Quasiparticle OR BCS Method

This Takes Into Account the Strong Pairing Part of the Effective Two-Body Interaction.

The Idea is to Go From Particle Picture to Quasiparticle Picture (New Mean Field) Through Bogoliubov or Quasiparticle (qp) Transformation. This Leads in the Lowest approximation, to Independent Quasiparticle Picture - Incorporates the Pairing Interaction.

The Quasiparticle/BCS Transformation :

$$a^{\dagger}_{\alpha} = U_{\alpha} C^{\dagger}_{\alpha} - V_{\alpha} \tilde{C}_{\alpha} \quad ; \quad \tilde{a}_{\alpha} = U_{\alpha} \tilde{C}_{\alpha} + V_{\alpha} C^{\dagger}_{\alpha}$$

The Inverse Transformation Is:

$$C^{\dagger}_{\alpha} = U_{\alpha} a^{\dagger}_{\alpha} + V_{\alpha} \tilde{a}_{\alpha} \quad ; \quad \tilde{C}_{\alpha} = U_{\alpha} \tilde{a}_{\alpha} - V_{\alpha} a^{\dagger}_{\alpha}$$

Here:

$$\tilde{C}_{\alpha} = S_{\alpha} C_{-\alpha} \quad ; \quad \tilde{a}_{\alpha} = S_{\alpha} a_{-\alpha}$$

With:

$$S_{\alpha} = (-1)^{j_{\alpha} - m_{\alpha}}$$

The qp (New) Operators $a_\alpha^\dagger$ (a_α) also Obey Fermion Commutation Rules.

This Requires

$$U_\alpha^2 + V_\alpha^2 = 1$$

$$V_\alpha = V_{-\alpha}, U_\alpha = U_{-\alpha}$$

The new or qp (Particle) Vacuum $|qp>$ ($|0>$) is Defined Through

$$\begin{aligned} a_\alpha|qp> &= 0 \text{ , and} \\ C_\alpha|0> &= 0. \end{aligned}$$

The qp or BCS State can be Expressed as

$$|\mathrm{BCS}\rangle = \prod_{\alpha>0} \left(\mathrm{U}_\alpha + \mathrm{V}_\alpha \mathrm{S}_\alpha \mathrm{C}_\alpha^\dagger \mathrm{C}_{-\alpha}^\dagger\right) |0\rangle$$

The qp (BCS) Transformation Does Not Conserve the Nucleon Number.
Therefore Introduce Lagrange Multiplier λ and Use the Hamiltonian H'

$$H' \rightarrow H - \lambda\hat{N}, \text{ where, } \hat{N} = \sum_{\alpha} C_{\alpha}^{\dagger} C_{\alpha}$$

H' Can be Written as:

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

$$= \sum_{\alpha}(\epsilon_{\alpha} - \lambda) C_{\alpha}^{\dagger} C_{\alpha} + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\mathcal{V}|\gamma\delta\rangle C_{\alpha}^{\dagger} C_{\beta}^{\dagger} C_{\delta} C_{\gamma}$$

Various Ways to Derive qp Equations:
We Follow here the Conventional Procedure.
Step I: Use Wick's Theorem to write the One Body and Two Body Particle Operators of the Hamiltonian in terms of Normal Products and Expectation Values / Contractions.
Step II: Express All These in terms of qp operators using qp Transformation. Evaluate the Expectation Values wrt qp Vacuum.
The Transformed Hamiltonian Contains Three Terms:

- H_0 a Constant with out any qp Operators

- Terms With Two qp Operators. This Contains Two Parts. The First H_{11} Contains Only $a^{\dagger} a$ Terms (Required For New Mean Field) While the Second H_{20}(H_{02}) Involves the Terms $a^{\dagger} a^{\dagger}$ (a a). This Dangerous Term has to be Equated to Zero

- Terms Involving four qp Operators (Hint) arising from $:C^{\dagger}C^{\dagger}CC:$, The Residual qp Interaction Needed While Going Beyond Mean Field

The Resulting qp Hamiltonian is:

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

$$= H_0 + H_{11} + H_{20} + H_{02} + H_{\text{int}}$$

Where

$$H_0 = \sum_\alpha \left(\varepsilon_a - \lambda + \frac{1}{2}\sum_\gamma V_c^2 \langle\alpha\gamma|\mathcal{V}|\alpha\gamma\rangle\right) V_a^2$$

$$+\frac{1}{2}\sum_\alpha U_a V_a \left(\frac{1}{2}\sum_\gamma \langle\alpha - \alpha|\mathcal{V}|\gamma - \gamma\rangle S_\alpha S_\gamma V_c U_c\right)$$

$$= \sum_\alpha \left((\tilde{\varepsilon}_a - \lambda)V_a^2 - \frac{1}{2}\Delta_\alpha U_a V_a\right)$$

$$\mathbf{H_{11}} = \sum_{\alpha} \left((\tilde{\varepsilon} - \lambda)_a \left(U_a^2 - V_a^2 \right) + 2\Delta_\alpha U_a V_a \right) a_\alpha^\dagger a_\alpha$$

$$\mathbf{H_{20}} = \sum_{\alpha} \left((\tilde{\varepsilon} - \lambda)_a U_a V_a - \frac{1}{2} \Delta_\alpha \left(U_a^2 - V_a^2 \right) \right) S_a a_a^\dagger a_{-a}^\dagger$$

$$\mathbf{H_{20}} = \mathbf{H_{02}}^\dagger$$

$$\bar{\varepsilon}_\alpha = \varepsilon_\alpha - \lambda + \Gamma_\alpha$$

$$\Gamma_\alpha = \frac{1}{2} \sum_{\alpha\beta} < \alpha\beta \,|V|\, \alpha\beta > V_\beta^2$$

Γ is Self Energy Contribution to New Mean Field. It is Usually Small and is Ignored

$$\Delta_a = -\frac{1}{2}\sum_{\beta} < \alpha - \alpha | V | \beta - \beta > S_\alpha S_\beta V_d U_d$$

Step III: We Need to Retain $H_0 + H_{11}$.

Equate $H_{20} = H_{02}^{\dagger}$ to Zero. This gives

$$(\overline{\varepsilon_a} - \lambda) U_a V_a = \frac{\Delta_a}{2}(U_a^2 - V_a^2)$$

Put $V_a = Sin\vartheta_a$, $U_a = Cos\vartheta_a$

Use $U_a^2 + V_a^2 = 1$ **To Get**

$$Tan(2\vartheta_a) = \frac{\Delta_a}{(\overline{\varepsilon}_a - \lambda)}$$

$$U_a^2 - V_a^2 = Cos(2\vartheta_a) = \frac{\overline{\varepsilon}_a - \lambda}{E_a}$$

$$E_a = ((\overline{\varepsilon}_a - \lambda)^2 + \Delta_a^2)^{1/2}$$

$$V_a^2 = \frac{1}{2}(1 - \frac{(\overline{\varepsilon}_a - \lambda)}{E_a})$$

We Get (Gap Eq.)

$$\Delta_a = -\frac{1}{2}\sum_{\beta} < \alpha -\alpha \,|V|\, \beta - \beta > S_\alpha S_\beta V_d U_d$$

$$= -\frac{1}{4}\sum_{c} < j_a^2 0 \,|V|\, j_c^2 0 > [\ \frac{2j_c+1}{2j_a+1}\ ]^{1/2} \frac{\Delta_c}{E_c}$$

The Lagrange Multiplier λ is Obtained Through the Requirement That

$$\sum_{\alpha} \langle C_\alpha^\dagger C_\alpha \rangle = \sum_{\alpha} V_\alpha^2 = N$$

N is the Nucleon Number (Number Eq.)

These qp or BCS (Gap and Number) are Coupled Highly Non-linear Set of Eqs.. → Are to be Solved Self-Consistently

Interpretation of λ:

The Expression $\langle C_\alpha^\dagger C_\beta \rangle = \delta_{\alpha\beta} V_\alpha^2$

→ $V_a^2 \; (U_a^2 = 1 - V_a^2)$

Occupation (Non-Occupation)Probability

$$V_a^2 = \frac{1}{2}\left[1 - \frac{(\tilde{\varepsilon}_a - \lambda)}{\sqrt{(\tilde{\varepsilon}_a - \lambda)^2 + \Delta_a^2}}\right]$$

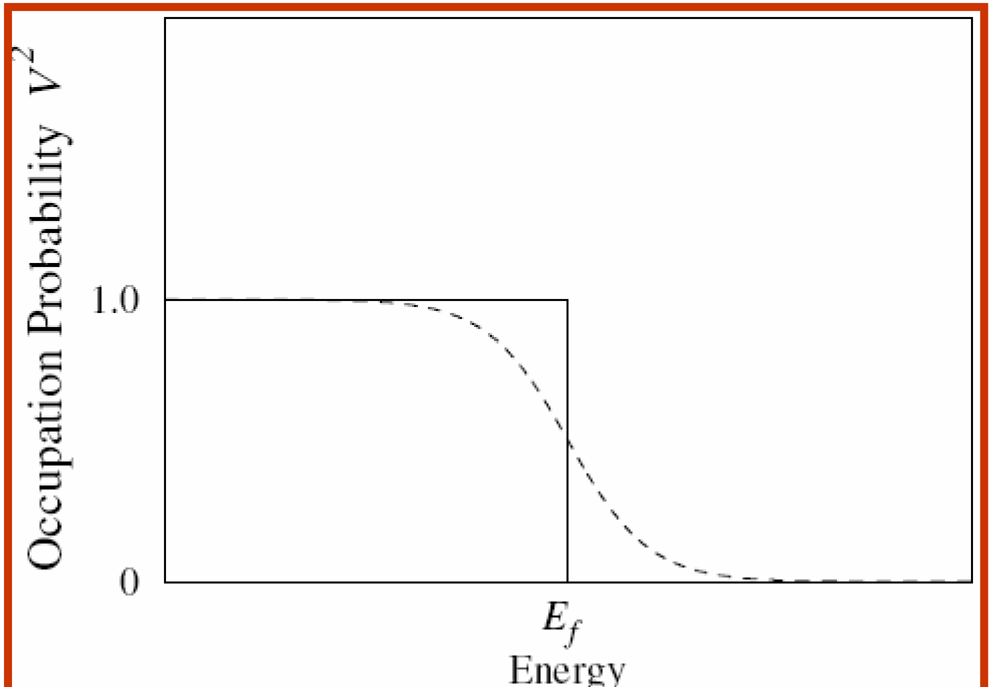
For $\tilde{\varepsilon}_a \gg \lambda$ $\quad V_a^2 \approx 0$

$\tilde{\varepsilon}_a \ll \lambda$ $\quad V_a^2 \approx 1$

AS $\tilde{\varepsilon}$ Approaches λ, V_a^2 Deviates From Unity (zero)

$$\tilde{\varepsilon}_a \leq \lambda,\ V_a^2 \geq 0.5;$$
$$\tilde{\varepsilon}_a \geq \lambda,\ V_a^2 \leq 0.5 \text{ and}$$
$$\tilde{\varepsilon}_a = \lambda,\ V_a^2 = 0.5\ .$$

<u>This Gives</u>



Interpretation of Δ

Inserting the Values of V's (U's), H_{11} becomes

$$H_{11} = \sum_{\alpha} \left[\frac{(\tilde{\varepsilon}_a - \lambda)(\tilde{\varepsilon}_a - \lambda)}{E_a} + 2\Delta_a \frac{\Delta_a}{2} \frac{(\tilde{\varepsilon}_a - \lambda)}{((\tilde{\varepsilon}_a - \lambda) E_a)} \right] a_{\alpha}^{\dagger} a_{\alpha}$$

$$\equiv \sum_{\alpha} E_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}$$

Neglect H_{int} → $H = H_0 + H_{11}$

Zero qp or |BCS> State Satisfies

$$a_{\alpha} |\mathrm{BCS}\rangle = 0$$

Even – Even Nuclei → 0, 2, 4 … qp
Odd-A Nuclei → 1, 3, 5 … qp

qp Energy $E_a = \sqrt{\left((\bar{\varepsilon}_a - \lambda)^2 + \Delta_a^2\right)} \geq \Delta_a$

Take Δ to be in dendent of α

For $\bar{\varepsilon}_a \simeq \lambda$ → $E_a \simeq \Delta$

The 2qp State Will be Atleast 2Δ above g.s.

For e – e Nuclei → gap 2Δ Between g.s & first Exc. State → Agree With Expt.

For Odd-A Nuclei: The g.s. → 1qp State Nearest to λ .
Energy $E_a \approx \Delta$, As $\tilde{\varepsilon}_a \approx \lambda$.
There Exist Other 1 qp Levels With Energy

$$E_{\beta \neq \alpha} = \sqrt{(\tilde{\varepsilon}_b - \lambda)^2 + \Delta^2}$$

$(\tilde{\varepsilon}_b - \lambda)$ **Being Small, So several 1 qp States Will Lie Close to Each Other → No Gap Between the g.s. And First Exc. State.**

Rough estimate of Δ

For N Valence Nucleons, The Energy of |BCS> or g.s. is:

$$E_N = \langle H \rangle = \langle H' \rangle + \lambda \langle \hat{N} \rangle = H_0(N) + \lambda N$$

The g.s Energy for Nuclei With N+(-) one Nucleons:

$$E_{N+1} = \langle H' \rangle + \lambda \langle \hat{N} \rangle \simeq H_0(N) + \lambda(N+1) + \Delta$$

$$E_{N-1} = \langle H' \rangle + \lambda \langle \hat{N} \rangle \simeq H_0(N) + \lambda(N-1) + \Delta$$

Thus

$$E_{N+1} + E_{N-1} - 2E_N = 2\Delta$$

So , For a Given N the Gap Δ Can be Obtained From Odd-Even Mass Difference Its Approximate Value is:

1.5 MeV for Ni isotopes and $N=50$ isotones
1.2 MeV for Sn isotopes and $N=82$ isotones
0.9 MeV for Pb isotopes.

Illustration: Ni - Isotopes

Core: ^{56}Ni → Z=28, N=28

Valence Levels: $1p_{3/2}$, $0f_{5/2}$ and $1p_{1/2}$

Energies: $\tilde{\varepsilon}_{3/2} = \varepsilon_{3/2} = 0.0$, $\tilde{\varepsilon}_{5/2} = \varepsilon_{5/2} = 0.78$

$\tilde{\varepsilon}_{1/2} = \varepsilon_{1/2} = 1.08$ MeV

Interaction: Empirical and Pairing

Table → Results For ^{60}Ni
( ) → Results With Pairing Int.

	λ	Δ	E	V
$1p_{3/2}$	0.064 (0.008)	1.352 (1.444)	1.353 (1.444)	0.724 (0.708)
$0f_{5/2}$		1.249 (1.444)	1.440 (1.637)	0.501 (0.597)
$1p_{1/2}$		1.352 (1.444)	1.691 (1.798)	0.447 (0.578)

Excited States: qp Configuration Mixing → H_{int}

Even – Even Nuclei → 0, 2 ,4 qp

Odd – A Nuclei → 1, 3 may be 5 qp

Advantages: Up to $\nu = 4$ (5) Space

Drawback: Non-conservation of N

→ Spurious States

Remedy → Number Projection

Broken Pair approximation (BPA)

BROKEN PAIR APPROXIMATION (BPA)

The SM gs State for 2 Identical Nucleons

$$s^{+}|0\rangle = \sum_{a} \frac{\hat{a}}{2} x_a A^{+}_{00}(aa)|0\rangle$$

$$\hat{a} = (2j_a + 1)^{1/2}$$

$$A^{+}_{JM}(ab) = \left[C^{+}_a \otimes C^{+}_b\right]_{JM}$$

gs - Φ_0 : P Pairs of Identical Nucleons

$$\Phi_0 \Rightarrow \left(s^+\right)^P |0\rangle = \left(\sum_a \frac{\hat{a}}{2} x_a A^+_{00}(aa) \right)^P |0\rangle$$

$$\Rightarrow \tau_+^P |0\rangle = \frac{1}{P!} \left(\prod_a u_a \frac{\hat{a}^2}{2} \right) \left(s^+\right)^P |0\rangle$$

$$x_a = v_a / u_a \; ; \; u_a^2 + v_a^2 = 1$$

The gs Parameters x (v or u) are obtained by:

$$\delta\left(\langle \Phi_0 \mid H \mid \Phi_0 \rangle / \langle \Phi_0 \mid \Phi_0 \rangle\right) = 0$$

Φ_0 :

Special Seniority 0 State

> 98% of ESM gs

2P – Particle Component of BCS State

If v/u ➔ v/u of BCS

Excited States: BPA Basis States

$$\tau^{+} \rightarrow A^{+}_{JM}(ab)$$

1 BPA Basis:

$$\left|\Phi_{JM}(ab)\right\rangle \Rightarrow A^{+}_{JM}(ab)\tau_{+}^{P-1}\left|0\right\rangle$$

Special Seniority 2 State

Diagonalise → Eigenvalues, Eigenvectors

^{60}Ni					
J^{π}	Expt.	ESM	$\nu \leq 2$	1bp	BCS2qp
0^+	0	0 (99.8)	0	0	0
	2.29	2.323 (95.8)	2.414	2.455	1.933
		3.268 (86.7)	3.415	3.645	2.977
2^+	1.33	1.421 (99.8)	1.418	1.421	0.946
	2.16	2.171 (76.6)	2.425	2.533	2.068
		2.578	2.866	3.481	2.994
3^+		2.758 (55.5)	3.439	3.506	2.991
		3.370 (30.0)	3.872	3.976	3.509
4^+	2.50	2.205 (91.9)	2.296	2.299	1.863
		2.798 (23.9)	3.497	3.565	3.205

	^{64}Ni				
J^{π}	Expt.	ESM	$\nu \leq 2$	1bp	BCS2qp
0^+	0	0 (99.8)	0	0	0
	2.27	2.156 (98.8)	2.180	2.188	1.720
		3.559 (81.2)	3.659	3.768	3.417
2^+	1.34	1.560 (99.7)	1.556	1.559	1.110
	2.89	2.371 (78.7)	2.479	2.492	2.084
		2.597 (64.9)	3.277	3.308	2.753
3^+		3.069 (36.6)	3.445	3.454	2.946
		3.477 (72.7)	3.766	3.804	3.340
4^+	2.61	2.257 (96.3)	2.292	2.307	1.835
		2.725 (34.1)	3.352	3.396	2.861

BE(2) Transition and Quadrupole Moments of Ni Isotopes

	$B(E2, 0_1^+ \rightarrow 2_1^+);\ e^2\ fm^4$			$Q(2_1^+); e\ fm^2$		
	ESM	**1bp**	**BCS2qp**	**ESM**	**1bp**	**BCS2qp**
^{58}Ni	**233**	**233**	**183**	**-14**	**-14**	**-8**
^{60}Ni	**386**	**390**	**303**	**-2**	**-5**	**-3**
^{62}Ni	**458**	**474**	**383**	**+2**	**+1**	**+1**
^{64}Ni	**410**	**431**	**343**	**+6**	**+8**	**+5**

1 (2) BPA: Good Approximation to Seniority 2 (4) Shell Model