Summary of the Mean-Field approach to the ground state properties of atomic nuclei

1. Variational Principle
2. Hartree-Fock theory
3. Effective interactions
4. Broken Symmetries
5. Symmetry Restoration
6. Pairing – BCS theory
7. Pairing – HFB theory

Variational Principle (Rayleigh-Ritz method)

$$\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_{\mathrm{g.s.}}$$

(note)

$$|\Psi\rangle = \sum_n C_n |\phi_n\rangle \Rightarrow \mathrm{lhs} = \frac{\sum_n C_n^2 E_n}{\sum_n C_n^2} \geq E_0$$

Strategy

Assume some simple form for $|\Psi\rangle$

⇒ Determine the parameters so that is at a minimum (*minimization*).

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Hartree-Fock Theory

many-body Hamiltonian:

$$H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j)$$

→ One-body approximation

$$H \sim \sum_{i=1}^{A} h(i) = -\sum_{i=1}^{A} \frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + V_{\text{eff}}(\boldsymbol{r}_i)$$

[independent particle motion in an effective potential well] many-body Hamiltonian: $$H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j)$$

→ One-body approximation

$$H \sim \sum_{i=1}^{A} h(i) = -\sum_{i=1}^{A} \frac{\hbar^2}{2m}\nabla_i^2 + V_{\text{eff}}(\boldsymbol{r}_i)$$

Two aspects:

- It is impossible to treat the N-body problem exactly (except for light systems).

# of parameters required: $M \sim p^{3N}$ $\quad 3 \leq p \leq 10$

→ $M \sim 10^{150} \quad (N = 100, p = 3)$

The Van Vleck catastrophe

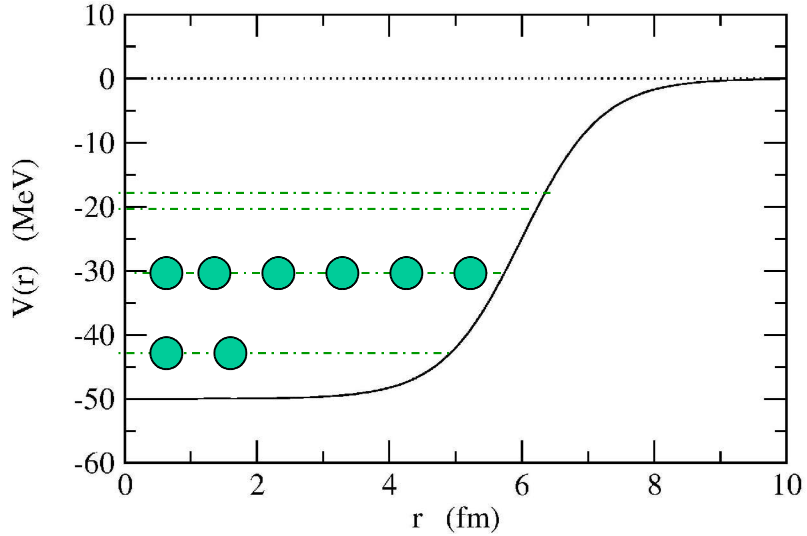
$$|\langle \phi_i | \phi_i^{\text{exact}} \rangle| = 1 - \epsilon \sim e^{-\epsilon} \qquad \epsilon \sim 10^{-2}$$

→ $|\langle \Psi | \Psi^{\text{exact}} \rangle| \sim |\langle \phi_i | \phi_i^{\text{exact}} \rangle|^N = \sim e^{-\epsilon N} \ll 1$

- **But, many experimental observables have a one- body character.**

Hartree-Fock Method

independent particle motion
in a potential well



$$\Psi(1,2,\cdots,A) = \mathcal{A}[\psi_1(1)\psi_2(2)\cdots\psi_A(A)]$$

$$= \frac{1}{\sqrt{A!}}\begin{vmatrix} \psi_1(1) & \psi_2(1) & \cdots & \psi_A(1) \\ \psi_1(2) & \psi_2(2) & \cdots & \psi_A(2) \\ \vdots & & & \\ \psi_1(A) & \psi_2(A) & \cdots & \psi_A(A) \end{vmatrix}$$

Slater determinant: antisymmetrization due to the Pauli principle

Minimization: $$\frac{\delta}{\delta\psi_i^*}[\langle\Psi|H-\epsilon|\Psi\rangle] = 0$$

Hartree-Fock equation: Schroedinger-type eq. with a mean-field potential

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\boldsymbol{r}) + \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r}) - \int \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}' = \epsilon_i\,\psi_i(\boldsymbol{r})$$

Density matrix:

$$\rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}') = \sum_i \psi_i^*(\boldsymbol{r}')\psi_i(\boldsymbol{r})$$

$$\rho_{\mathsf{HF}}(\boldsymbol{r}) = \sum_i \psi_i^*(\boldsymbol{r})\psi_i(\boldsymbol{r}) = \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r})$$

Iteration Procedure

V_{HF}: depends on ψ_i $\longleftarrow$ non-linear problem

Iteration: $\{\psi_i\} \rightarrow \rho_{\mathsf{HF}} \rightarrow V_{\mathsf{HF}} \rightarrow \{\psi_i\} \rightarrow \cdots$

Observables

i) One-body operators $\hat{Q} = \sum_{i=1}^{A} Q(\boldsymbol{r}_i)$

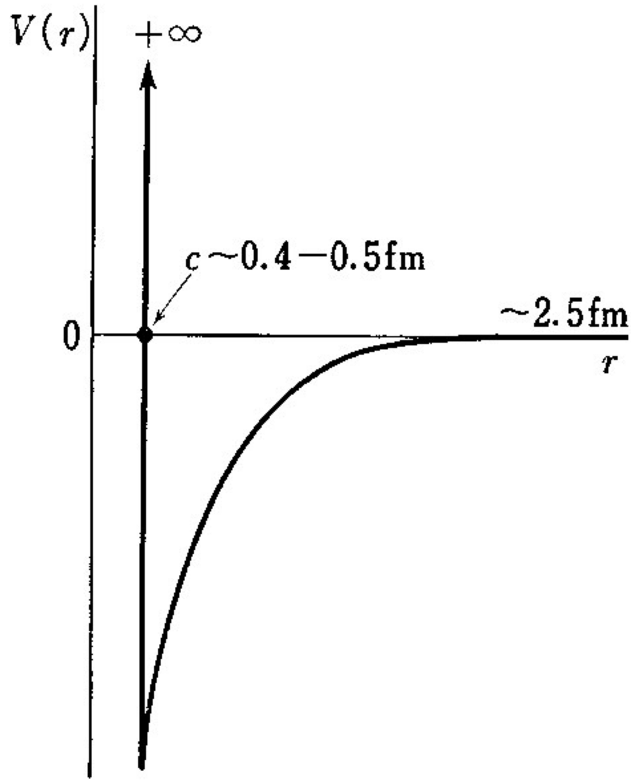
$$\langle \hat{Q} \rangle = \int d\boldsymbol{r}\, \rho_{\mathrm{HF}}(\boldsymbol{r}) Q(\boldsymbol{r})$$

ii) Total Energy $H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m} \boldsymbol{\nabla}_i^2 + \frac{1}{2} \sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j)$

$$E = \langle \Psi | H | \Psi \rangle = \frac{1}{2} \left(E_{\mathrm{kin}} + \sum_i \epsilon_i \right)$$

Effective Interaction

Nucleon-nucleon interaction
in vacuum



Existence of short range
repulsive core

Nucleon-nucleon interaction
in-medium

Bruckner's G-matrix

phenomenological effective
interactions

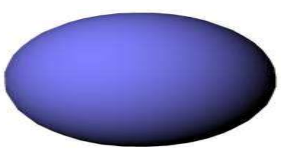
- Skyrme interaction
- Gogny interaction
- RMF

Broken Symmetries

$$H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j) \rightarrow -\sum_{i=1}^{A} \frac{\hbar^2}{2m} \nabla_i^2 + V_{\mathrm{HF}}(\boldsymbol{r}_i)$$

Energy minimization by breaking symmetries

Example: nuclear deformation



- The existence of rotational bands

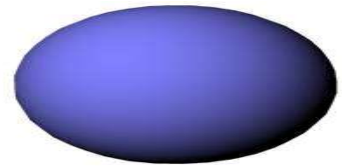
$$E_I = \frac{I(I+1)\hbar^2}{2\mathcal{J}}$$

"^{180}Hf is *intrinsically* deformed."

(MeV)		
1.084	——	8^+
0.641	——	6^+
0.309	——	4^+
0.093	——	2^+
0	——	0^+

^{180}Hf

➢ Rotational symmetry



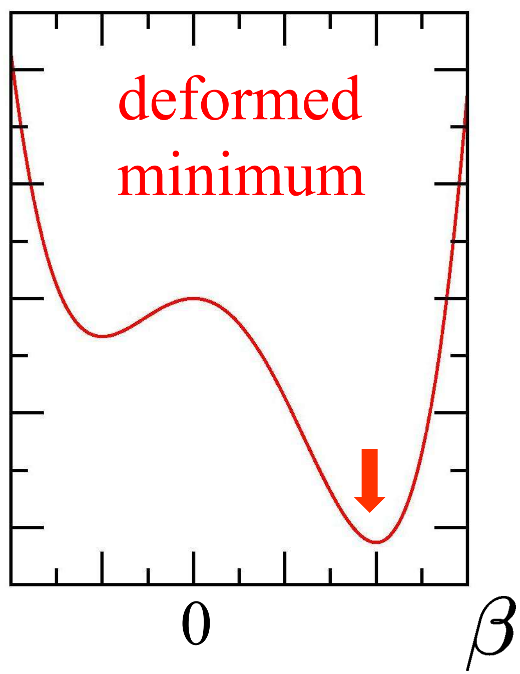
Deformed solution

Constrained Hartree-Fock method

minimize $H' = H - \lambda \hat{Q}_{20}$ with a Slater determinant w.f.

$\hat{Q}_{20} = \sum_i r_i^2 Y_{20}(\hat{\boldsymbol{r}}_i)$: quadrupole operator

λ : Lagrange multiplier, to be determined so that $\langle \hat{Q}_{20} \rangle = Q \propto R^2 \beta$



Symmetry Restoration

$$
\begin{aligned}
|\Psi_{\text{proj}}\rangle &= \int d\Omega\, D^{I*}_{MK}(\Omega)|\Psi_{\Omega K}\rangle \\
&= \int d\Omega\, D^{I*}_{MK}(\Omega)\hat{R}(\Omega)|\Psi_K\rangle
\end{aligned}
$$

Rotated wave function: $|\Psi_\Omega\rangle = \hat{\mathcal{R}}(\Omega)|\Psi\rangle$

(deformed HF solution)

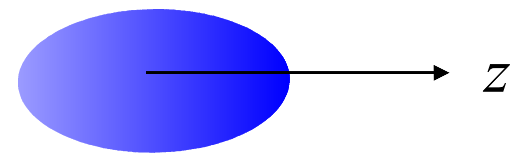
(note) $\hat{\mathcal{R}}(\Omega)|\phi_{IK}\rangle = \sum_M |\phi_{IM}\rangle \underbrace{\langle\phi_{IM}|\hat{\mathcal{R}}(\Omega)|\phi_{IK}\rangle}_{D^I_{MK}(\Omega)}$

$$D^I_{M0}(\phi,\theta,\chi) = \sqrt{\frac{4\pi}{2I+1}}Y^*_{IM}(\theta,\phi)$$

$$\int d\Omega D^{I*}_{MK}(\Omega)D^{I'}_{M'K'}(\Omega) = \frac{8\pi^2}{2I+1}\delta_{I,I'}\delta_{M,M'}\delta_{K,K'}$$

Projection Operator

Consider a HF state with the axial symmetry



$$|\Psi_K\rangle = \sum_I C_I |\Psi_{IK}\rangle$$

rotated state:

$$|\Psi_\Omega\rangle = \hat{\mathcal{R}}(\Omega)|\Psi\rangle = \sum_{I,M} C_I\, D^I_{MK}(\Omega)|\Psi_{IM}\rangle$$

$$\begin{aligned} |\Psi_{\mathrm{proj}}\rangle &= \int d\Omega\, D^{I*}_{MK}(\Omega)|\Psi_\Omega\rangle \\ &= \frac{8\pi^2}{2I+1} C_I\,|\Psi_{IM}\rangle \end{aligned}$$

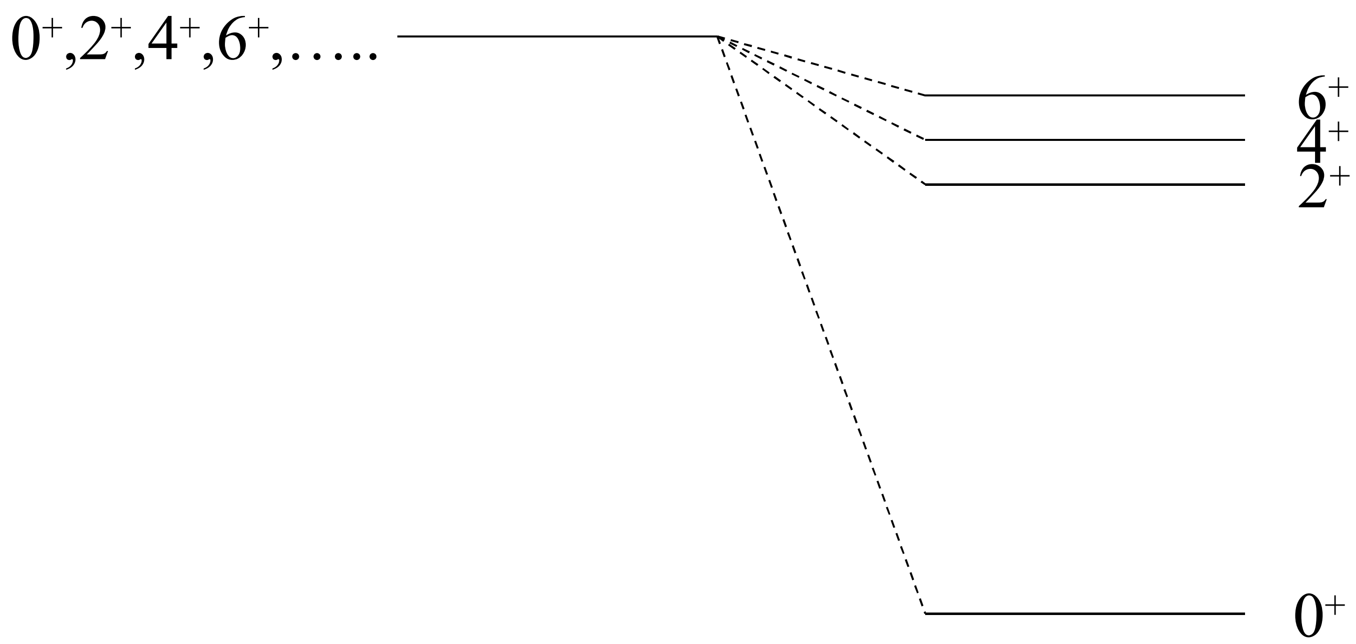
or

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2}\int D^{I*}_{MK}(\Omega)\hat{\mathcal{R}}(\Omega)\, d\Omega = |IM\rangle\langle IK|$$

Pairing Correlations

Effects of the residual interaction

$$H=\sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2+V_{\mathrm{HF}}(i)\right)+\underline{\underline{\frac{1}{2}\sum_{i,j}^{A}v(\boldsymbol{r}_i,\boldsymbol{r}_j)-\sum_i V_{\mathrm{HF}}(i)}}$$



without residual interaction

with residual interaction

$^{210}_{84}Po_{126} = {}^{208}_{82}Pb_{126} + 2p$

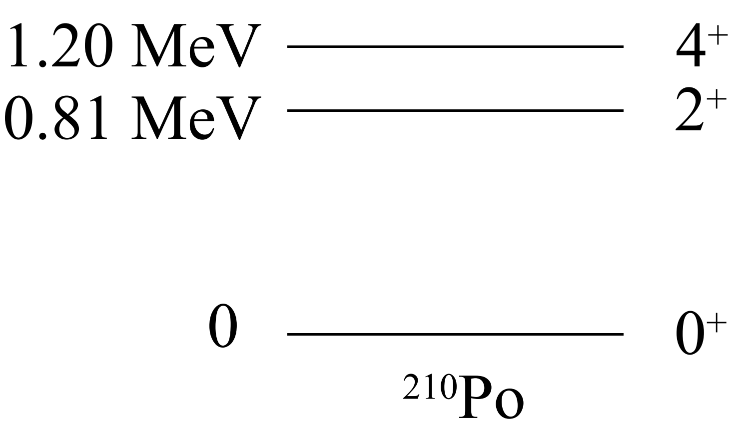
expectation of the indep. particle model:

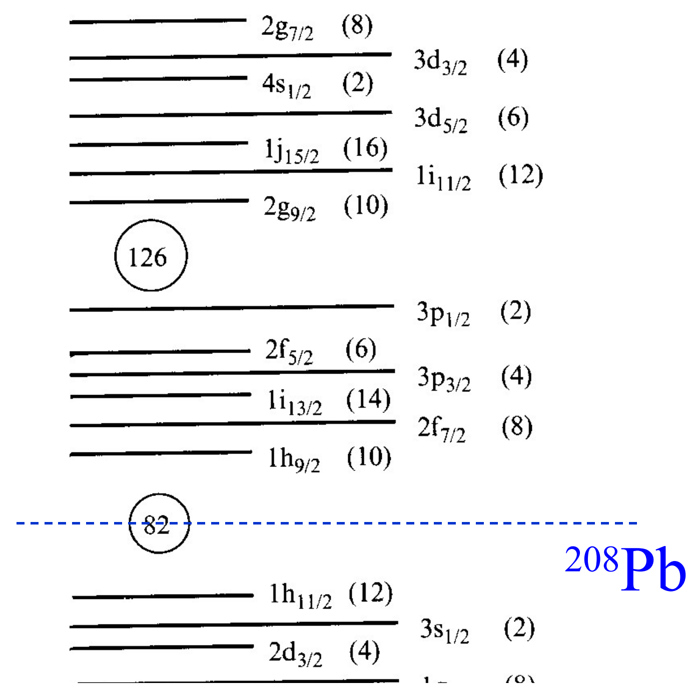
E=0: $[h_{9/2} \otimes h_{9/2}]^I$ $(I=0,2,4,6,8)$

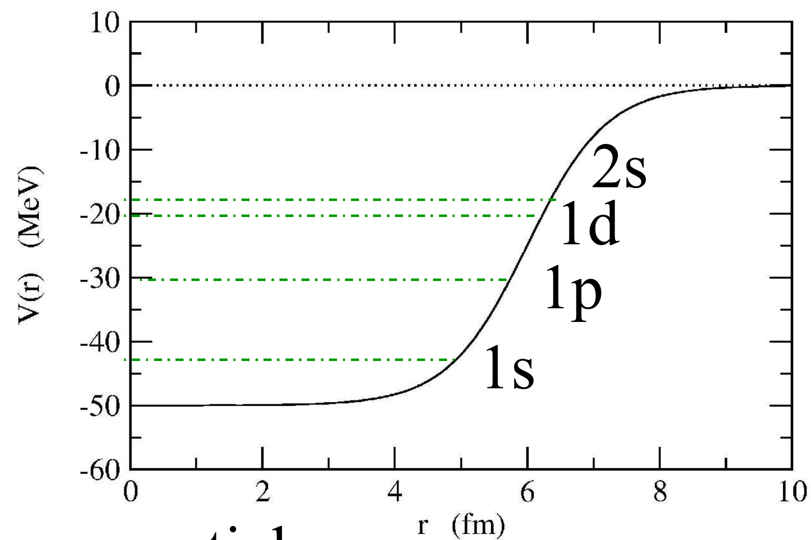
E=0.89 MeV: $[h_{9/2} \otimes f_{7/2}]^I$ $(I=1,2,3,4,5,6,7,8)$

⇨ # of states below 1 MeV: 13

observed spectra:







The ground state spin of nuclei

- Even-even nuclei: 0^+
- Even-odd nuclei: the spin of the valence particle

The BCS theory

Many-particles in non-degenerate levels
~ mean-field approx. for the pairing channel ~

Solve the pairing Hamiltonian

$$H = \sum_{\nu} \epsilon_{\nu}(a_{\nu}^{\dagger}a_{\nu} + a_{\bar{\nu}}^{\dagger}a_{\bar{\nu}}) - G\left(\sum_{\nu>0} a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger}\right)\left(\sum_{\nu>0} a_{\bar{\nu}}a_{\nu}\right)$$

in the mean-field approximation

- The Bardeen, Cooper, Schrieffer (BCS) ansatz

$$|\Psi\rangle = \prod_{\nu>0}\left(u_{\nu} + v_{\nu}\, a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger}\right)\Big|0\Big\rangle$$

(note) $\left\langle a_{\nu}^{\dagger}a_{\nu}\right\rangle = |v_{\nu}|^2$: occupation probability

Minimize $\langle H' \rangle = \left\langle \sum_{\nu} \epsilon_{\nu}(a_{\nu}^{\dagger}a_{\nu} + a_{\bar{\nu}}^{\dagger}a_{\bar{\nu}}) - GP^{\dagger}P - \lambda\hat{N} \right\rangle$

with $\langle\Psi|\hat{N}|\Psi\rangle = 2\sum_{\nu>0} v_{\nu}^2 = N$

$$\begin{pmatrix} \epsilon_\nu - \lambda & \Delta \\ \Delta & -\epsilon_\nu + \lambda \end{pmatrix} \begin{pmatrix} u_\nu \\ v_\nu \end{pmatrix} = E_\nu \begin{pmatrix} u_\nu \\ v_\nu \end{pmatrix}$$

$$u_\nu^2 = \frac{1}{2}\left(1 - \frac{\epsilon_\nu - \lambda}{E_\nu}\right)$$

$$v_\nu^2 = \frac{1}{2}\left(1 + \frac{\epsilon_\nu - \lambda}{E_\nu}\right)$$

$$E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}$$

Pairing gap: $\Delta = G\langle P^\dagger \rangle = G \sum_{\nu>0} u_\nu v_\nu$

$$\Delta = \frac{G}{2} \sum_{\nu>0} \frac{\Delta}{E_\nu}$$

(Gap equation)

i) Trivial solution: always exists

$$\Delta = 0$$

$$v_\nu^2 = 1 \quad (\epsilon_\nu \leq \lambda)$$
$$\quad = 0 \quad (\epsilon_\nu > \lambda)$$

$$|\Psi\rangle = \prod_{\nu>0} a_\nu^\dagger a_{\bar{\nu}}^\dagger |0\rangle$$

G a/o $N \longrightarrow$ large

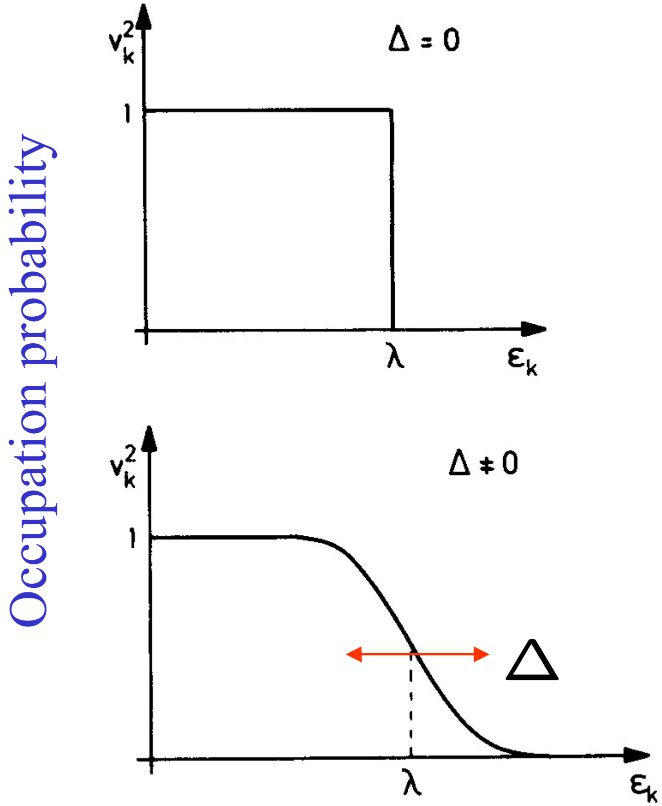
ii) Superfluid solution

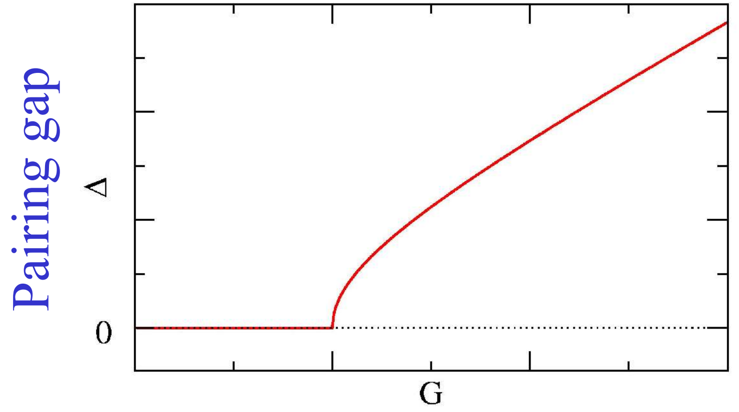
$$\Delta \neq 0$$

$$v_\nu^2 < 1$$

$$|BCS\rangle = \prod_{\nu>0} \left(u_\nu + v_\nu\, a_\nu^\dagger a_{\bar{\nu}}^\dagger\right) \big|\, 0\rangle$$

Number fluctuation





Normal-Superfulid phase transition

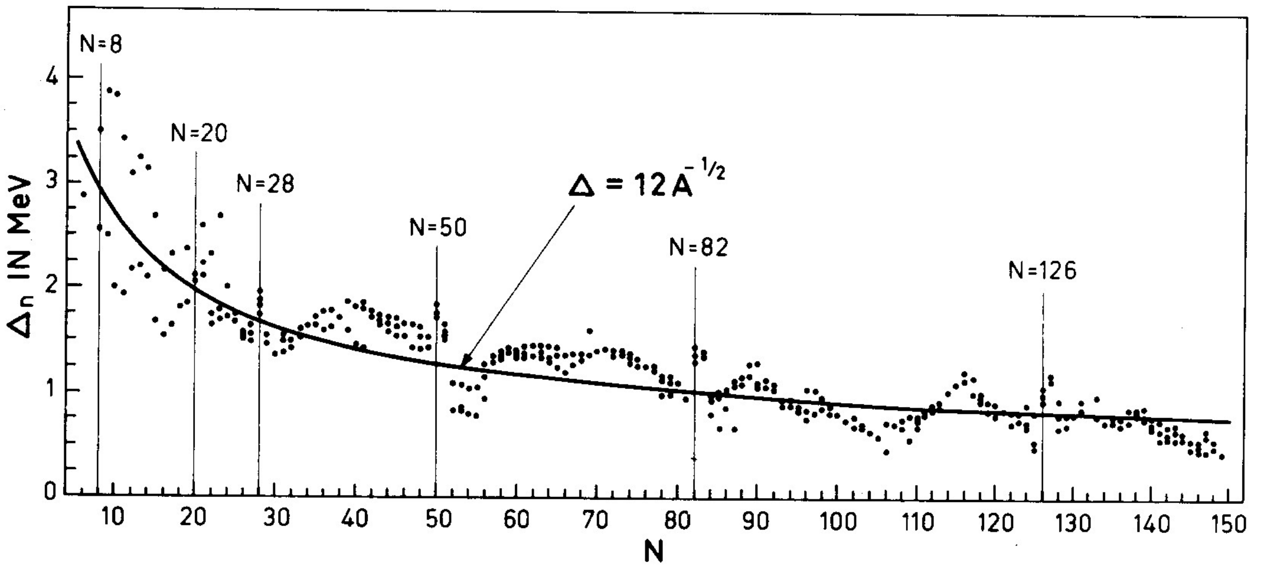
Even-odd mass difference and pairing gap

$$B_{\text{pair}} = \Delta \quad \text{(for even – even)}$$
$$= 0 \quad \text{(for even – odd)}$$
$$= -\Delta \quad \text{(for odd – odd)}$$

$$E(N+2,Z) = E(N,Z) + 2\lambda$$
$$E(N+1,Z) = E(N,Z) + \lambda + \Delta$$

$$-\Delta_n \sim [E(N+2,Z) - 2E(N+1,Z) + E(N,Z)]/2$$

Or $$\Delta_n \sim (\Delta_n(N) + \Delta_n(N-1))/2$$



Bohr-Mottelson ('69)

Hartree-Fock-Bogoliubov (HFB) Theory

~ generalization and unification of HF and BCS methods ~

BCS: u,v factors

HFB: u,v *functions*

$$|HFB\rangle = \prod_{\alpha} \beta_{\alpha} |0\rangle$$

generalized Bogoliubov transformation

$$\beta_{\alpha}^{\dagger} = \int d\boldsymbol{r} \, \left\{ U_{\alpha}(\boldsymbol{r}) \, c_{\boldsymbol{r}}^{\dagger} + V_{\alpha}(\boldsymbol{r}) \, c_{\boldsymbol{r}} \right\}$$

minimize

$$\langle HFB | H - \lambda \hat{N} | HFB \rangle$$

For a local and zero-range interaction:

$$\langle \boldsymbol{r}_1\boldsymbol{r}_2|v|\boldsymbol{r}_3\boldsymbol{r}_4\rangle = v(\boldsymbol{r}_1)\delta(\boldsymbol{r}_1-\boldsymbol{r}_3)\delta(\boldsymbol{r}_2-\boldsymbol{r}_4)\cdot\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$$

$$\begin{pmatrix} \hat{h}(\boldsymbol{r})-\lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r})^* & -\hat{h}(\boldsymbol{r})+\lambda \end{pmatrix}\begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

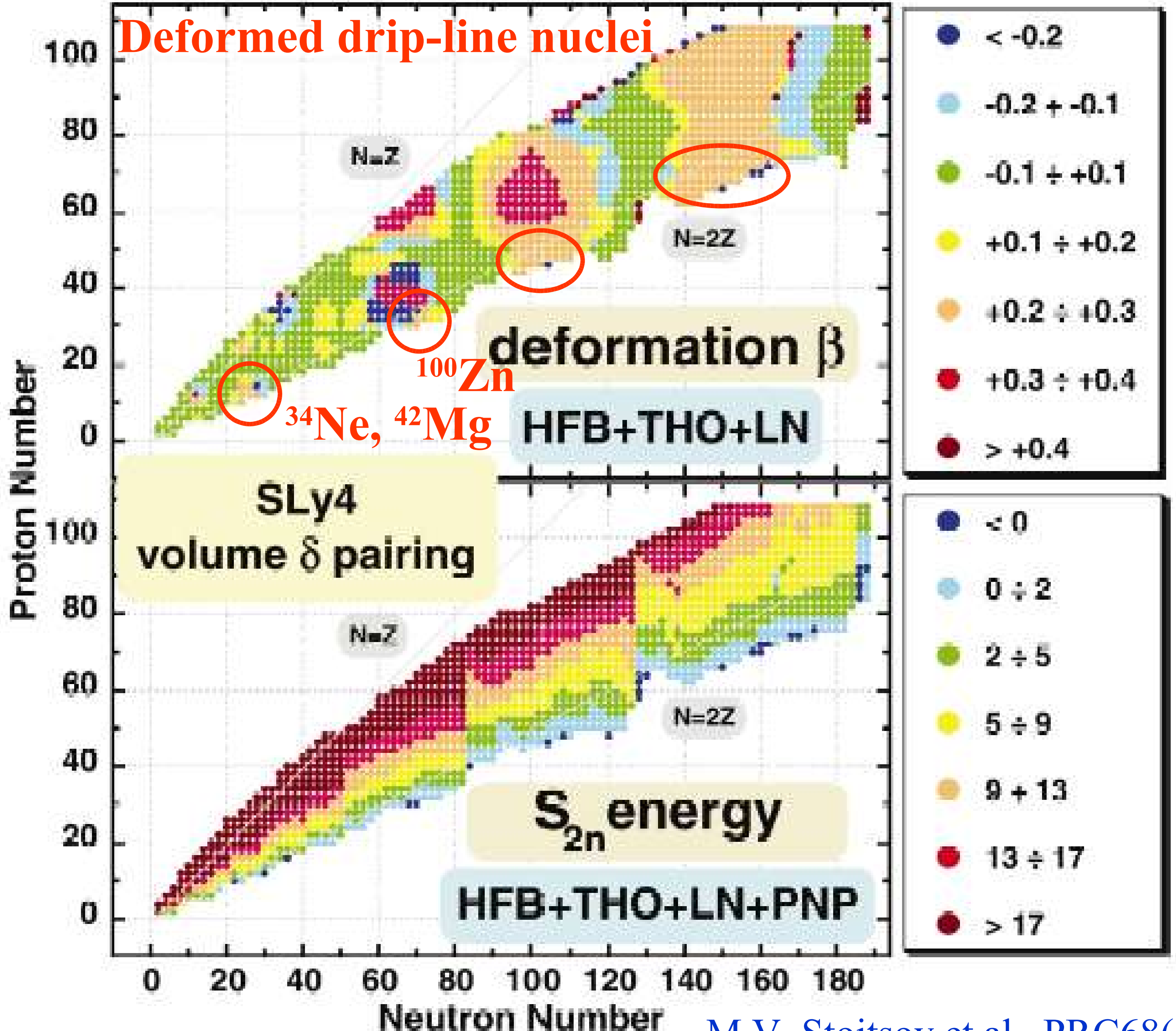
$$\begin{aligned} \hat{h}(\boldsymbol{r}) &= -\frac{\hbar^2}{2m}\nabla^2 + V_{\rm HF}(\boldsymbol{r}), \quad V_{\rm HF}(\boldsymbol{r}) = v(\boldsymbol{r})\rho(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r}) &= v(\boldsymbol{r})\tilde{\rho}(\boldsymbol{r})/2 \\ \rho(\boldsymbol{r}) &= \sum_\alpha |V_\alpha(\boldsymbol{r})|^2, \quad \tilde{\rho}(\boldsymbol{r}) = -\sum_\alpha U_\alpha(\boldsymbol{r})V_\alpha^*(\boldsymbol{r}) \end{aligned}$$

Ortho-normalization:

$$\int d\boldsymbol{r}\,[U_\alpha^*(\boldsymbol{r})U_{\alpha'}(\boldsymbol{r}) + V_\alpha^*(\boldsymbol{r})V_{\alpha'}(\boldsymbol{r})] = \delta_{\alpha,\alpha'}$$

(note) in condensed matter physics: *Bogoliubov-de Gennes Equations*

Deformed drip-line nuclei



M.V. Stoitsov et al., PRC68('03)054312