Hartree Fock (HF) Mean Field Theory

We have

$$[H, J^2] = 0 ,$$

$$H \mid \Psi_J\rangle = E_J \mid \Psi_J\rangle ,$$

$$J^2 \mid \Psi_J\rangle = J(J+1) \mid \Psi_J\rangle .$$

HF Does not deal directly with | Ψ_J > instead determines by Minimizing E_J. In independent particle picture

Many Body HF Wave Function Φ Is

$$\Phi = \mathcal{A}\prod_i^A \phi_i \; ; \quad H \rightarrow H_{eff} = \sum_i^A h(i) , \quad h \mid \phi_i\rangle = \varepsilon_i \mid \phi_i\rangle .$$

Φ Is obtained through $\delta\langle\Phi \mid H \mid \Phi\rangle = 0$.

The HF s.p. states ϕ_i is expanded in terms of s.p. basis states $\mid \alpha >\equiv\mid nljm\tau_3 >$

$$\mid \phi_i >\equiv\mid i >= \sum_\alpha x_\alpha^i \mid \alpha >,$$

The Real Expansion Coeff. $x_\alpha^i =< \alpha \mid i >$ **are Variational Parameters**

These Orthonormal Sets of s.p. States Satisfy:

$$< i \mid i' >= \delta_{ii'} = \sum_{\alpha} x_{\alpha}^{i*} x_{\alpha}^{i'}$$

$$< \alpha \mid \beta >= \delta_{\alpha\beta} = \sum_{i} x_{\alpha}^{i*} x_{\beta}^{i}$$

One Uses

$$\delta[\langle \Phi \mid H \mid \Phi \rangle - \sum_{i} \varepsilon_i \sum_{\alpha} x_{\alpha}^{i*} x_{\alpha}^{i}] = 0$$

Where ε_i are Lagrange Multipliers

The Expectation Value

$$\langle \Phi \mid H \mid \Phi \rangle = \sum_{i}^{occ} < i \mid t \mid i > + \frac{1}{2} \sum_{ii'}^{occ} < ii' \mid v \mid ii' >$$

$$= \sum_{i}^{occ} \sum_{\alpha} e_{\alpha} x_{\alpha}^{i*} x_{\alpha}^{i} + \frac{1}{2} \sum_{ii'}^{occ} \sum_{\alpha\beta\gamma\delta} x_{\alpha}^{i*} x_{\beta}^{i'*} < \alpha\beta \mid v \mid \gamma\delta > x_{\gamma}^{i} x_{\delta}^{i'}$$

e_{α} **is Eigen Energy of** $\mid \alpha >$

'occ' **Stands for Sum Over Lowest A Occupied States**

With

$$\rho_{\delta\beta} = \sum_{i'}^{occ} x_{\beta}^{i'*} x_{\delta}^{i'}$$

And Manipulation of Summation Indices . One Gets

$$e_{\mu} x_{\mu}^{k} + \sum_{\beta\gamma\delta} < \mu\beta \mid v \mid \gamma\delta > \rho_{\delta\beta} x_{\gamma}^{k} = \varepsilon_{k} x_{\mu}^{k}$$

Define One Body HF Potential

$$\Gamma_{\mu\gamma} = \sum_{\beta\delta} < \mu\beta \mid v \mid \gamma\delta > \rho_{\delta\beta}$$

The HF Equation Now Becomes

$$\sum_{\gamma}[(e_{\gamma} - \varepsilon_k)\delta_{\mu\gamma} + \Gamma_{\mu\gamma}]x_{\gamma}^{k} = 0$$

This is an Eigen Value Equation With One Body HF Hamiltonian h_{HF}

$$< \mu \mid h_{HF} \mid \gamma >= e_{\gamma}\delta\mu\gamma + < \mu \mid \Gamma \mid \gamma >$$

The Diagonalization of this HF Matrix Yields HF s.p. Energies ε **and wave functions (Through Vectors X) Defining** ϕ

The HF Matrix Requires Γ Which in Turn Requires ρ .
It has to be Solved Iteratively. One starts With Initial Guess $\rho^{(i)}$ (of Nilsson Hamiltonian) and calculates New $\rho^{(f)}$, Which Forms the New Input.
This Procedure is Continued Till the Desired Convergence is Achieved.

HF Total Energy

$$
\begin{aligned}
E_{HF} &= \sum_{i}^{occ} < i \,|\, t \,|\, i > + \frac{1}{2} \sum_{ii'}^{occ} < ii' \,|\, v \,|\, ii' > \\
&= \sum_{i} [\varepsilon_i - \frac{1}{2} < i \,|\, \Gamma \,|\, i >] \\
&= \sum_{i} \varepsilon_i + |\delta E|
\end{aligned}
$$

δE is Positive for Attractive Potential. Thus HF Overestimates the Total Energy.

For Spherical Nuclei the Summation in the Expansion is Over Nodal Quantum Number n

HF Wave function $|\Phi>$ is not an Eigen State of Total Angular Momentum J^2 . The State with Good J and Projection M (on the Lab. Fixed z-axis is written as

$$|\Psi_{JM}>= n_J P^J_{MK} \,|\, \Phi\rangle$$

n_J is normalization and Projector P is

$$P^J_{MK} = \frac{2J+1}{8\pi^2}\int d\Omega D^{J*}_{MK}(\Omega)R(\Omega)$$

D is the Well Known Rotation Matrix

The Energy becomes (Choose M=K.)

$$
\begin{aligned}
E_{JK} &= \, < JK|H|JK > / < JK|JK > \\
&= \frac{< \Phi|P^{J\dagger}_{KK} H P^{J}_{KK}|\Phi >}{< \Phi|P^{J\dagger}_{KK} P^{J}_{KK}|\Phi >} \\
&= \frac{< \Phi|H P^{J}_{KK}|\Phi >}{< \Phi|P^{J}_{KK}|\Phi >}
\end{aligned}
$$

Illustration:

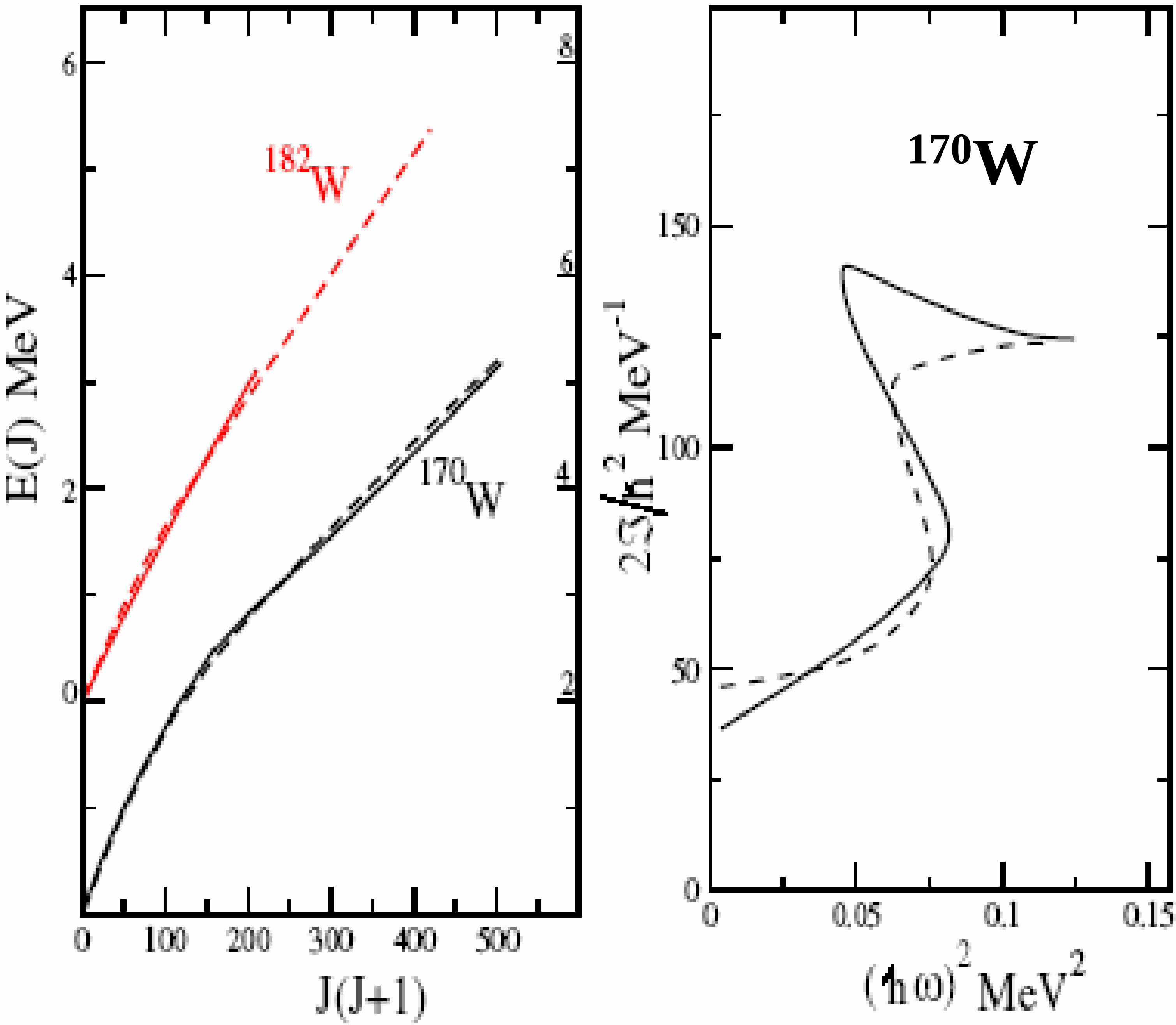
W Isotopes (Z = 74)

Step 1: Core: Z = 40, N = 70
Valance Levels: $2\hbar\omega$ **, Both for p & n**

Step 2: HF Basis States

Step 3: Interaction – Pairing + Q.Q

Step 4: Diagonalisation of HF Matrices



E(J) MeV
6
4
2
0
8
6
4
2
182W
170W
0
100
200
300
400
500
J(J+1)
170W
2ℑ/ħ² MeV⁻¹
150
100
50
0
0
0.05
0.1
0.15
(ħω)² MeV²

Backbending

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

$$\frac{\hbar^2}{2\Im_I} = \frac{\partial E_I}{\partial (I(I+1))} = \frac{E_I - E_{I-2}}{2(2I-1)}$$

$$\Im_I \omega_I = \hbar\sqrt{(I(I+1))} = \hbar\bar{I}\ ;$$

$$\hbar\omega_I = \frac{\partial E_I}{\partial \bar{I}} \approx \frac{E_I - E_{I-2}}{\left(2 - \frac{1}{2I}\right)}$$

Hartree-Fock-Bogoliubov (HFB) Theory

The Quasi-particle Operators b are Defined of the Basis Space Operators c

$$
\begin{aligned}
b_i^\dagger &= \sum_\alpha (A_{\alpha i} A_\alpha^\dagger + B_{\alpha i} c_\alpha) \\
b_i &= \sum_\alpha (B_{\alpha i}^* c_\alpha^\dagger + A_{\alpha i}^* c_\alpha)
\end{aligned}
$$

The Inverse Transformation Reads

$$
\begin{aligned}
c_\alpha^\dagger &= \sum_i (A_{\alpha i}^* b_i^\dagger + B_{\alpha i} b_i) \\
c_\alpha &= \sum_i (B_{\alpha i}^* b_i^\dagger + A_{\alpha i} b_i)
\end{aligned}
$$

The HFB g.s. is Defined Through

$$b_i \mid HFB\rangle = 0 \qquad |HFB> = \prod_i b_i|0>$$

$|0>$ **Being the Real Vacuum**

|HFB > is not an Eigen Function of the Particle Number Operator

$$\hat{N} = \sum_{\alpha} c_{\alpha}^{\dagger} c_{\alpha}$$

This can be Rectified by Introducing Lagrange Multiplier and Working with the New Hamiltonian

$$H' \;=\; H - \lambda \hat{N}$$

$$= \sum_{\alpha} (e_\alpha - \lambda) c^\dagger_\alpha c_\alpha + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} < \alpha\beta|v|\gamma\delta > c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$$

In the Independent Quasiparticle Picture We Should Have

$$[H', b^\dagger_i] = E_i b^\dagger_i$$

$$[H', b_i] = -E_i b_i$$

Evaluating These Commutators

$$[H', b_i^\dagger] \;=$$

$$\sum_{\alpha\gamma} \{[((e_\alpha - \lambda)\delta_{\alpha\gamma} + \Gamma_{\alpha\gamma})A_{\gamma i} + \Delta_{\alpha\gamma} B_{\gamma i}]c_\alpha^\dagger$$

$$-[((e_\alpha - \lambda)\delta_{\alpha\gamma} + \Gamma^*_{\alpha\Gamma})B_{\gamma i} + \Delta^*_{\alpha\gamma} A_{\gamma i}]c_\alpha\}$$

HF Potential Γ **and Pairing Potential** Δ **are:**

$$\Gamma_{\alpha\gamma} = \sum_{\beta\delta} < \alpha\beta|v|\gamma\delta > \rho_{\delta\beta}$$

$$\Delta_{\alpha\beta} = \frac{1}{2}\sum_{\gamma\delta} < \alpha\beta|v|\gamma\delta > \kappa_{\delta\gamma}$$

One Body HF Density ρ and Pairing Matrix κ are;

$$
\begin{aligned}
\rho_{\delta\beta} &= <HFB|c^{\dagger}_{\beta}c_{\delta}|HFB> \\
&= (B^{*}\tilde{B})_{\delta\beta} \\
\kappa_{\delta\gamma} &= <HFB|c_{\delta}c_{\gamma}|HFB> \\
&= (AB^{\dagger})_{\delta\gamma} \,,
\end{aligned}
$$

Here $\tilde{B}$ Stands for Transpose of B

The Commutator Should be Equated To

$$E_i \sum_{\alpha}(A_{\alpha i}c^{\dagger}_{\alpha} + B_{\alpha i}c_{\alpha})$$

For Each Value of α

This Equality Leads To HFB Equations:

$$\begin{pmatrix} \bar{\Gamma} & \Delta \\ -\Delta^* & -\bar{\Gamma}^* \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = E \begin{pmatrix} A \\ B \end{pmatrix}$$

With :

$$\bar{\Gamma}_{\alpha\gamma} = (e_\alpha - \lambda)\delta_{\alpha\gamma} + \Gamma_{\alpha\gamma}$$

The Total HFB Energy can be Calculated as:

$\mathbf{E_{HFB}} =$

$$\sum_{\alpha\gamma} (e_\alpha \delta_{\alpha\gamma} + \frac{1}{2} \Gamma_{\alpha\gamma}) \rho_{\gamma\alpha} + \frac{1}{2} \sum_{\alpha\beta} \Delta_{\alpha\beta} \kappa^*_{\beta\alpha}$$

- HFB Equations Have to be Solved Iteratively.
- Initial Guess for Bogoliubov Transformation Coefficients A and B →
- Through Hartree – Nilsson OR Nilsson – BCS Calculations Such That

$$A_{\alpha i} = x_{\alpha}^{i} U_{i} \quad \textbf{and} \quad B_{\alpha i} = x_{\alpha}^{i} V_{i}$$

Where x are the HF Expansion Coeff. And V, U are the Standard BCS Occupation Parameters.