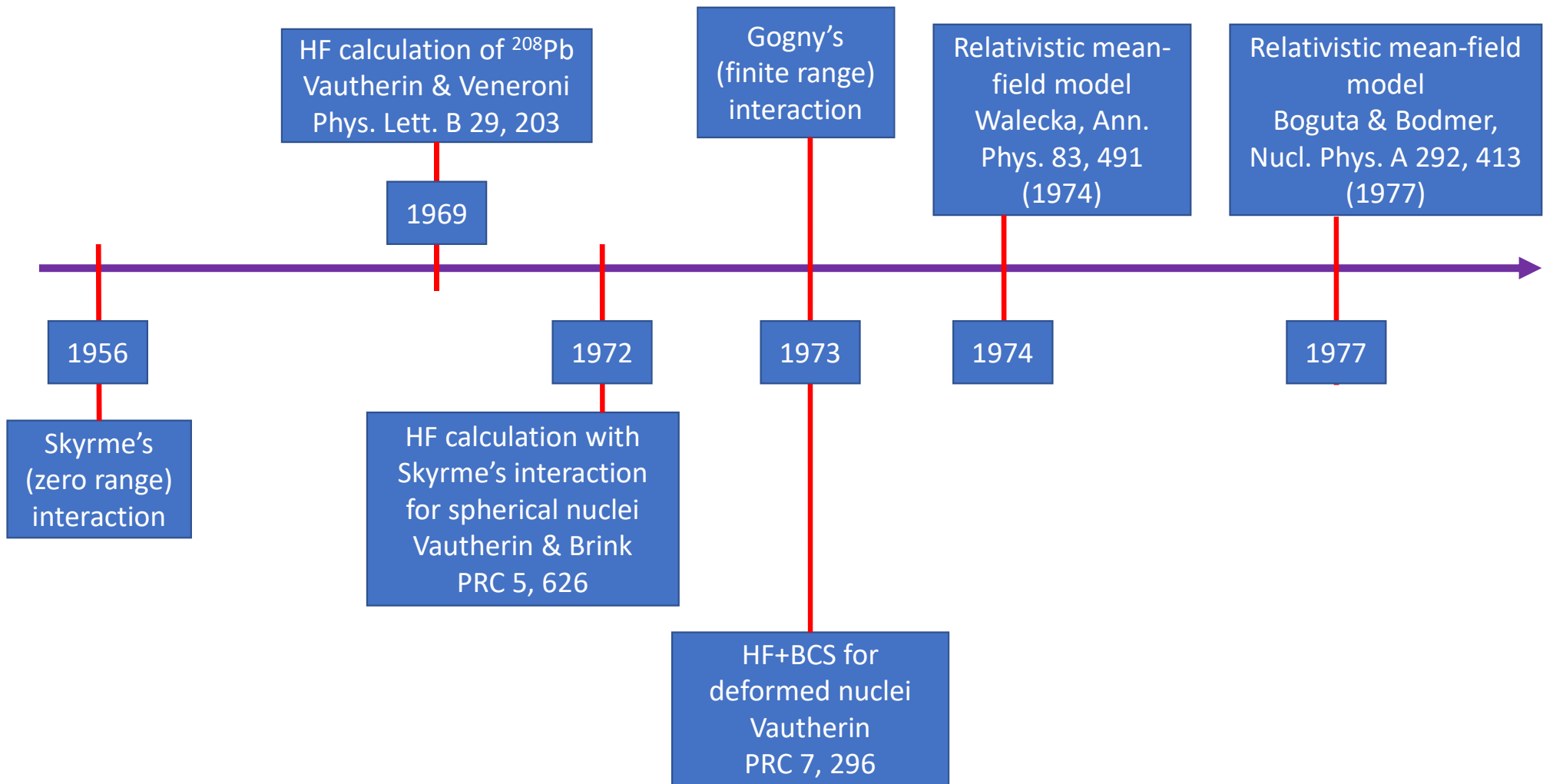
and with $s = 1/2$, we have after substituting j into the equation

$$\langle \hat{l} \cdot \hat{s} \rangle = \begin{cases} \boxed{\dfrac{\hbar^2}{2} l \qquad ; \text{for } j = l + \frac{1}{2}} \\[2ex] -\dfrac{\hbar^2}{2}(l+1); \text{for } j = l - \frac{1}{2} \end{cases}$$

Attractive when spin and orbital angular momentum are aligned.

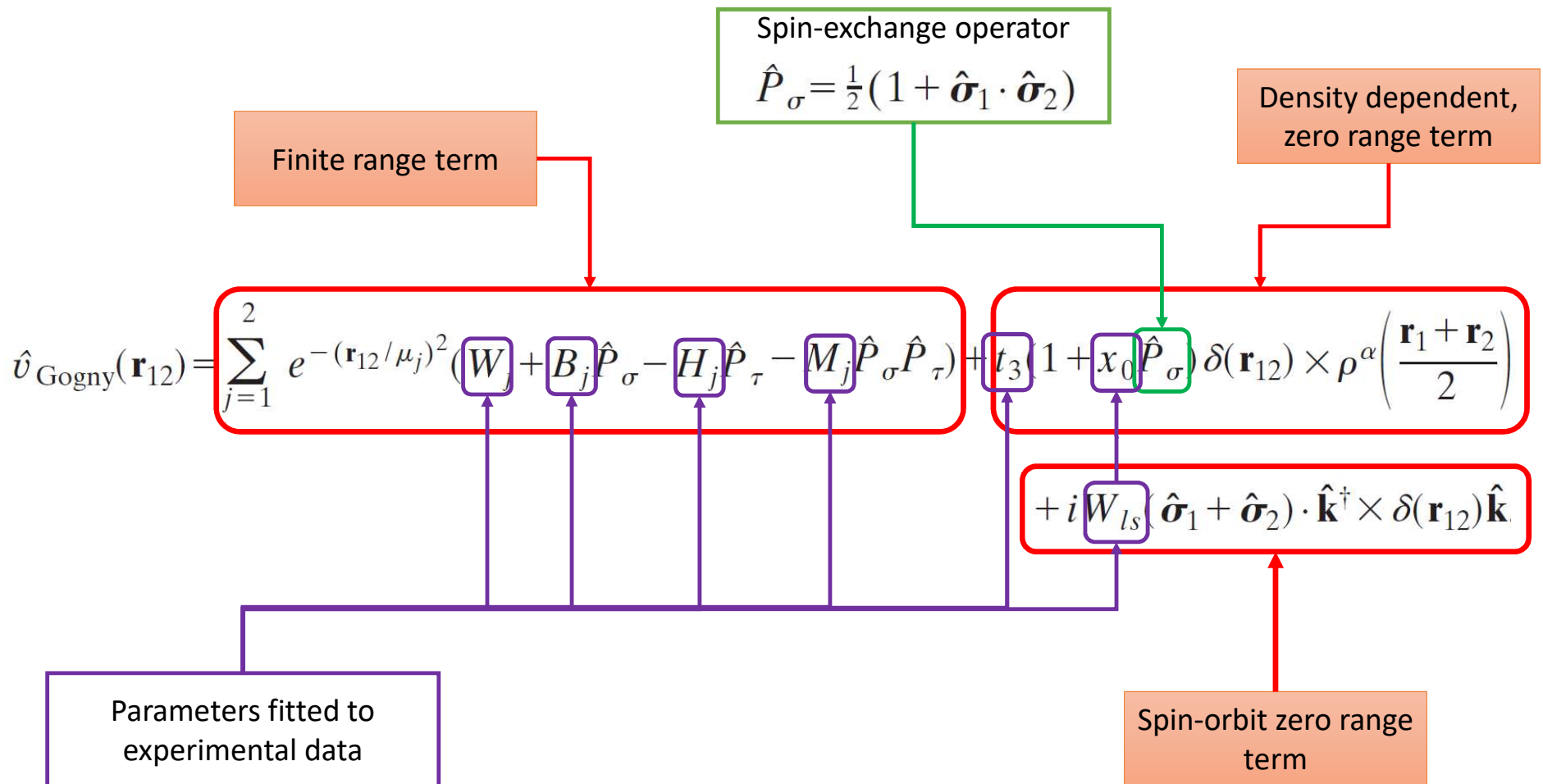Magic numbers were explained after introducing spin-orbit term

Wood Saxon

Wood Saxon + spin-orbit

Choices of effective interaction

HF calculation of ^{208}Pb
Vautherin & Veneroni
Phys. Lett. B 29, 203

1969

Gogny's
(finite range)
interaction

Relativistic mean-field model
Walecka, Ann.
Phys. 83, 491
(1974)

Relativistic mean-field model
Boguta & Bodmer,
Nucl. Phys. A 292, 413
(1977)

1956

1972

1973

1974

1977

Skyrme's
(zero range)
interaction

HF calculation with
Skyrme's interaction
for spherical nuclei
Vautherin & Brink
PRC 5, 626

HF+BCS for
deformed nuclei
Vautherin
PRC 7, 296

Choices of effective interaction: Gogny interaction

Spin-exchange operator

$$\hat{P}_\sigma = \tfrac{1}{2}(1 + \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2)$$

Finite range term

Density dependent, zero range term

$$\hat{v}_{\text{Gogny}}(\mathbf{r}_{12}) = \sum_{j=1}^{2} e^{-(\mathbf{r}_{12}/\mu_j)^2}(W_j + B_j\hat{P}_\sigma - H_j\hat{P}_\tau - M_j\hat{P}_\sigma\hat{P}_\tau) + t_3(1 + x_0\hat{P}_\sigma)\delta(\mathbf{r}_{12}) \times \rho^\alpha\!\left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right)$$

$$+ i\,W_{ls}(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2) \cdot \hat{\mathbf{k}}^\dagger \times \delta(\mathbf{r}_{12})\hat{\mathbf{k}}$$

Parameters fitted to experimental data

Spin-orbit zero range term

Choices of effective interaction: Skyrme interaction

The Skyrme interaction can be written as

$$V(\mathbf{r}_1,\mathbf{r}_2) = V_c(\mathbf{r}_1,\mathbf{r}_2) + V_{DD}(\mathbf{r}_1,\mathbf{r}_2) + V_{s.o}(\mathbf{r}_1,\mathbf{r}_2)$$

Central term

$$V_c(\mathbf{r}_1,\mathbf{r}_2) = t_0(1+x_0 P_\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2)$$
$$+ \frac{1}{2}(t_1+x_1 P_\sigma)[\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k}^2 + \mathbf{k}^{\dagger^2}\delta(\mathbf{r}_1-\mathbf{r}_2)]$$
$$+ t_2(1+x_2 P_\sigma)\mathbf{k}^\dagger \delta(\vec{\mathbf{r}_1}-\vec{\mathbf{r}_2})\mathbf{k}$$

Spin-orbit term

$$V_{s.o}(\mathbf{r}_1,\mathbf{r}_2) = iW_0(\sigma^{(1)}+\sigma^{(2)})\cdot\mathbf{k}^\dagger \times \delta(\vec{\mathbf{r}_1}-\vec{\mathbf{r}_2})\mathbf{k}$$

Momentum operator

$$\mathbf{k} = \frac{1}{2i}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$

Density dependent term

$$V_{DD}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{6}t_3(1+x_3 P_\sigma)\rho^\alpha \delta(\vec{\mathbf{r}_1}-\vec{\mathbf{r}_2})$$

The Skyrme parameters are t_i, x_i and W_0 with $i = [1,2,3]$ are obtained from fit to some nuclear properties.

Part 5:
Skyrme's energy density functional

Skryme energy-density functional

The expectation value of the many-body Hamiltonian operator for a wave function written as a normalized Slater determinant is

$$E = \langle \Psi_{HF} | \hat{H} | \Psi_{HF} \rangle = \int \mathscr{H}(\mathbf{r}) \, d\mathbf{r} = \int \left(\mathscr{H}_{kin}(\mathbf{r}) + \mathscr{H}_c(\mathbf{r}) + \mathscr{H}_{DD}(\mathbf{r}) + \mathscr{H}_{s.o}(\mathbf{r}) + \mathscr{H}_{Coul}(\mathbf{r}) \right) d\mathbf{r}$$

They are written as Hamiltonian densities with contributions from

Kinetic energy

$$\mathscr{H}_{kin}(\mathbf{r}) = \left(1 - \frac{1}{A} \right) \frac{\hbar^2}{2m} \tau$$

Central

$$\mathscr{H}_c(\mathbf{r}) = B_1 \rho^2 + B_{10} \mathbf{s}^2 + B_3(\rho\tau - \mathbf{j}^2) + B_{14}(\overleftrightarrow{J}^2 - \mathbf{s} \cdot \mathbf{T}) + B_5 \rho \triangle \rho + B_{18} \mathbf{s} \cdot \triangle \mathbf{s}$$
$$+ \sum_q \{ B_2 \rho_q^2 + B_{11} \mathbf{s}_q^2 + B_4(\rho_q \tau_q - \mathbf{j}_q^2) + B_{15}(\overleftrightarrow{J}_q^2 - \mathbf{s}_q \cdot \mathbf{T}_q) \} + B_6 \rho_q \triangle \rho_q + B_{19} \mathbf{s}_q \cdot \triangle \mathbf{s}_q$$

Density dependent

$$\mathscr{H}_{DD}(\mathbf{r}) = \rho^\alpha \left[B_7 \rho^2 + B_{12} \mathbf{s}^2 + \sum_q (B_8 \rho_q^2 + B_{13} \mathbf{s}_q^2) \right]$$

Spin-orbit

$$\mathscr{H}_{s.o}(\mathbf{r}) = B_9 \left[\rho \nabla \cdot \mathbf{J} + \mathbf{j} \cdot \nabla \times \mathbf{s} + \sum_q (\rho_q \nabla \cdot \mathbf{J}_q + \mathbf{j}_q \cdot \nabla \times \mathbf{s}_q) \right]$$

Coulomb

$$\mathscr{H}_{Coul}(\mathbf{r}) \approx \frac{1}{2} \rho_p(\mathbf{r}) V_{CD}(\mathbf{r}) - \frac{3}{4} e^2 \left(\frac{3}{\pi} \right)^{\frac{1}{3}} \rho_p^{\frac{4}{3}}(\mathbf{r})$$

Skyrme energy-density functional – coupling constants

The coupling constants B_j with $j = [1,19]$ are written in terms of the Skyrme parameters t_i, x_i and W_0.

$$B_1 = \frac{t_0}{2}\left(1 + \frac{x_0}{2}\right)$$

$$B_2 = -\frac{t_0}{2}\left(\frac{1}{2} + x_0\right)$$

$$B_3 = \frac{1}{4}\left[t_1\left(1 + \frac{x_1}{2}\right) + t_2\left(1 + \frac{x_2}{2}\right)\right]$$

$$B_4 = -\frac{1}{4}\left[t_1\left(\frac{1}{2} + x_1\right) - t_2\left(\frac{1}{2} + x_2\right)\right]$$

$$B_5 = -\frac{1}{16}\left[3t_1\left(1 + \frac{x_1}{2}\right) - t_2\left(1 + \frac{x_2}{2}\right)\right]$$

$$B_6 = \frac{1}{16}\left[3t_1\left(\frac{1}{2} + x_1\right) + t_2\left(\frac{1}{2} + x_2\right)\right]$$

$$B_7 = \frac{t_3}{12}\left(1 + \frac{x_3}{2}\right)$$

$$B_8 = -\frac{t_3}{12}\left(\frac{1}{2} + x_3\right)$$

$$B_9 = -\frac{W_0}{2}$$

$$B_{10} = \frac{1}{4}t_0 x_0$$

$$B_{11} = -\frac{1}{4}t_0$$

$$B_{12} = \frac{1}{24}t_3 x_3$$

$$B_{13} = -\frac{t_3}{24}$$

$$B_{14} = -\frac{1}{8}\left(t_1 x_1 + t_2 x_2\right)$$

$$B_{15} = \frac{1}{8}\left(t_1 - t_2\right)$$

$$B_{18} = -\frac{1}{32}\left(3t_1 x_1 - t_2 x_2\right)$$

$$B_{19} = \frac{1}{32}\left(3t_1 + t_2\right)$$

Skryme energy-density functional – local densities

Kinetic energy

$$\mathcal{H}_{kin}(\mathbf{r}) = \left(1 - \frac{1}{A}\right)\frac{\hbar^2}{2m}\,\tau$$

Time-even local densities

Kinetic energy density

$$\tau(\mathbf{r}) = \sum_k v_k^2 \left(\nabla[\phi_k]^\dagger(\mathbf{r})\right) \cdot \nabla[\phi_k](\mathbf{r})$$

Spin-orbit

$$\mathcal{H}_{s.o}(\mathbf{r}) = B_9\left[\rho\nabla\cdot\mathbf{J} + \mathbf{j}\cdot\nabla\times\mathbf{s} + \sum_q \left(\rho_q\nabla\cdot\mathbf{J}_q + \mathbf{j}_q\cdot\nabla\times\mathbf{s}_q\right)\right]$$

Particle density

$$\rho(\mathbf{r}) = \sum_k v_k^2 [\phi_k]^\dagger(\mathbf{r})[\phi_k](\mathbf{r})$$

Spin current density

$$J_{\mu\nu}(\mathbf{r}) = \frac{1}{2i}\sum_k v_k^2 \left\{[\phi_k]^\dagger(\mathbf{r})\sigma_\nu\nabla_\mu[\phi_k](\mathbf{r}) - \left(\nabla_\mu[\phi_k]^\dagger(\mathbf{r})\right)\sigma_\nu[\phi_k](\mathbf{r})\right\}$$

Skryme energy-density functional – local densities

Time-odd local densities
➢ Do not contribute for ground-state of even-even nucleus

Spin kinetic density

$$\mathbf{T}_\mu(\mathbf{r}) = \sum_k v_k^2 \left(\nabla[\phi_k]^\dagger(\mathbf{r}) \right) \cdot \sigma_\mu \nabla[\phi_k](\mathbf{r})$$

Central

$$\mathcal{H}_c(\mathbf{r}) = B_1\rho^2 + B_{10}\mathbf{s}^2 + B_3(\rho\tau - \mathbf{j}^2) + B_{14}(\overleftrightarrow{J}^2 - \mathbf{s} \cdot \mathbf{T}) + B_5\rho\triangle\rho + B_{18}\mathbf{s}\cdot\triangle\mathbf{s}$$
$$+ \sum_q \{B_2\rho_q^2 + B_{11}\mathbf{s}_q^2 + B_4(\rho_q\tau_q - \mathbf{j}_q^2) + B_{15}(\overleftrightarrow{J}_q^2 - \mathbf{s}_q\cdot\mathbf{T}_q)\} + B_6\rho_q\triangle\rho_q + B_{19}\mathbf{s}_q\cdot\triangle\mathbf{s}_q$$

Spin-orbit

Spin density

$$\mathbf{s}(\mathbf{r}) = \sum_k v_k^2 [\phi_k]^\dagger(\mathbf{r})\sigma[\phi_k](\mathbf{r})$$

$$\mathcal{H}_{s.o}(\mathbf{r}) = B_9\left[\rho\nabla\cdot\mathbf{J} + \mathbf{j}\cdot\nabla\times\mathbf{s} + \sum_q (\rho_q\nabla\cdot\mathbf{J}_q + \mathbf{j}_q\cdot\nabla\times\mathbf{s}_q)\right]$$

Current density

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2i}\sum_k v_k^2\left\{ \left(\nabla[\phi_k]^\dagger(\mathbf{r})\right)[\phi_k](\mathbf{r}) - [\phi_k]^\dagger(\mathbf{r})\nabla[\phi_k](\mathbf{r})\right\}$$

Application of variational principle to obtain HF equations

The Hartree-Fock equations to be solved iteratively are obtained by varying the total energy with respect to ϕ_i

$$\frac{\delta}{\delta\phi_j(\mathbf{r})}\left(E[\phi_k] - \sum_{k,\tau,\sigma} e_k \int d\mathbf{r}\,|\phi_k(\mathbf{r})|^2\right) = 0$$
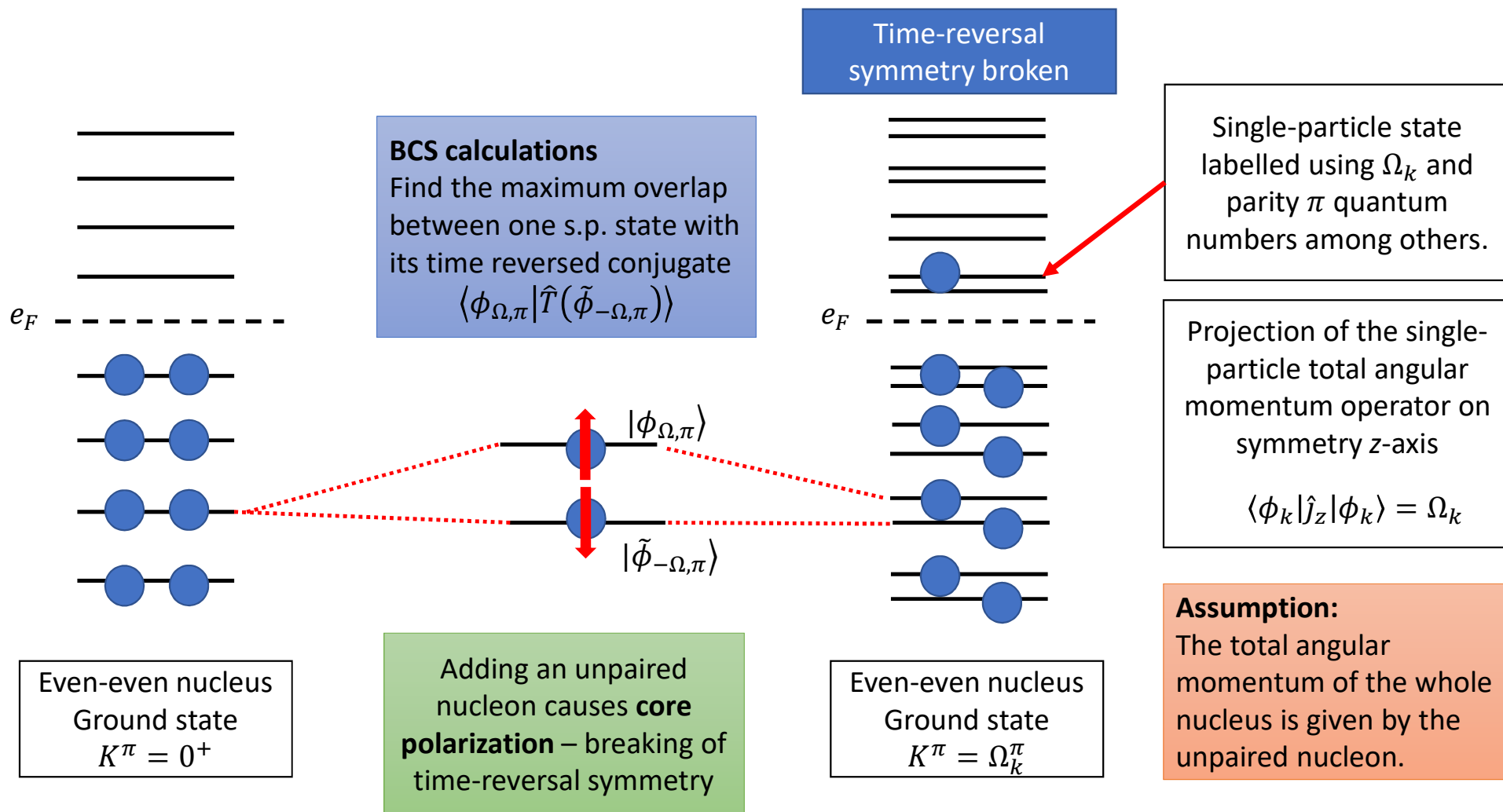
The HF equations in coordinate space given below are written in terms of local densities and Skyrme's coupling constants.

$$\langle\mathbf{r}|\hat{h}_{HF}^{(q)}|\phi_k\rangle = -\nabla\cdot\left(\frac{\hbar^2}{2m_q^*(\mathbf{r})}\nabla[\phi_k](\mathbf{r})\right) + \left(U_q(\mathbf{r}) + \delta_{qp}U_{Coul}(\mathbf{r})\right)[\phi_k](\mathbf{r})$$

$$+ i\mathbf{W}_q(\mathbf{r})\cdot\left(\sigma\times\nabla[\phi_k](\mathbf{r})\right) - i\sum_{\mu,v}\left\{\left(W_{q,\mu v}^{(J)}(\mathbf{r})\sigma_v\nabla_\mu[\phi_k](\mathbf{r})\right)\right.$$

$$\left. + \nabla_\mu\left(W_{q,\mu v}^{(J)}(\mathbf{r})\sigma_v[\phi_k](\mathbf{r})\right)\right\} - \frac{i}{2}\left\{\mathbf{A}_q(\mathbf{r})\cdot\nabla[\phi_k](\mathbf{r}) + \nabla\cdot\left(\mathbf{A}_q[\phi_k](\mathbf{r})\right)\right\}$$

$$+ \mathbf{S}_q(\mathbf{r})\cdot\sigma[\phi_k](\mathbf{r}) - \nabla\cdot\left(\left(\mathbf{C}_q(\mathbf{r})\cdot\sigma\right)\nabla[\phi_k](\mathbf{r})\right)$$

Time-odd potentials

Vanishes when time-reversal symmetry is preserved.

Breaking of time-reversal symmetry at the mean-field level

Time-reversal symmetry broken

BCS calculations
Find the maximum overlap between one s.p. state with its time reversed conjugate
$$\langle \phi_{\Omega,\pi} | \hat{T}(\tilde{\phi}_{-\Omega,\pi}) \rangle$$

e_F

$|\phi_{\Omega,\pi}\rangle$

$|\tilde{\phi}_{-\Omega,\pi}\rangle$

e_F

Single-particle state labelled using Ω_k and parity π quantum numbers among others.

Projection of the single-particle total angular momentum operator on symmetry z-axis
$$\langle \phi_k | \hat{j}_z | \phi_k \rangle = \Omega_k$$

Assumption:
The total angular momentum of the whole nucleus is given by the unpaired nucleon.

Even-even nucleus
Ground state
$K^\pi = 0^+$

Adding an unpaired nucleon causes **core polarization** – breaking of time-reversal symmetry

Even-even nucleus
Ground state
$K^\pi = \Omega_k^\pi$

Part 6:
Expansion of s.p. wave functions

Expanding on deformed harmonic oscillator basis states

HF equation to be solved:

$$\hat{h}_{HF}|k\rangle = e_k|k\rangle$$

$$\hat{h}_{HF}\phi_k(r,\sigma,q) = e_k\phi_k(r,\sigma,q)$$

The wave function can be expanded on any orthonormal basis states for e.g.

$$\phi_k(\mathbf{r},\sigma,q) = \chi_q \sum_{\alpha} C_{\alpha}^{(k)} \boxed{\varphi_{\alpha}(\mathbf{r},\sigma)}$$

Cartesian coordinate

Deformed harmonic oscillator
$$\alpha \equiv \{n_r, n_z, l_z, s_z\}$$
$r = \{r, z, \varphi\}$ (cylindrical coord.)

Recap:
1-dimensional SE with harmonic oscillator potential

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x)$$

Eigenvalue:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

Hermite polynomial

Eigenfunction:

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\,2^n n! x_0}}e^{-x^2/2x_0^2}\boxed{H_n\left(\frac{x}{x_0}\right)}$$

Recap:
Radial equation of hydrogen atom

$$-\frac{\hbar^2}{2\mu}\frac{d^2 U(r)}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{r}\right]U(r) = EU(r)$$

Eigenvalue:

$$E_n = -\frac{\mu e^4}{2\hbar^2}\frac{1}{n^2} = -\frac{e^2}{2a_0}\frac{1}{n^2}$$

Associated Laguerre polynomial

Eigenfunction:

$$R_{nl}(r) = N_{nl}\left(\frac{2r}{na_0}\right)^l e^{-r/na_0}\boxed{L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right)}$$

Expanding on deformed harmonic oscillator basis states

When expanding the s.p. wave function on deformed harmonic oscillator, it is written as

$$\phi_k(\mathbf{r}, \sigma, q) = \chi_q \sum_\alpha C_\alpha^{(k)} \boxed{\varphi_\alpha(\mathbf{r}, \sigma)}$$

$$\varphi_\alpha(\mathbf{r}, \sigma) = \Gamma_{s_z}(\sigma) \boxed{\psi_{n_z}(z)} \boxed{\psi_{n_r}^{l_z}(r)} \frac{e^{il_z\varphi}}{\sqrt{2\pi}}$$

$$\psi_{n_z}(z) = N_{n_z} \boxed{\beta_z^{1/2}} e^{-\xi^2/2} \boxed{H_{n_z}(\xi)}$$

$$\psi_{n_r}^{l_z}(r) = N_{n_r}^{l_z} \boxed{\beta_\perp} \sqrt{2}\, \eta^{l_z/2} e^{-\eta/2} \boxed{L_{n_r}^{l_z}(\eta)}$$

Hermite polynomial

Assoc. Laguerre polynomial

$$\beta_z = \sqrt{m\omega_z/\hbar}$$

$$\beta_\perp = \sqrt{m\omega_\perp/\hbar}$$

A truncation in the expansion is made using

$$\hbar\omega_\perp(n_\perp + 1) + \hbar\omega_z\left(n_z + \frac{1}{2}\right) \le \hbar\omega_0(N_0 + 2)$$

Two parameters to be optimized namely

$$\beta_0 = \sqrt{\frac{m\omega_0}{\hbar}} \qquad q \equiv \frac{\omega_\perp}{\omega_z}$$

with $\omega_0^3 = \omega_\perp^2 \omega_z$ for a given basis size N_0.

Part 7:
Examples of HF+BCS calculations

# Global microscopic calculations of ground-state spins and parities for odd-mass nuclei

Calculated GS spin-parity compared to experiment

Calculated GS spin-parity compared to experiment
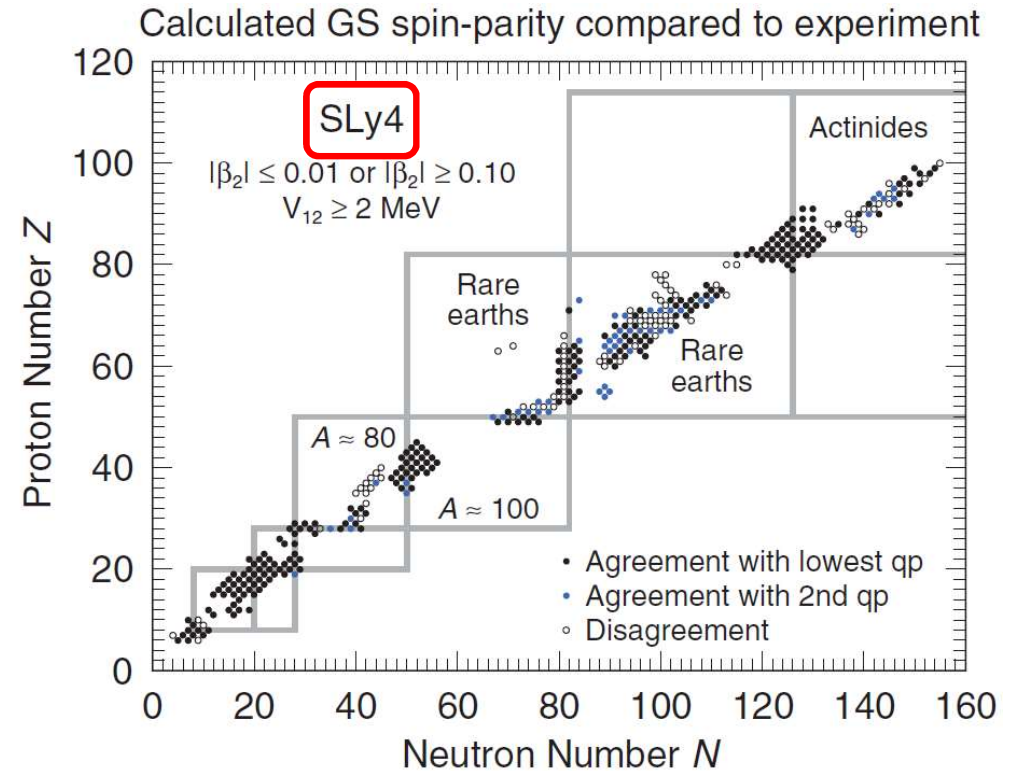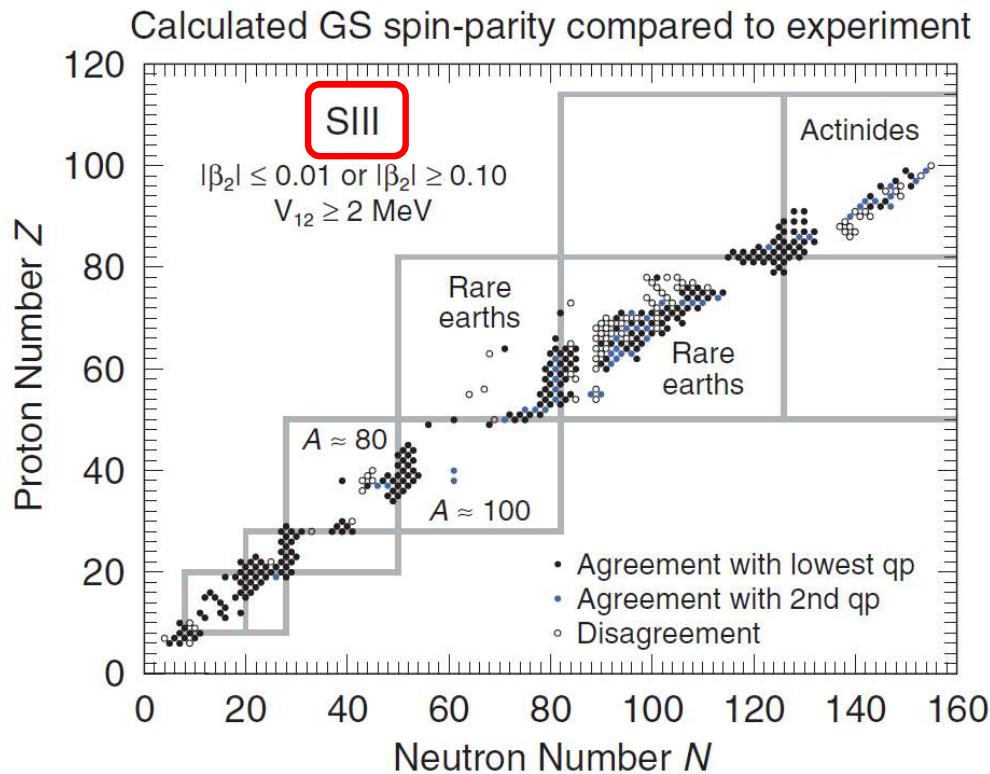
"...the overall agreement is similar for the SIII and SLy4 Skyrme forces and about 5% less good for the SkM∗ force."

Large-scale self-consistent nuclear mass calculations
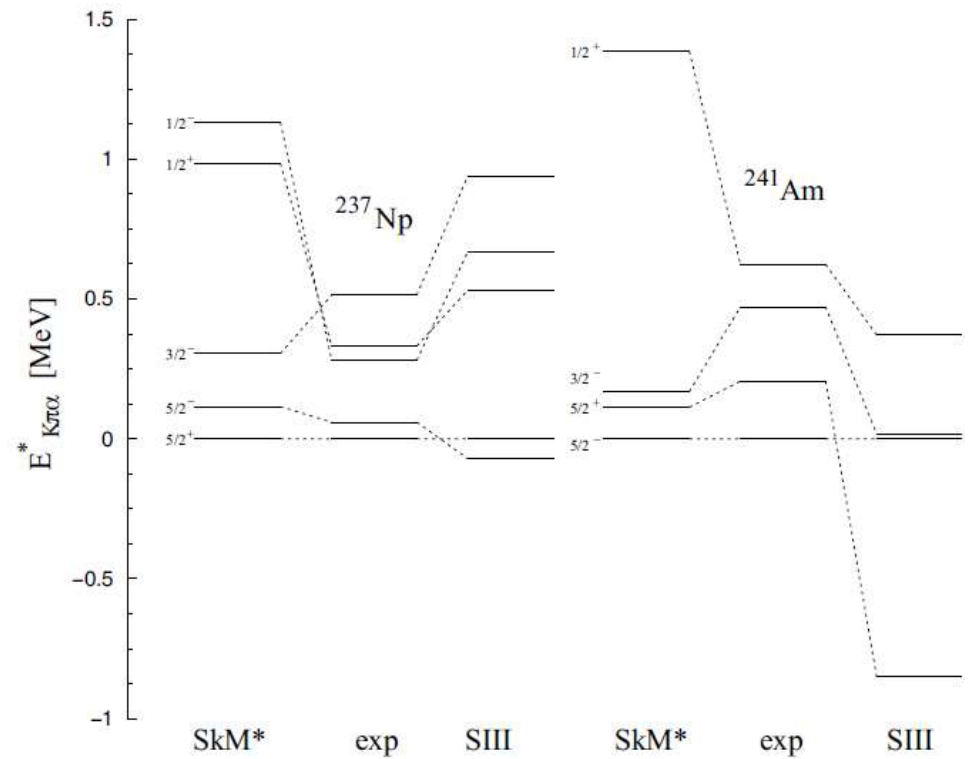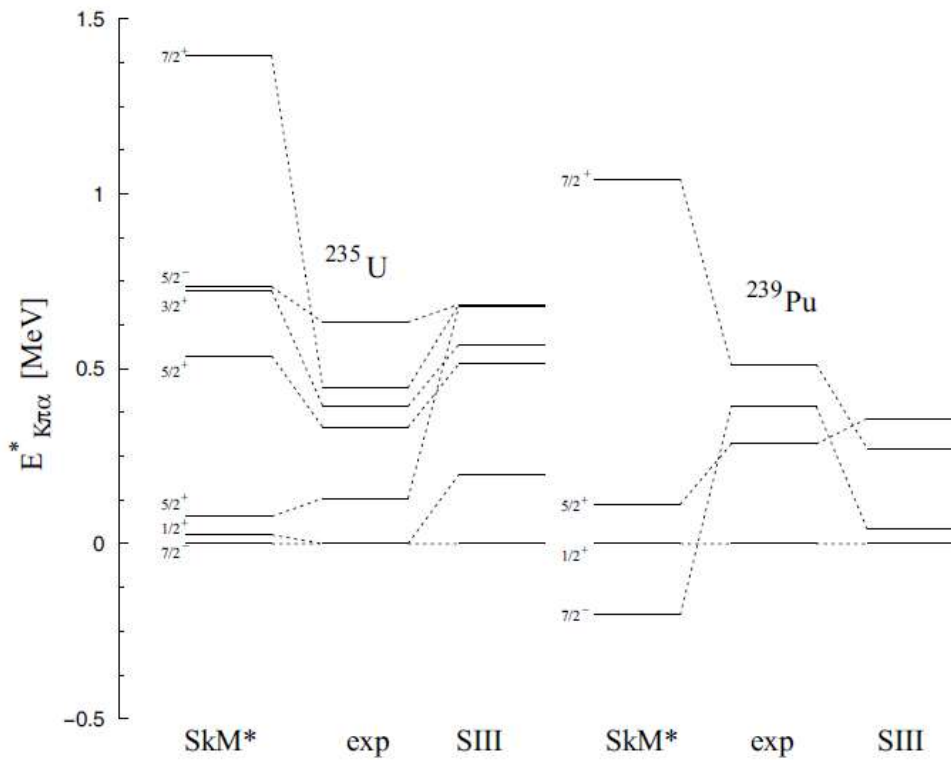
M.V. Stoitsov, J. Dobaczewski, W. Nazarewicz and P. Borycki, Int. J. Mass Spectrom. 251 (2006)
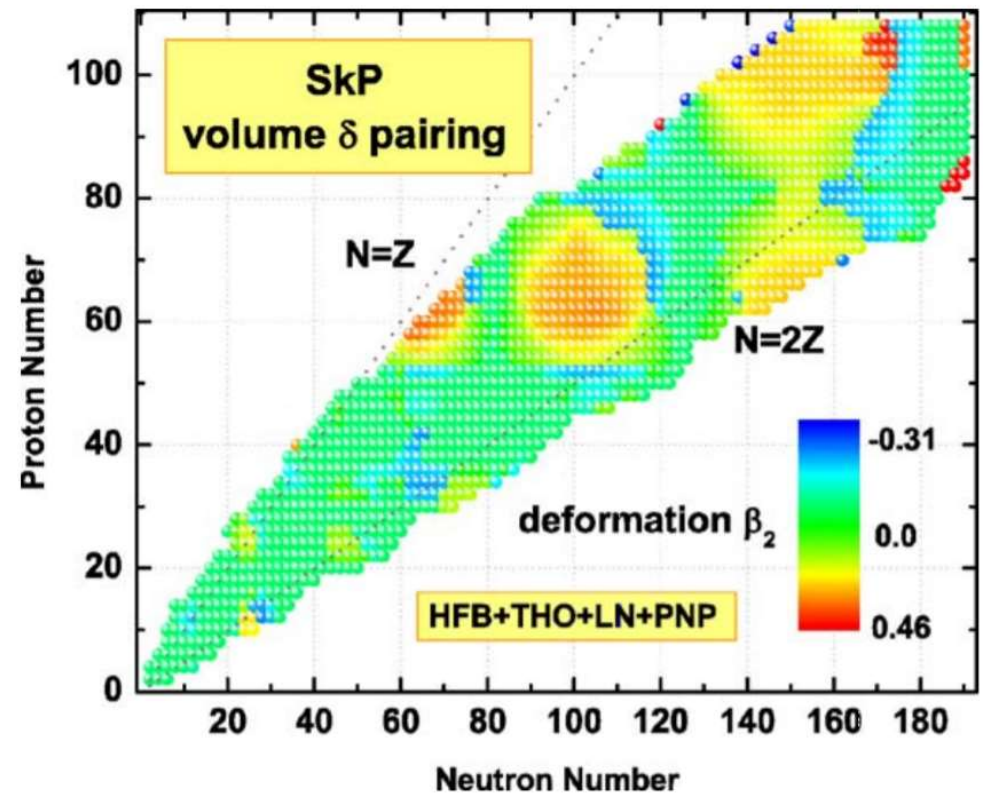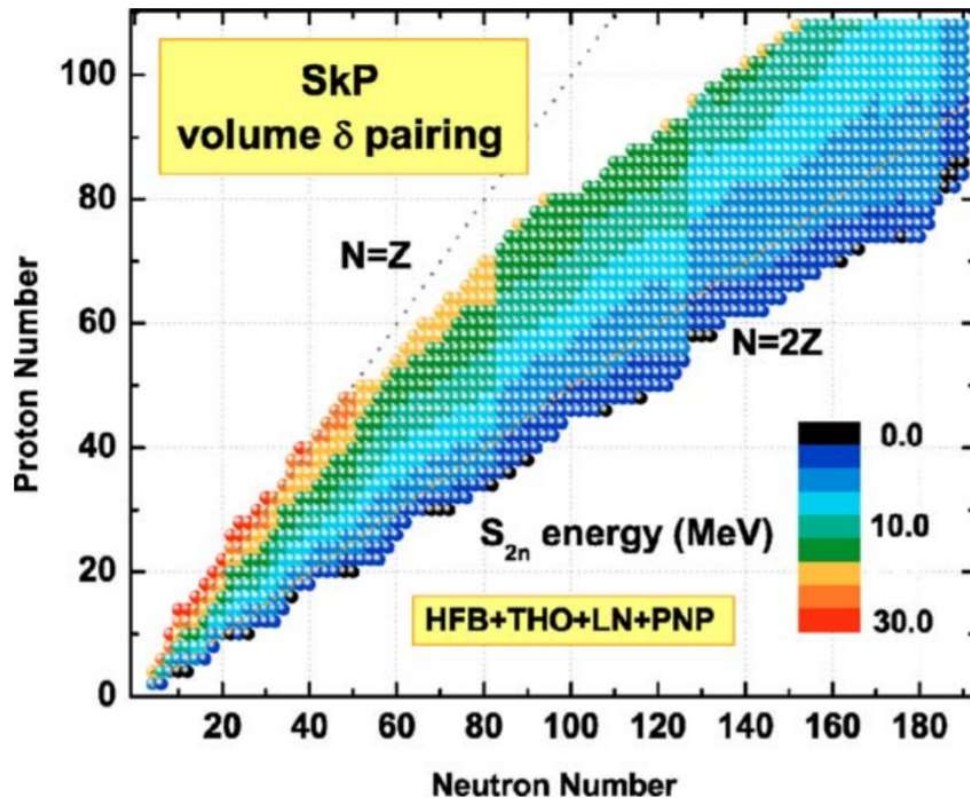
Band-head spectra of low-energy single-particle excitations in some well-deformed, odd-mass heavy nuclei within a microscopic approach

M.-H. Koh, D.D. Duc, T.V. Nhan Hao, H.T. Long, P. Quentin and L. Bonneau, Eur. Phys. J A 52 (2016)

Part 8:
Constrained Hartree-Fock

Constraining to a desired nuclear shape

Unconstrained HF calculation yields solution at the **local extrema (minima).** A constraint is added to study nuclear properties at a certain deformation.
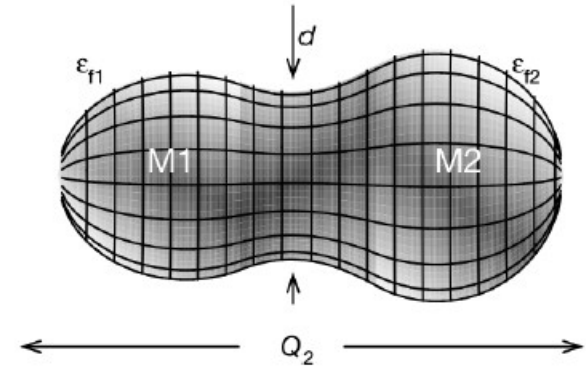
$$\hat{H}' = H + f(\mu_l, \langle \hat{Q}_{lm} \rangle)$$

Multipole moments

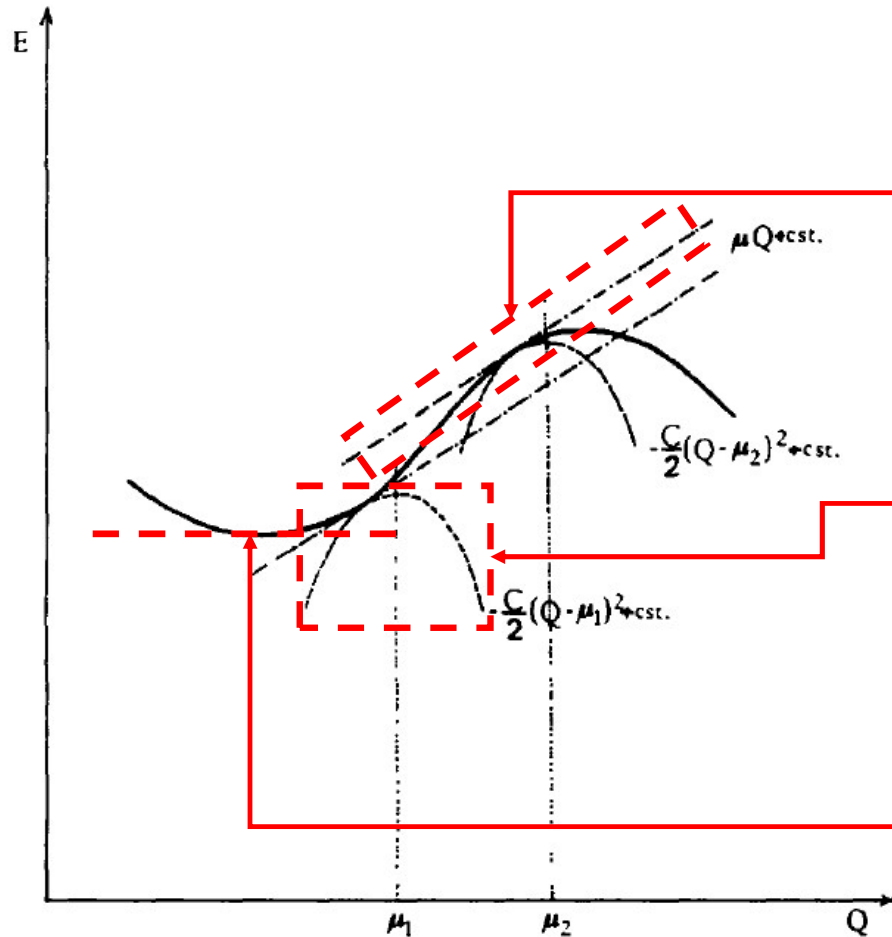**Parity asymmetric shapes**

Octupole moment

$$Q_{30} = \langle \hat{Q}_{30} \rangle = \int d\mathbf{r}\, \rho(\mathbf{r})\, r^3\, Y_3^0(\theta, \varphi)$$

Axial & parity symmetric shapes

Quadrupole moment
$$Q_{20} = \langle \hat{Q}_{20} \rangle = \int d\mathbf{r}\, \rho(\mathbf{r})(2z^2 - r^2)$$

Hexadecapole moment
$$Q_{40} = \langle \hat{Q}_{40} \rangle = \int d\mathbf{r}\, \rho(\mathbf{r})\, r^4\, Y_4^0(\theta, \varphi)$$

Axially asymmetric shapes

Non-axial quadrupole moment
$$Q_{22} = \langle \hat{Q}_{22} \rangle = \int d\mathbf{r}\, \rho(\mathbf{r})(x^2 - y^2)$$

Ways to constraint nuclear deformation

Linear constraint

$$f\left(\mu_l, \langle \hat{Q}_{lm} \rangle\right) = -\mu \langle \hat{Q}_{lm} \rangle$$

Search for a point in which the slope is equal to μ.

Quadratic constraint

$$f(\mu_l, \langle \hat{Q}_{lm} \rangle) = \frac{1}{2} C_l (\langle \hat{Q}_{lm} \rangle - \mu_l)^2$$

Calculations with __no constraint__

$$f\left(\mu_l, \langle \hat{Q}_{lm} \rangle\right) = 0$$
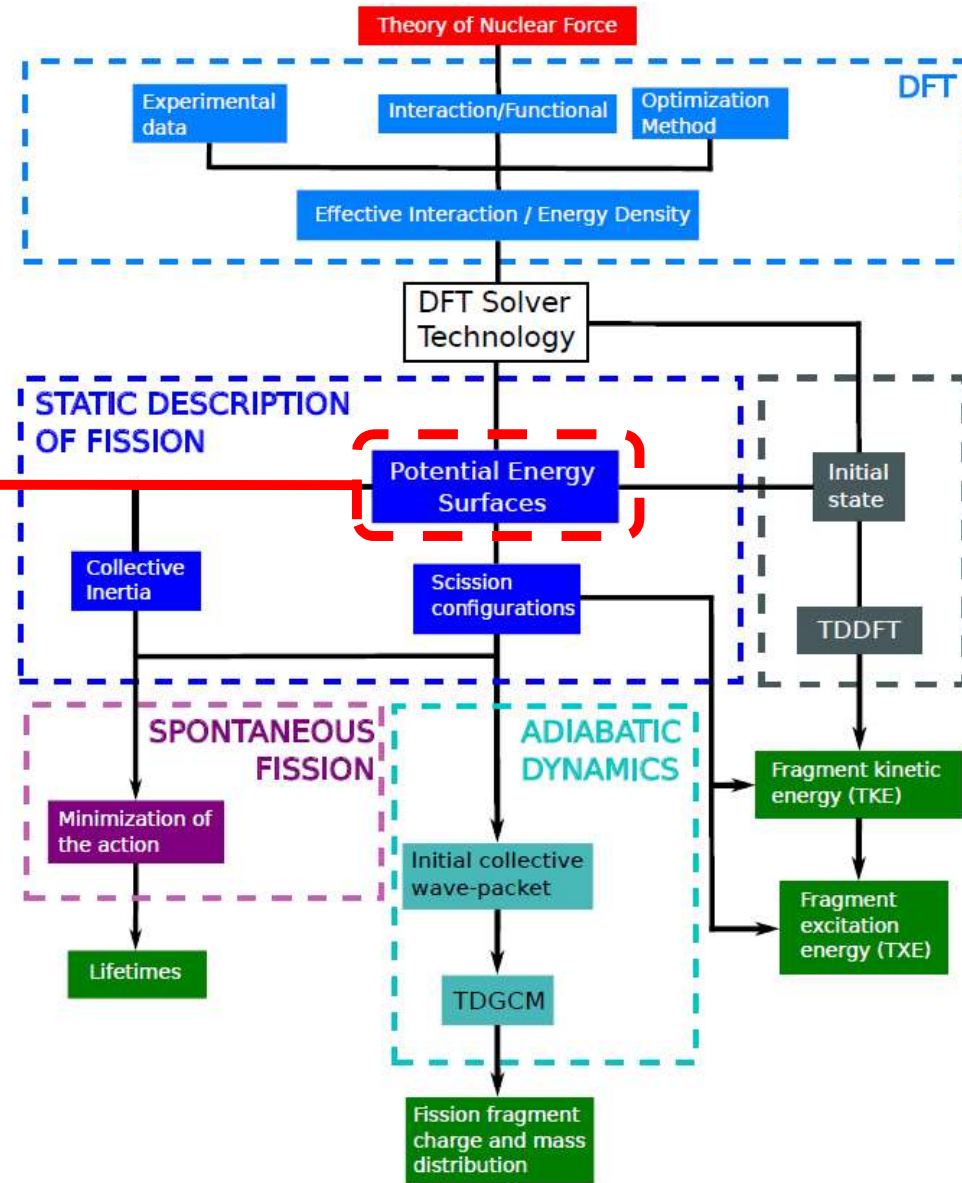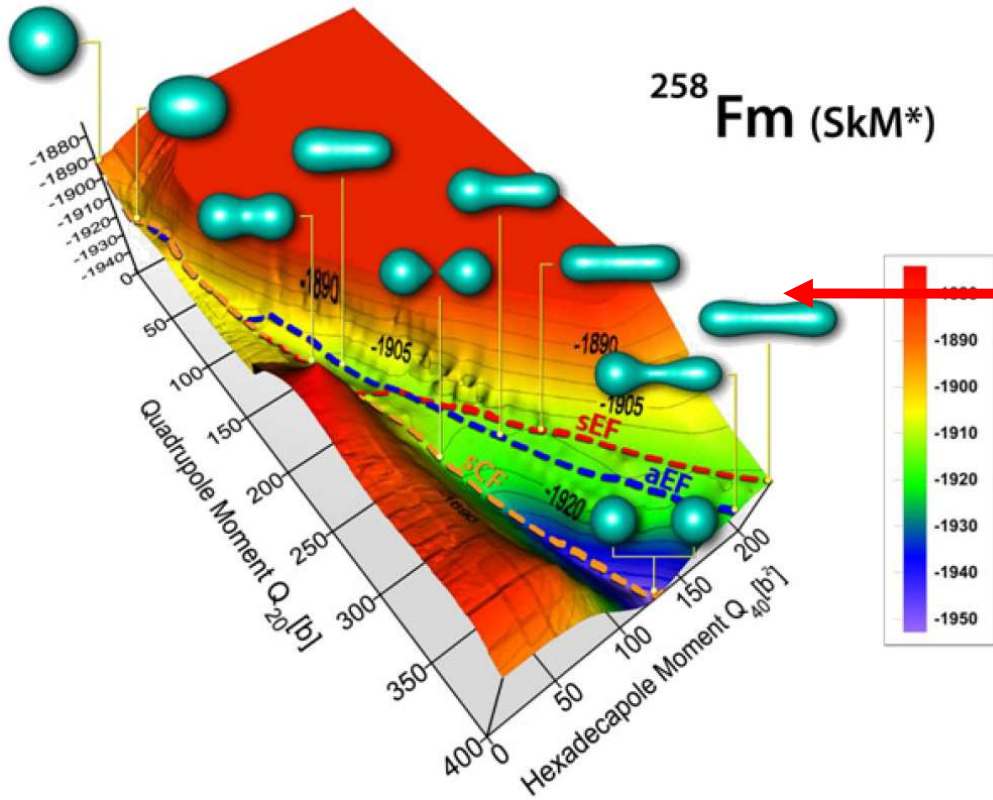
yields solution at the local extrema.

From H. Flocard, P. Quentin, A.K. Kerman and D. Vautherin, Nucl. Phys. A 203, 433 (1973)

Part 9:
Application of HF+BCS to large nuclear deformation
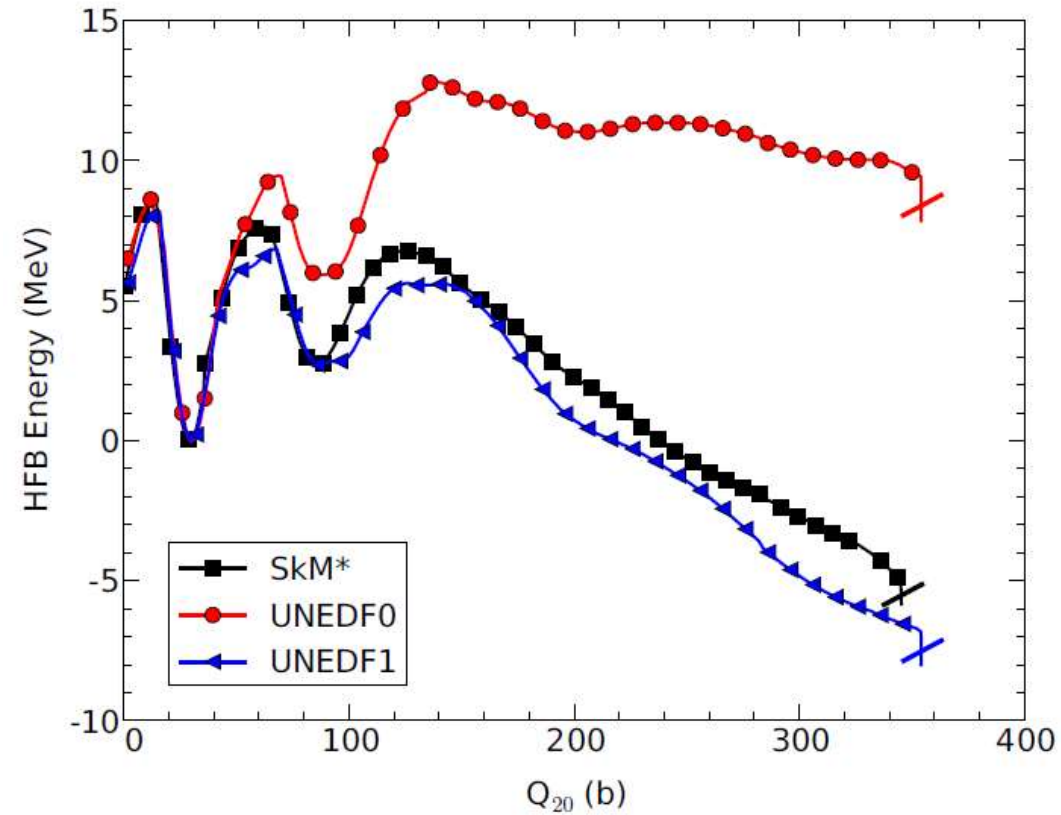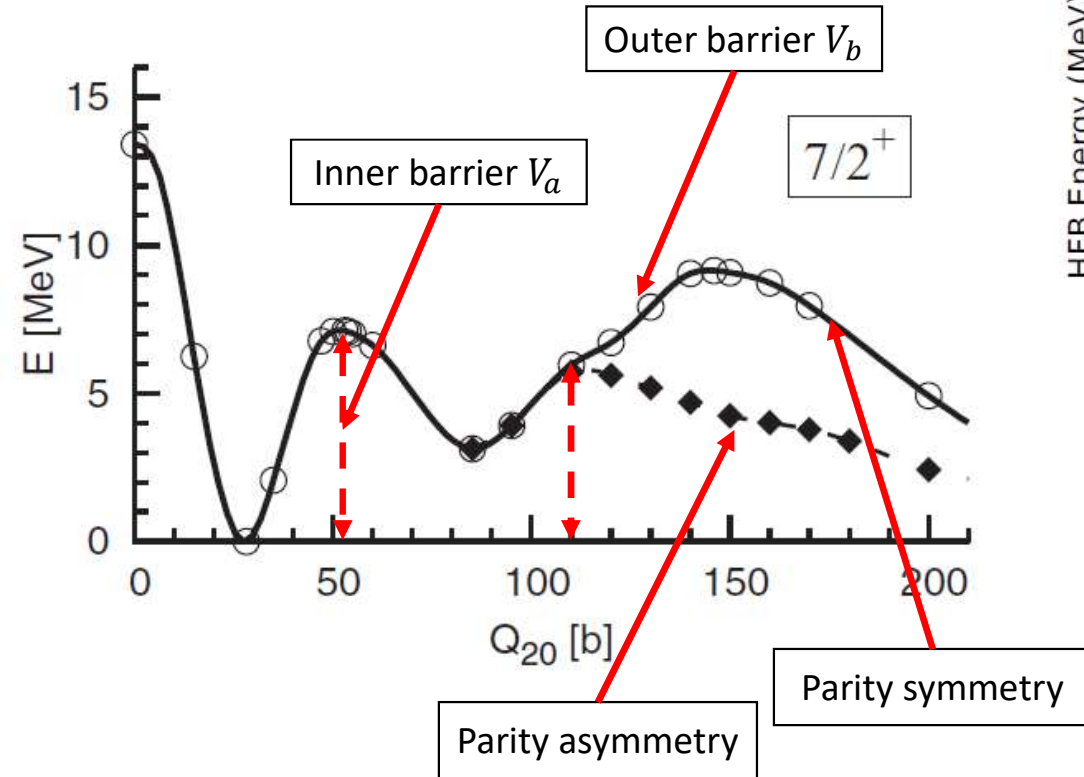
Overview of nuclear theory studies

N. Schunck & L.M. Robledo
Microscopic theory of nuclear fission: a review
Rep. Prog. Phys. 79, 116301 (2016)

Calculations of deformation energies

Deformation energy of odd-mass ^{239}Pu
M.-H. Koh, L. Bonneau, P. Quentin, T.V. Nhan Hao and H. Wagiran, Phys. Rev. C 95, 014315 (2017)

Outer barrier V_b

Inner barrier V_a

$7/2^+$

Parity symmetry

Parity asymmetry

N. Schunck, D. Duke, H. Carr, and A. Knoll, Phys. Rev. C 90, 054305 (2014)

Fission cross-section modelling

Fission cross-section modelling

$$\sigma_e^{J\pi}(E_e) = \frac{\pi}{k_e^2}(2J+1)\, T_e^{J\pi}(E_e)$$

Transmission coefficient(s) across the barriers

$$T_j(E,J^\pi) = \sum_d \mathscr{P}_j(E,V_{jd}^{J\pi}) + \int_{E_d}^{E_{max}^*} \mathscr{P}(E,V_j^{J\pi}(\varepsilon))\,\rho(\varepsilon,J,\pi)\,d\varepsilon$$

$$\mathscr{P}_j^{HW}(E,V_{jd}^{J\pi}) = \left[1 + \exp\left(2\pi\frac{V_{jd}^{J\pi} - E}{\hbar\,\omega_{jd}^{J\pi}}\right)\right]^{-1}$$

Barrier penetrability within Hill-Wheeler approach

Input parameters obtained from nuclear structure info

Deformation energy:
Total binding energy as a function of nuclear shape

Stationary states in the potential well & top of fission barriers

E^* [MeV]

Transition states on top of each barrier A and B

i= υ_A i= υ_B

i=3
i=2
i=1

i=3
i=2
i=1

Class–I states

S_n

Second well

First well

V_A

Class–II vibrational states

V_B

LDM

SCM

Deformation (ε)