Hartree-Fock-Bogoliubov Theory

From Stable to Weakly-Bound Nuclei

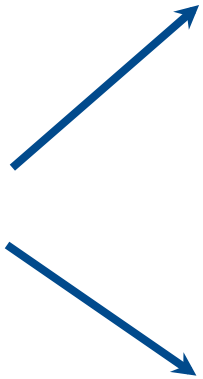
Theories of Nuclear Structure

microscopic

Ab initio approaches - start from a given NN force
-no core shell model
-coupled cluster calculations
-unitary correlator method

Large scale **Shell Model** calculations

Microscopic models based on effective interactions or energy-density functionals

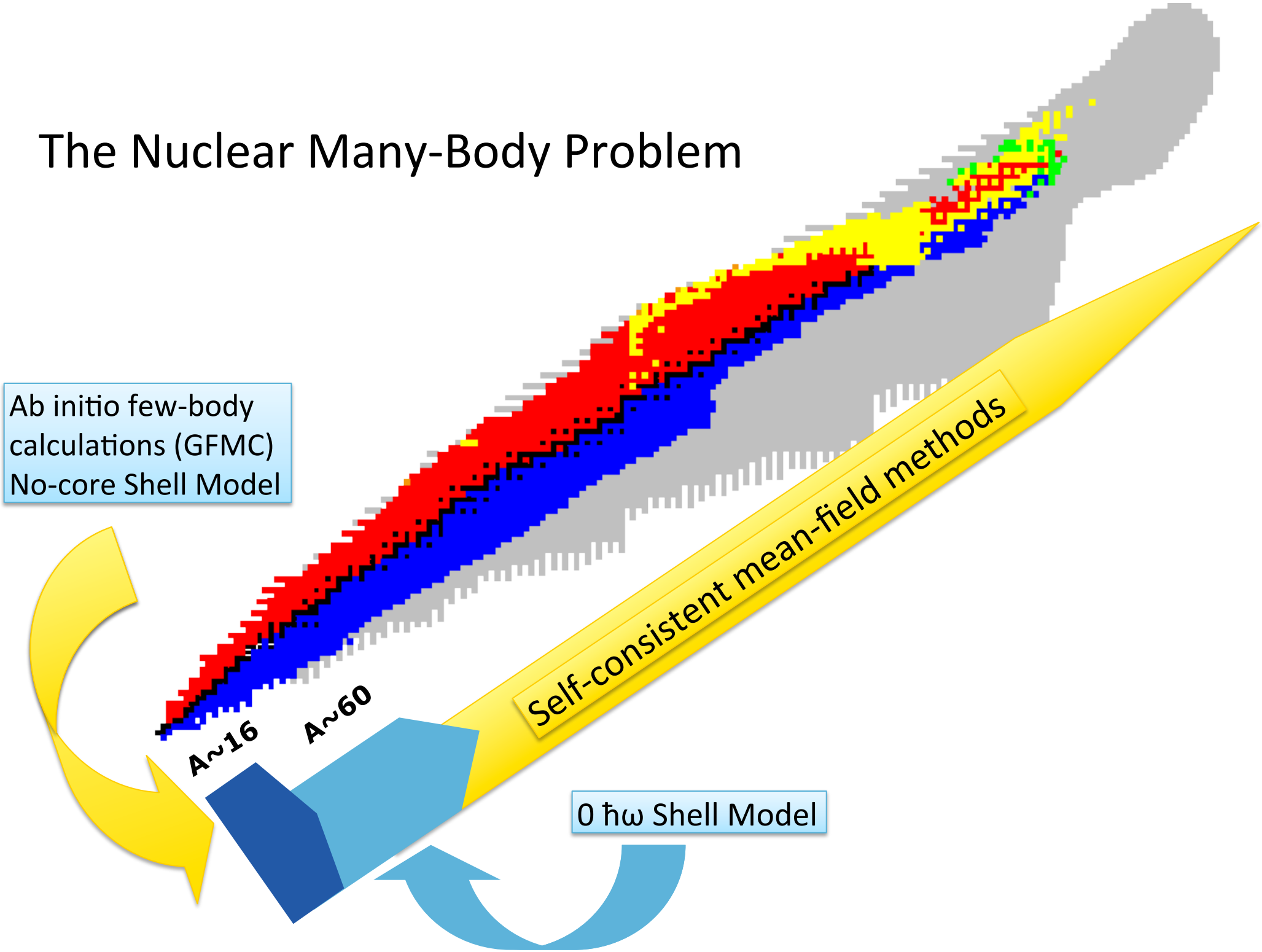


Self-consistent mean-field models

Mac-mic approach
-liquid drop model plus shell corrections
-phenomenological input

phenomenological

The Nuclear Many-Body Problem



Self-consistent mean-field models

Mean-field approximation: the dynamics of the nuclear many-body system is represented by independent nucleons moving in a self-consistent potential.

Self-consistent potential: corresponds to the actual density distribution for a given nucleus.

Advantages of the SCMF approach:

- ✧ use of global effective nuclear interactions (used for all nuclei!)
- ✧ can be applied to arbitrarily heavy systems, including superheavy nuclei
- ✧ intuitive picture of intrinsic shapes

The General Variational Principle

$$E[\Psi] = \frac{<\Psi|H|\Psi>}{<\Psi|\Psi>}$$

→ any state which makes the functional E[Ψ] stationary, when |Ψ> is allowed to vary over the whole Hilbert space, is an eigenstate of the hamiltonian H with the eigenvalue E.

→ variation: $<\Psi| \rightarrow <\Psi| + <\delta\Psi|$

$$\delta E[\Psi] = 0 \quad \Longrightarrow \quad <\delta\Psi|H - E|\Psi> = 0$$

If this is satisfied for any variation ⇒ $H|\Psi> = E|\Psi>$

Trial wave function:

✧ single Slater determinant ≡ **Hartree-Fock approximation**
✧ quasi-particle vacuum ≡ **Hartree-Fock-Bogoliubov approximation**
✧ linear combination of a finite number of Slater determinants ≡ **Shell Model**
✧ continuous superposition of Slater determinants ≡ **Hill-Wheeler equation**

The Hartree-Fock Approximation

1. Basics of a mean-field description

The basic building block of any mean-field model is a set of single-nucleon wave functions:

$$\{\psi_i(\vec{x}), i = 1, \ldots, N_{\rm wf}\}\,, \quad \vec{x} = (\vec{r}, \sigma, \tau)$$

✧ the number of single-particle wave functions N_{wf} is larger than the number of nucleons A

$$a_i^+ = \int d^3r \sum_{\sigma t} \psi_i(\vec{x})\; a_x^+$$

Creation operator for a nucleon in a single-particle state ***i***

Creation operator for eigenstates of position

HF approximation: the state of a nucleus is described by a Slater determinant:

$$|\Phi\rangle \equiv \det\{\psi_i(\vec{x}), i = 1, \ldots, A\}$$

$$\hat{a}_i^+|\Phi\rangle = 0 \quad 1 \le i \le A \qquad\qquad \hat{a}_i|\Phi\rangle = 0 \quad i > A$$

2. Single-particle density matrix

$$\rho_{ij} = < i|\rho|j > = < \Phi|a_j^+ a_i|\Phi >$$

→ the density operator associated with the Slater determinant |Φ> can be expressed in terms of the single-nucleon orbitals:

$$\rho = \sum_i^A |\psi_i >< \psi_i| = \sum_i n_i |\psi_i >< \psi_i|$$

A completely antisymmetric state |Φ> is a Slater determinant if and only if the corresponding density matrix ρ is a projector onto the Hilbert space spanned by occupied single-particle orbitals:

$$\rho^2 = \rho$$

3. Hartree-Fock equations

The hamiltonian of the system : sum of a kinetic energy term and a two-body potential:

$$H = \sum_{ij} < i|T|j > a_i^+ a_j + \frac{1}{4} \sum_{ijkl} < ij|V|kl > a_i^+ a_j^+ a_l a_k$$

→ the expectation value in a Slater determinant |Φ >:

$$E[\rho] =< \Phi|H|\Phi >= \sum_{ij} < i|T|j > \rho_{ji} + \frac{1}{2} \sum_{ijkl} < ij|V|kl > \rho_{ki}\rho_{lj}$$

defines the energy E as a functional of the single-particle density matrix ρ associated with the state |Φ >.

the variational equation:

$$\delta\{E[\rho] - \mathrm{tr}\Lambda(\rho^2 - \rho)\} = 0$$

The Hartree-Fock hamiltonian:

→ hermitian operator in the space of single-particle states

$$h_{ij} \equiv < i|h|j >= \frac{\partial E[\rho]}{\partial \rho_{ji}}$$

From the variational equation: $\Rightarrow$ $[h, \rho] \equiv h\rho - \rho h = 0$

the Hartree-Fock equation

The solution of the Hartre-Fock equation is a single-particle basis in which both h and ρ are diagonal.

$$h|\lambda_\nu >= e_\nu|\lambda_\nu >$$ HF orbitals

$h = h[\rho]$ $\Rightarrow$ the HF equation is non-linear!

Iterative solution:

1) initial guess for the HF orbitals $|\lambda_\nu > \implies \rho = \sum_{\nu=1}^{A} |\lambda_\nu >< \lambda_\nu|$

2) with this density matrix ρ construct the HF hamiltonian h

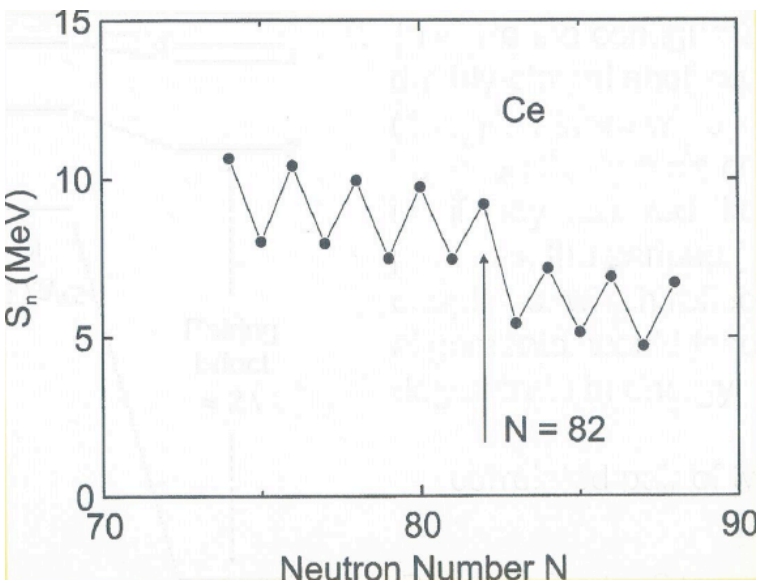
3) Diagonalize h: new set of HF orbitals $|\lambda'_\nu >$

Repeat steps 2) and 3) until two successive calculations give the same HF orbitals to a desired accuracy:
self-consistent HF hamiltonian

Empirical evidence for pairing correlations

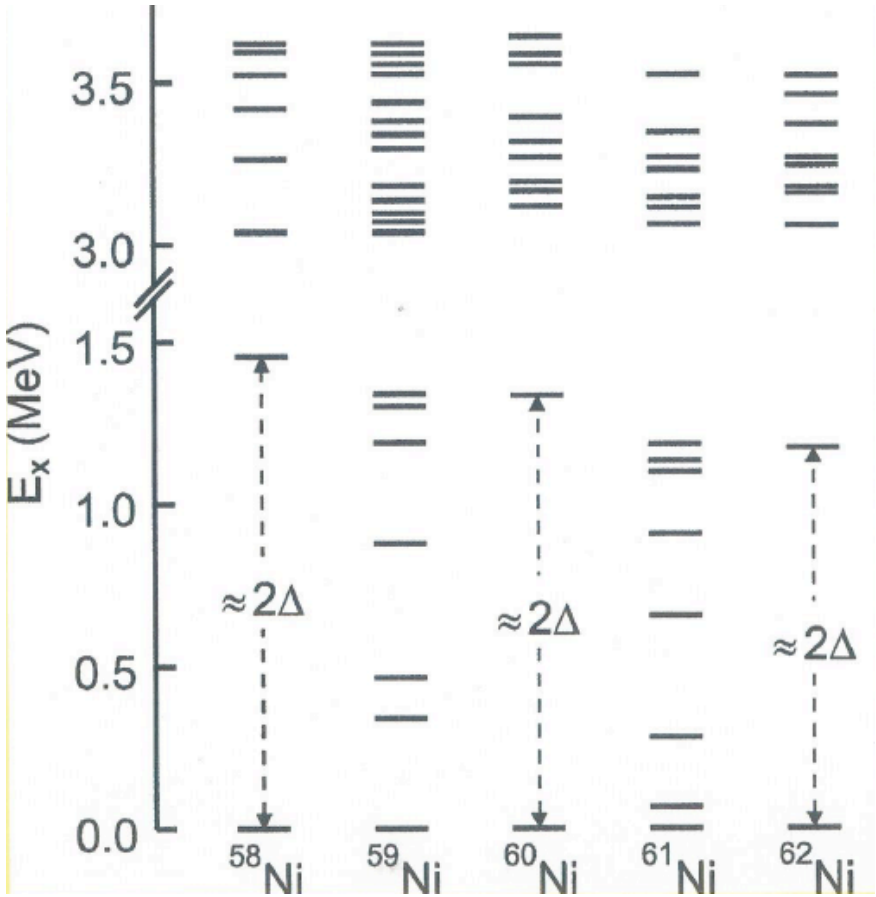
For even-even nuclei the ground-state has always zero angular momentum, i.e. the residual interaction lowers this particular state with respect to other ang. momentum combinations.

Odd-even effect: even-even nuclei are bound more tightly than neighboring odd-A nuclei.



One-neutron separation energies in Ce.

In even-even nuclei there is an energy gap of 1-2 MeV between the ground state and the lowest singe-particle excitations.



Two nucleons in the same shell:

$$|nljj; J = 0M = 0\rangle = \sum_m < jmj - m|00 > |jm\rangle|j - m\rangle = \frac{1}{\sqrt{2j+1}} \sum_m (-)^{j-m}|jm\rangle|j - m\rangle$$

This state will have the lowest energy for a short-range interaction. In the state J = 0 the nucleons are relatively close (the spatial overlap of the two nucleon densities is maximal), whereas they are not in higher angular momentum states.

For nuclei between closed shells, the nucleons (except the last one) will be paired off . This configuration will be most favorable energetically. To excite even-even nuclei, either a pair has to be lifted to a higher shell or it has to be broken. For odd nuclei, the odd unpaired nucleon can simply be lifted to higher orbits.

Pairing in a degenerate single-j shell

… general two-body interaction: $$V(1,2) \rightarrow \frac{1}{4} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta|V|\gamma\delta\rangle a^+_\alpha a^+_\beta a_\delta a_\gamma$$

PAIRING HAMILTONIAN:

$$H_P = -G \sum_{m,m'>0} a^+_{jm} a^+_{j-m} a_{j-m'} a_{jm'} (-)^{2j+m+m'}$$

a) Two particles in a single-j shell $2\Omega = 2j+1$ degenerate states.

The number of states occupied by 2 nucleons: $$N = \begin{pmatrix} 2j+1 \\ 2 \end{pmatrix}$$

Number of states of the form |m –m>: $$\Omega = \frac{2j+1}{2}$$

Example: $j = \frac{9}{2}$ $m = \frac{9}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, -\frac{7}{2}, -\frac{9}{2}$

In matrix representation the pairing Hamiltonian reads:

$$H_P = -G \begin{bmatrix} \overbrace{\begin{matrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \dots & \dots & \dots & \dots \\ 1 & 1 & \dots & 1 \\ 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \end{matrix}}^{\Omega} & \begin{matrix} 0 & \dots & 0 \\ 0 & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & 0 \\ 0 & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & 0 \end{matrix} \end{bmatrix}$$

with the two-nucleon basis arranged so that the first Ω states are those of the form |m –m >.

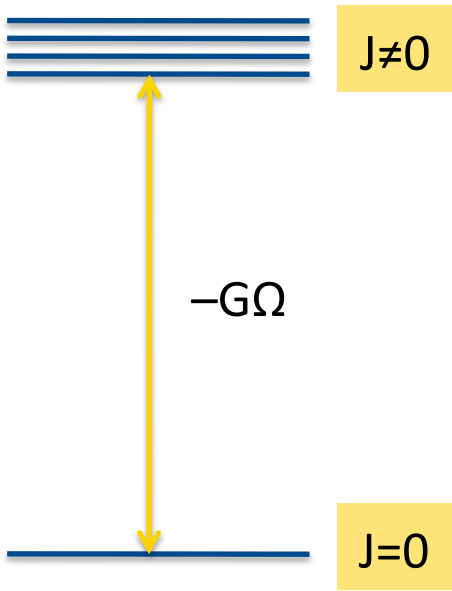
$$|\psi_0\rangle = \frac{1}{\sqrt{\Omega}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \frac{1}{\sqrt{\Omega}} \sum_{m>0} (-)^{j+m} a^+_{jm} a^+_{j-m} |0\rangle$$

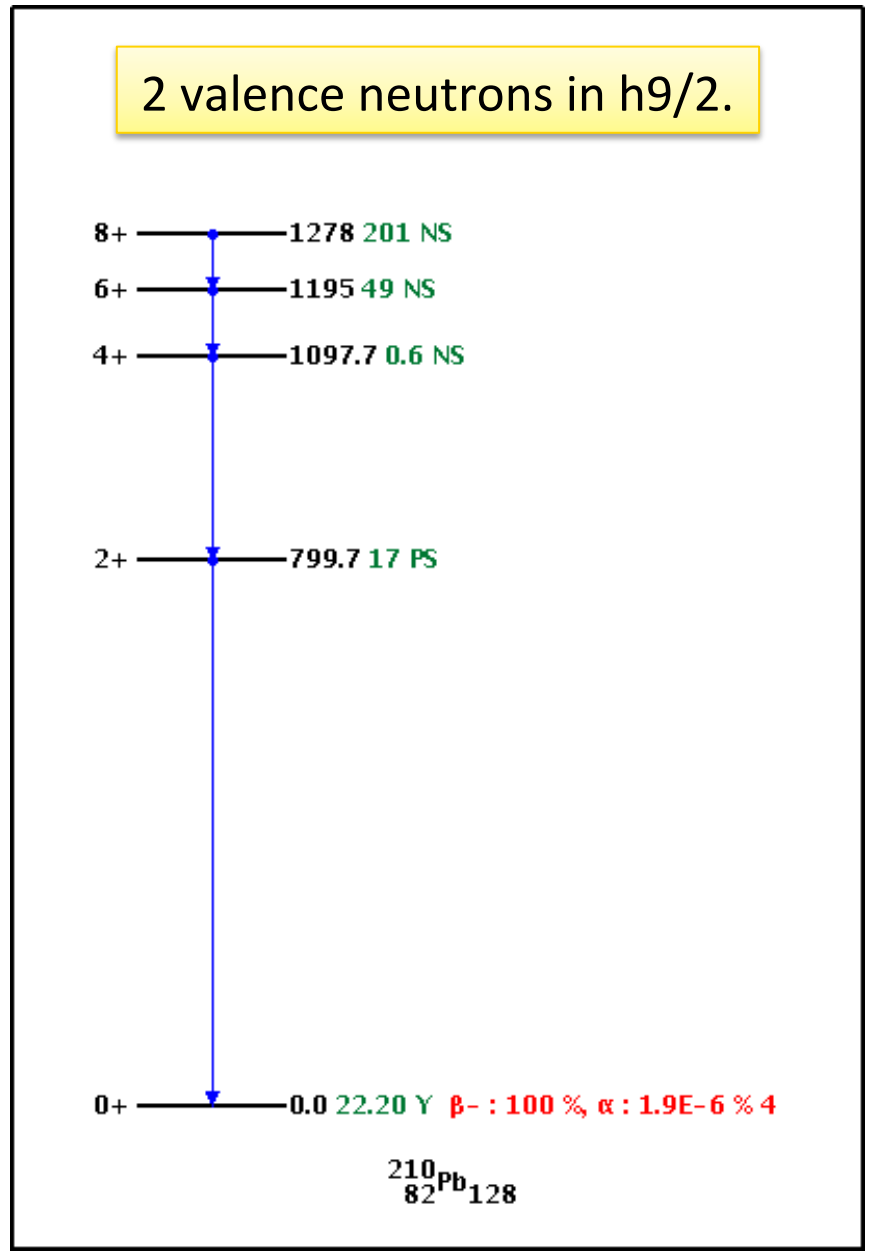
closed shell

is the lowest energy eigenstate of H_P with $E_0 = - G\Omega$.

Since the eigenvalue of this state is equal to the trace of the matrix H_P, all other eigenstates of H_P which are orthogonal to $|\psi_0\rangle$ must be degenerate with eigenvalue zero. This is because the sum of all eigenvalues equals the trace of the Hamiltonian matrix and because this particular matrix H_P is negative definite.

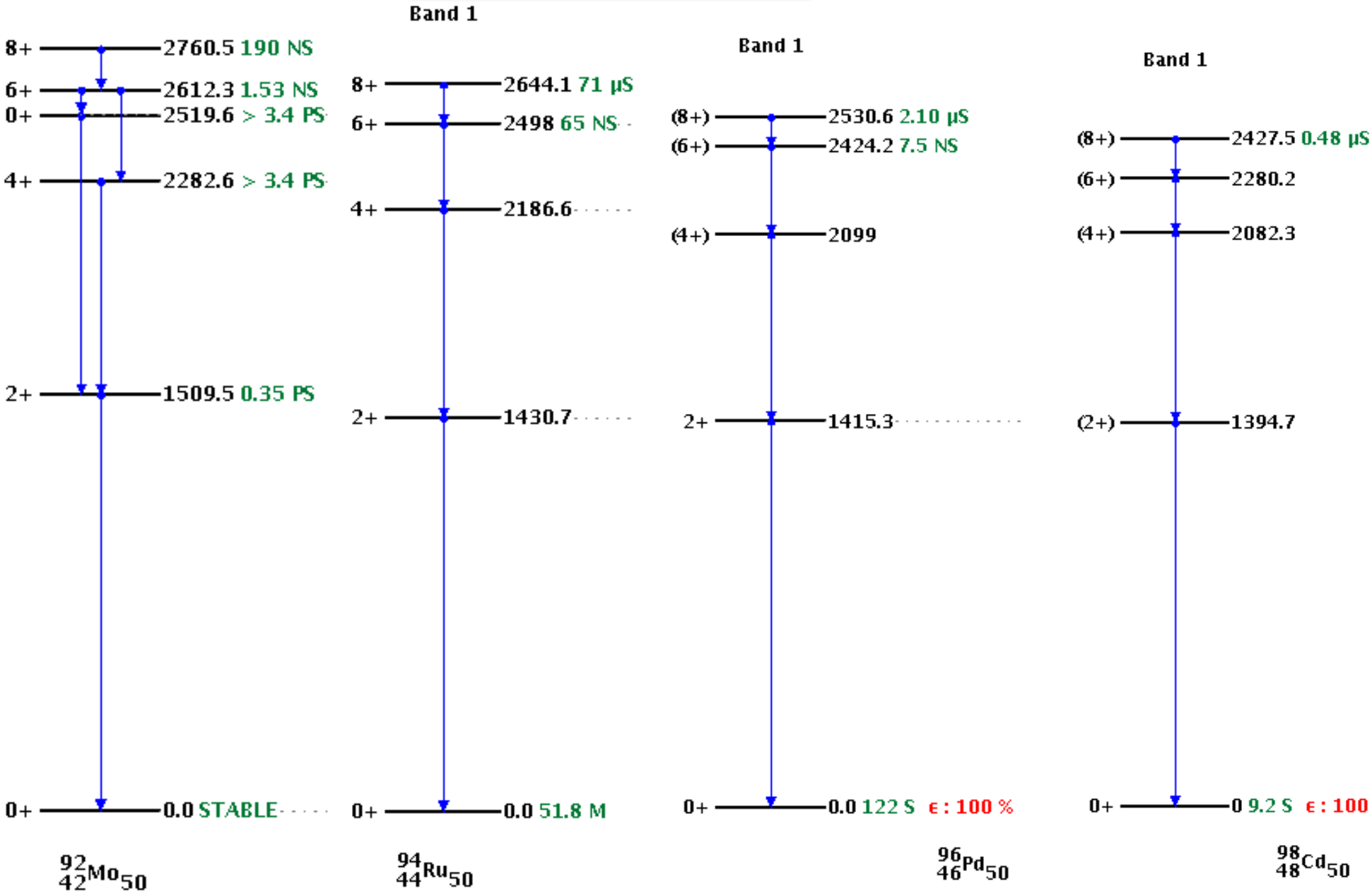
$|\psi_0\rangle$ is shifted downward in energy by $-G\Omega$.
All other states with $J\neq 0$ are not affected.





b) n – particles in a single-j shell

Filling the 1g9/2 orbital.



The Hartree-Fock-Bogoliubov Approximation

Pure Slater determinants ⇒ occupation numbers n={0,1}. This is strictly valid only for doubly magic nuclei. All others have partially occupied shells with a high density of almost degenerate states that are mixed by the residual two-body interaction: **nuclear pairing scheme.**

1. Pairing correlations

→ concept of independent quasi-particles defined by the Bogoliubov transformation:

$$b_n^+ = \sum_i (U_{in}\, a_i^+ + V_{in}\, a_i)$$

which relates single-particle states to quasiparticle states. In compact notation:

$$\begin{pmatrix} b \\ b^+ \end{pmatrix} = \mathcal{W}^+ \begin{pmatrix} a \\ a^+ \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

⇒ the transformation matrix is unitary.

The ground state of the system is determined by the condition that it is the quasi-particle vacuum:

$$b_n|\Phi\rangle = 0 \qquad \forall n$$

→ quasi-particle wave functions in coordinate space:

$$\phi_n = \begin{pmatrix} \phi_n^{(U)}(\vec{x}) \\ \phi_n^{(V)}(\vec{x}) \end{pmatrix} = \begin{pmatrix} \sum_i U_{in}\psi_i(\vec{x}) \\ \sum_i V_{in}\psi_i(\vec{x}) \end{pmatrix}$$

the single-particle density: $\rho_{ij} = \langle\Phi|a_j^+ a_i|\Phi\rangle = (V^* V^T)_{ij} = \rho_{ji}^*$

the pair tensor: $\kappa_{ij} = \langle\Phi|a_j a_i|\Phi\rangle = (V^* U^T)_{ij} = -\kappa_{ji}$

The completely antisymmetric state $|\Phi>$ is a quasiparticle vacuum if and only if the associated **generalized density matrix**

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$$

satisfies the relations: $\mathcal{R}^2 = \mathcal{R} \qquad \mathcal{R}^+ = \mathcal{R}$

2. Hartree-Fock-Bogoliubov equations

→ derived from the variational principle by using a quasiparticle vacuum as the trial wave function.

The qp vacuum is not an eigenstate of the particle number operator → additional constraint: the average number of particles = number of particles in the system.

$$< \Phi|N|\Phi >=< \Phi|\sum_i a_i^+ a_i|\Phi >= \mathrm{tr}\rho = \bar{N}$$

⇒ minimize the expectation value of the hamiltonian:

$$\begin{aligned} \hat{H} &= H - \mu N \\ &= \sum_{ij} < i|T-\mu|j > a_i^+ a_j + \frac{1}{4}\sum_{ijkl} < ij|V|kl > a_i^+ a_j^+ a_l a_k \end{aligned}$$

$$E[\rho,\kappa] \equiv < \Phi|\hat{H}|\Phi >\equiv E[\mathcal{R}]$$

$$\delta E[\rho,\kappa,\kappa^*] = \sum_{ij}\frac{\partial E}{\partial \rho_{ij}}\delta\rho_{ij} + \frac{1}{2}\sum_{ij}\left[\frac{\partial E}{\partial \kappa_{ij}^*}\delta\kappa_{ij}^* + \frac{\partial E}{\partial \kappa_{ij}}\delta\kappa_{ij}\right]$$

Hartree-Fock hamiltonian

$$h_{ij} = \frac{\partial E[\mathcal{R}]}{\partial \rho_{ji}} = h^*_{ji}$$

Pairing field

$$\Delta_{ij} = \frac{\partial E[\mathcal{R}]}{\partial \kappa^*_{ij}} = -\Delta_{ji}$$

$$h_{ij} = < i|T - \mu|j > + \sum_{kl} < ik|V|jl > \rho_{lk}$$

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} < ij|V|kl > \kappa_{kl}$$

DEF. the quasiparticle hamiltonian:

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

⇒ the variational equation reads: $\delta\{E[\mathcal{R}] - \mathrm{tr}\Lambda(\mathcal{R}^2 - \mathcal{R})\} = 0$

Hartree-Fock-Bogoliubov equation

$$[\mathcal{H}, \mathcal{R}] = 0$$

$$\begin{pmatrix} h & \Delta \\ -\Delta & -h^* \end{pmatrix} \begin{pmatrix} U_n \\ V_n \end{pmatrix} = e_n \begin{pmatrix} U_n \\ V_n \end{pmatrix}$$

$\mathcal{H} = \mathcal{H}[\mathcal{R}]$ → The HFB equation is nonlinear. Solution by **iteration**.

1) initial guess for the density and pair matrices ρ and κ

2) calculate the Hartree-Fock hamiltonian h and pairing field Δ

3) solve the eigenvalue HFB equation

4) from the eigenvectors evaluate the new density and pair matrices. The trace of the density matrix will not, in general, be equal to the number of particles in the system -> change the chemical potential $\mu \rightarrow \mu + \delta\mu$ until the trace equals the desired number of particles.

5) repeat steps 2) → 4) until two successive calculations give the same density and pair matrices to a desired accuracy.

The stationary value of the energy functional:

$$E = < \Phi | H | \Phi > = \mu \bar{N} + \mathrm{tr}(h\rho - \kappa^* \Delta) - < \Phi | V | \Phi >$$

1. Quasiparticle basis ϕ_n → diagonalizes the generalized one-body matrix R.
2. Canonical basis ψ_i → diagonalizes the one-body density ρ.
3. Hartee-Fock basis → diagonalizes the mean-field Hamiltonian h.

3. Symmetries and constraints

i) symmetries related to the shape of the nucleus – spherical, axial quadrupole, triaxial quadrupole, octupole

ii) time-reversal symmetry – for even-even nonrotating nuclei. The creation of a quasiparticle or the rotation of the nucleus breaks time-reversal symmetry.

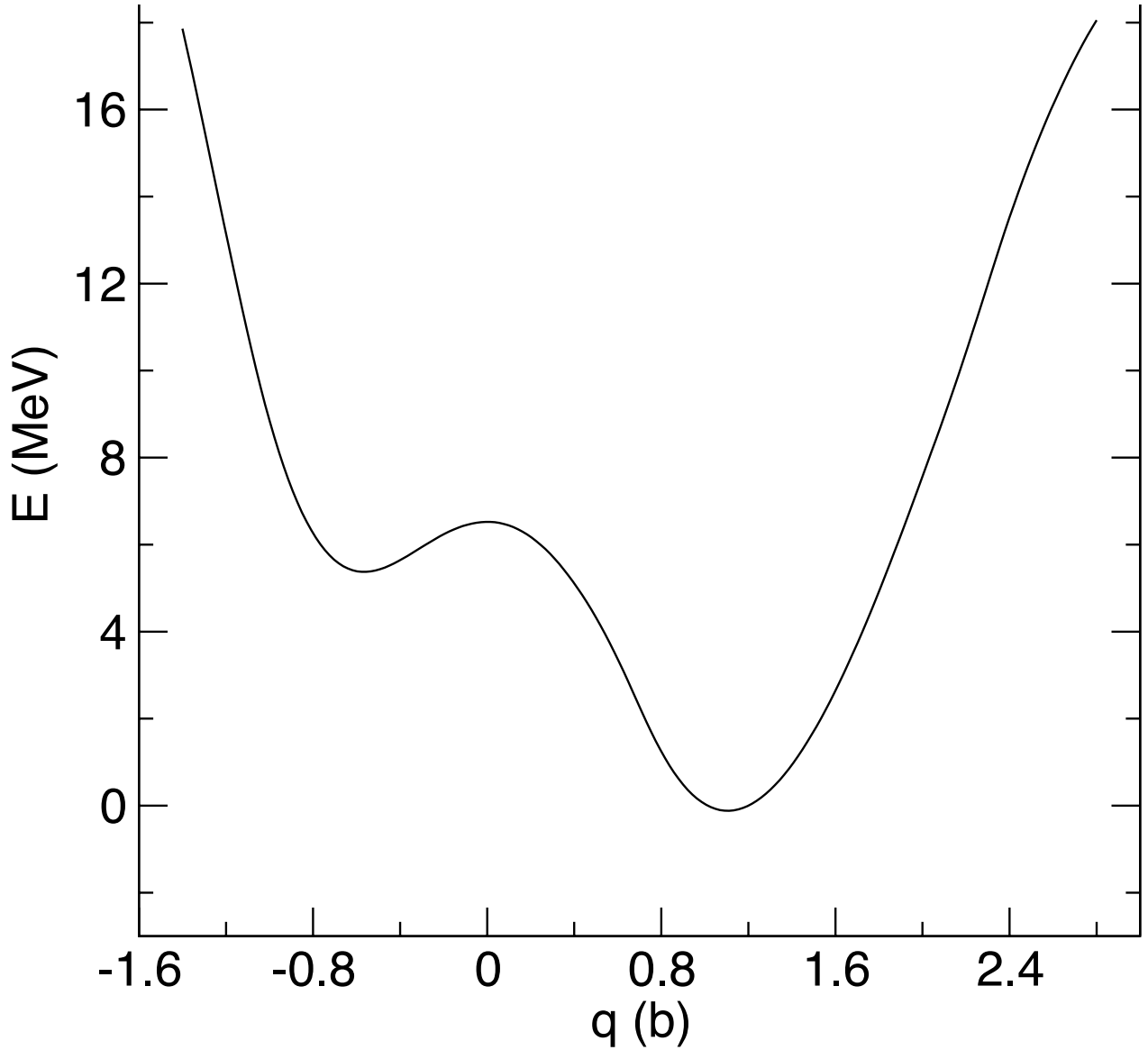
The landscape of the energy as a function of a shape degree of freedom is explored with the help of constraints.

The equations of motion are obtained by minimization of a Routhian:

$$E = \langle \hat{H} \rangle - \sum_{q=p,n} \lambda_q \langle \hat{N}_q \rangle - \sum_{\alpha} \lambda_\alpha \langle \hat{Q}_\alpha \rangle$$

with a constraint on the expectation value:

$$\langle \hat{Q}_\alpha \rangle \equiv \langle \Phi | \hat{Q}_\alpha | \Phi \rangle = Q_\alpha$$



→ Routhian:

$$\hat{H}' = \hat{H} - \lambda \hat{Q}$$

$$\lambda = \frac{dE}{dq}$$

collective coordinate

4. The BCS approximation

→ well defined only in the case of time-reversal invariance -> Kramers degeneracy of single-particle states: $\epsilon_n = \epsilon_{\bar{n}}$ for time-conjugate partners $\phi_n, \phi_{\bar{n}}$

The BCS approximation: forces the pairing potential to be diagonal in the basis of the eigenstates of the mean-field potential:

$$\Delta = \begin{pmatrix} 0 & d \\ -d^T & 0 \end{pmatrix}$$

$$d_{n\bar{m}} = \delta_{nm} d_{n\bar{m}}, \quad h\varphi_n = \epsilon_n \varphi_n$$

The pairing problem reduces to the determination of occupation amplitudes by solving the gap equation:

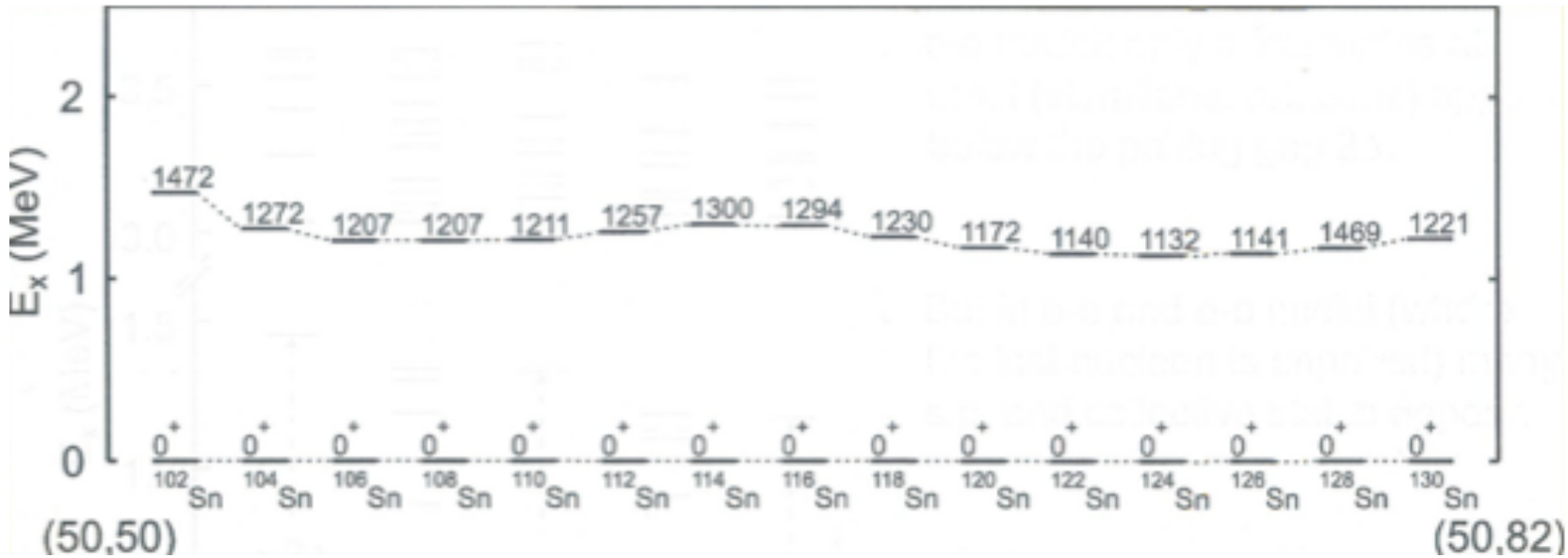
$$(\varepsilon_n - \mu)(u_n^2 - v_n^2) + 2d_{n\bar{n}} u_n v_n = 0$$

The two-component wave functions become simply:

$$\phi_n^{(U)} = u_n \varphi_n \qquad \phi_n^{(V)} = v_n \varphi_n$$

n-particles in non-degenerate shells: BCS

2^+_1 excitation energies in Sn isotopes:



… between 2 and 30 nucleons (1 to 15 pairs) are distributed over the available five neutron orbitals 2d5/2, 1g7/2, 1h11/2, 3s1/2, 2d3/2.

… consider a general trial wave function: $|\tilde{0}\rangle = \prod_{\nu>0}(u_\nu + v_\nu a^+_\nu a^+_{\bar{\nu}})|0\rangle$

BCS ground state. Not an eigenstate of the number operator.

closed shell

… normalization: $\langle\tilde{0}|\tilde{0}\rangle = \prod_{\nu>0}(u^2_\nu + v^2_\nu)$

… particle number: $\langle\tilde{0}|\hat{n}|\tilde{0}\rangle = \sum_{\nu>0} 2v^2_\nu$

… particle number uncertainty: $\Delta n^2 = \langle\tilde{0}|\hat{n}^2|\tilde{0}\rangle - \langle\tilde{0}|\hat{n}|\tilde{0}\rangle^2 = 4\sum_{\nu>0} u^2_\nu v^2_\nu$

The uncertainty in the particle number arises from those single-particle states that are fractionally occupied, i.e. $u^2_\nu \neq 0, 1 \qquad v^2_\nu \neq 0, 1$

The coefficients u_υ and v_υ are determined from a constrained variational calculation:

$$\delta\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = 0$$

$$\mathcal{H} = H - \lambda\hat{n} = \sum_{\nu>0}(\epsilon_\nu - \lambda)(a^+_\nu a_\nu + a^+_{\bar{\nu}} a_{\bar{\nu}}) - G\sum_{\mu,\nu>0} a^+_\mu a^+_{\bar{\mu}} a_{\bar{\nu}} a_\nu$$

The Lagrange multiplier is chosen such that the average particle number equals the actual number of valence particles:

$$\langle\tilde{0}|\hat{n}|\tilde{0}\rangle = n$$

From: $$\frac{\partial}{\partial n}\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = 0 \Longrightarrow \lambda = \frac{\partial}{\partial n}\langle\tilde{0}|H|\tilde{0}\rangle$$

The BCS transformation from particle creation and annihilation operators to "quasiparticle" operators:

$$\begin{aligned} c^+_\nu &= u_\nu a^+_\nu - v_\nu a_{\bar{\nu}} \\ c_\nu &= u_\nu a_\nu - v_\nu a^+_{\bar{\nu}} \end{aligned}$$

$$\begin{aligned} a^+_\nu &= u_\nu c^+_\nu + v_\nu c_{\bar{\nu}} \\ a_\nu &= u_\nu c_\nu + v_\nu c^+_{\bar{\nu}} \end{aligned}$$

inverse transformation

The BCS state is, by construction, the quasiparticle vacuum:

$$c_\nu|\tilde{0}\rangle = 0 \quad \forall\nu$$

Rewrite the Hamiltonian in terms of quasiparticle operators:

$$\mathcal{H} = U_0 + H_{11} + H_{20} + H_{02} + H_{\rm res}$$

$$\begin{aligned} H_{11} &\sim c^+c \\ H_{20} &\sim c^+c^+ \\ H_{\rm res} &\sim c^+c^+c^+c^+ + c^+c^+c^+c + c^+c^+cc + \text{h.c.} \end{aligned}$$

Because of the normal order of the operators, the expectation value of the interacting terms in the BCS state vanishes, and the ground-state energy:

$$\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = U_0 = \sum_{\nu>0}\left[2(\epsilon_\nu - \lambda)v_\nu^2 - Gv_\nu^4\right] - G\left[\sum_{\nu>0} u_\nu v_\nu\right]^2$$

The variational problem: $\delta\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = 0 \Longrightarrow \dfrac{d}{dv_\nu}U_0 = 0$

From: $v_\nu^2 + u_\nu^2 = 1$ ⟹ $\dfrac{d}{dv_\nu} = \dfrac{\partial}{\partial v_\nu} - \dfrac{v_\nu}{u_\nu}\dfrac{\partial}{\partial u_\nu}$

$$\frac{d}{dv_\nu}U_0 = 0 \quad \Longrightarrow \quad 2(\epsilon'_\nu - \lambda)u_\nu v_\nu = \Delta(u_\nu^2 - v_\nu^2) \quad \bigstar$$

DEF. the pairing gap:

$$\Delta \equiv G\sum_{\nu>0} u_\nu v_\nu$$

$$\epsilon'_\nu \equiv \epsilon_\nu - G v_\nu^2$$

includes the self-energy correction for a particle in a given orbital υ interacting, via the constant pairing force, with an extra pair of nucleons.

… solutions:

$$u_\nu^2 = \frac{1}{2}\left[1 + \frac{(\epsilon'_\nu - \lambda)}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}}\right]$$

$$v_\nu^2 = \frac{1}{2}\left[1 - \frac{(\epsilon'_\nu - \lambda)}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}}\right]$$

Two equations are needed to determine the chemical potential λ and the pairing gap Δ.

Insert the solutions for u_υ and v_υ into: $\Delta \equiv G \sum_{\nu>0} u_\nu v_\nu$

$$\frac{2}{G} = \sum_{\nu>0} \frac{1}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}}$$

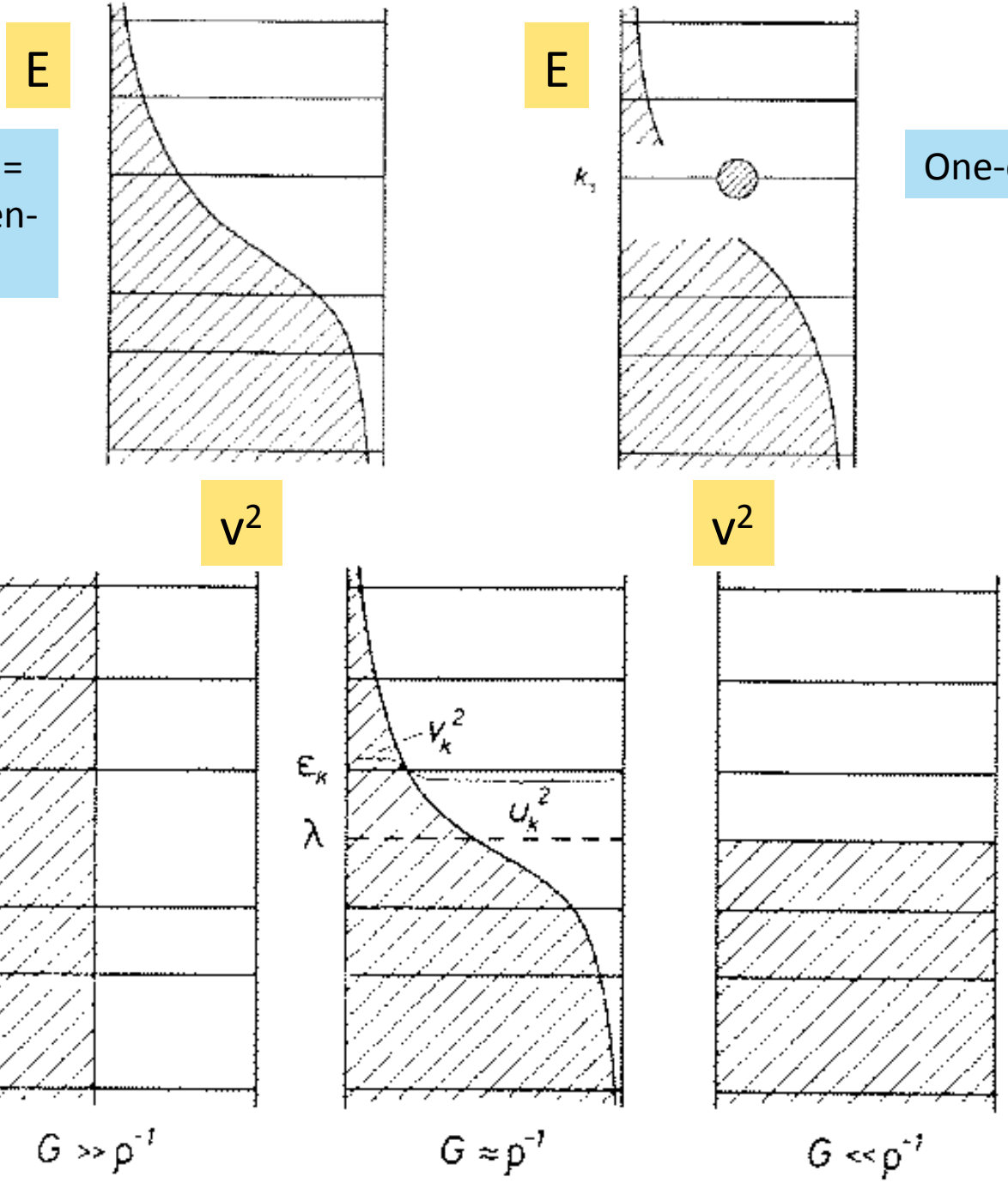
Gap equation

… plus the particle number condition:

$$n = \sum_{\nu>0} \left[1 - \frac{(\epsilon'_\nu - \lambda)}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}} \right]$$

For a given set of single-particle energies, particle number n, and pairing strength G, these two coupled equations have to be solved simultaneously for the unknown quantities λ and Δ (solution by iteration).

Quasiparticle vacuum= ground state of an even-even nucleus.



One-quasiparticle state.

Population v^2 of pairs in single-particle levels for different ratios of the pairing strength to the average distance between single-particle levels.