Pairing correlation between nucleons and the BCS theory

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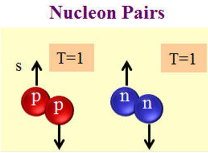
Outline

Introduction

Introduction: evidence of pairing correlation



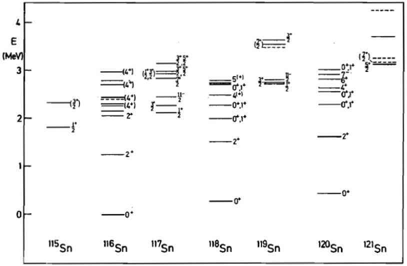
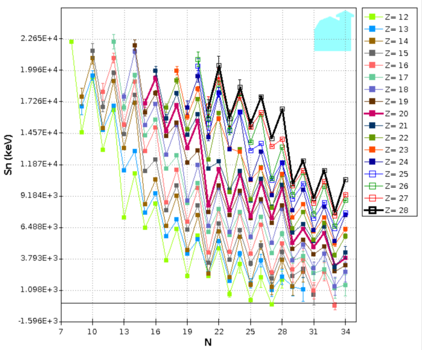


Figure 6.1. Excitation spectra of the $_{50}$Sn isotopes.



- even-even nuclei are bound more tightly than odd nuclei.
- in even-even nuclei there is an energy gap of 1-2 MeV between the ground state and the lowest single-particle excitation.

Introduction: evidence of pairing correlation

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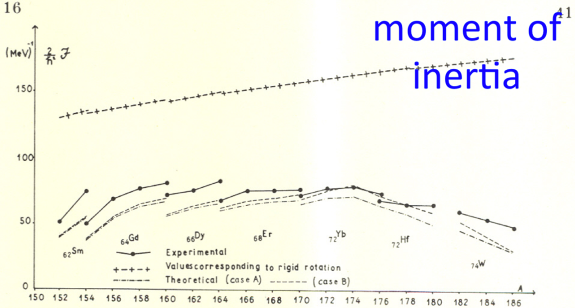
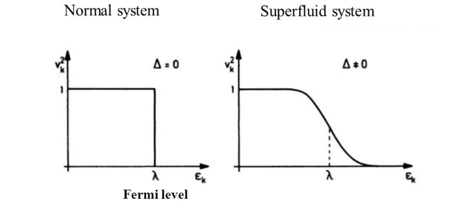


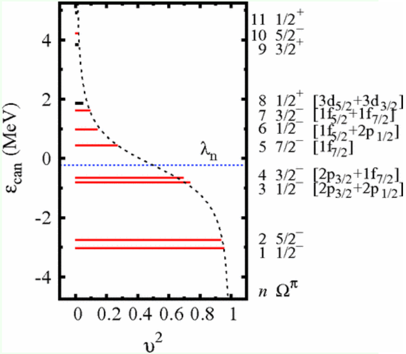
Fig. 17. *Moments of inertia of even-even nuclei in region I.* The figure exhibits by the crossed line the rigid moment of inertia corresponding to $R_0 = 1.2 \times A^{1/3} f$. The empirical values given as filled circles do not include any correction for the rotation-vibration interaction. The dashed and dot-and-dash lines refer to calculations corresponding to the choice of $\Delta_p = P_p$ and $\Delta_n = P_n$ with an assumed single-particle level spectrum ε_ν as given according to the alternative cases A and B of table I.

- To explain the moment of inertia we need to take into the account nuclear pairing interaction.

Introduction: occupation probability



Neutrons in ^{44}Mg



S.G. Zhou et al., Phys. Rev. C 82, 011301(R) (2010)

The two-particle system

The wave function of two-particle system

The normalized angular-momentum (J) coupled wave function of two-particle system:

$$|ab;JM\rangle = \mathcal{N}_{ab}(J)\left[c_a^\dagger c_b^\dagger\right]_{JM}|0\rangle$$
$$= \mathcal{N}_{ab}(J)\sum_{m_\alpha m_\beta} C^{JM}_{j_a m_\alpha j_b m_\beta} c_\alpha^\dagger c_\beta^\dagger|0\rangle$$
$$\mathcal{N}_{ab}(J) = \frac{\sqrt{1+\delta_{ab}(-1)^J}}{1+\delta_{ab}}$$

where $\mathcal{N}_{ab}(J)$ is a normalization factor. The label a stands for $n_a l_a j_a$. The $C^{JM}_{j_a m_\alpha j_b m_\beta}$ is the Clebsch-Gordon coefficient.

The wave function of two-particle system

- The Clebsch-Gordan (CG) coefficients:
  Let $\mathbf{j}_1$ and $\mathbf{j}_2$ be two angular momenta with projections m_1 and m_2 on the quantization axis. A CG coefficients represents the probability amplitude that $\mathbf{j}_1$ and $\mathbf{j}_2$ are coupled into a resultant angular momentum $\mathbf{j}$ with projection m.
  In accordance with the vector addition rules $\mathbf{j}_1 + \mathbf{j}_2 = \mathbf{j}$, the CG coefficient vanishes unless the triangular conditions (triangular inequalities) are fulfilled, i.e.,

$$|j_1 - j_2| \le j \le j_1 + j_2$$

and the requirement

$$m_1 + m_2 = m$$

is satisfied. The CG coefficients satisfy the following conditions:

1. j_1, j_2, j are integer or half-integer non-negative numbers;
2. m_1, m_2, m are integer or half-integer (positive or negative) numbers;
3. $|m_1| \le j_1, |m_2| \le j_2, |m| \le j$
4. $j_1 + m_1, j_2 + m_2, j + m, j_1 + j_2 + j$ are integer non-negative numbers.
5. $\sum_{j=|j_1-j_2|}^{j_1+j_2}(2j+1) = (2j_1+1)(2j_2+1)$.

The absolute value of a CG coefficient is given by $\Omega = (\alpha, \beta, \gamma)$

$$\left|C^{jm}_{j_1 m_1 j_2 m_2}\right|^2 = \frac{2j+1}{8\pi}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma D^{j_1}_{m_1 m_1}(\Omega) D^{j_2}_{m_2 m_2}(\Omega) D^{j*}_{mm}(\Omega)$$

The phase of the CG coefficients may be chosen in different ways. If the Condon-Shortley convention is chosen, the CG coefficients are real.

The wave function of two-particle system

- The Clebsch-Gordan (CG) coefficients:
  The CG coefficients are elements of the unitary matrix which performs direct and inverse transformations between state vectors $|j_1 m_1 j_2 m_2\rangle$ and $|j_1 j_2 jm\rangle$

$$C^{jm}_{j_1 m_1 j_2 m_2} = \langle j_1 m_1 j_2 m_2 \mid j_1 j_2 jm\rangle = \langle j_1 j_2 jm \mid j_1 m_1 j_2 m_2\rangle$$

The unitarity relation is

$$\sum\nolimits_{m_1 m_2} C^{jm}_{j_1 m_1 j_2 m_2} C^{j' m'}_{j_1 m_1 j_2 m_2} = \delta_{jj'} \delta_{mm'}$$
$$\sum\nolimits_{j(m)} C^{jm}_{j_1 m_1 j_2 m_2} C^{jm}_{j_1 m_1' j_2 m_2'} = \delta_{m_1 m_1'} \delta_{m_2 m_2'}$$

The direct product of two irreducible tensors $\mathfrak{T}_{j_1 m_1}$ and $\mathfrak{R}_{j_2 m_2}$ may be decomposed into irreducible tensors. The coefficients of this decomposition are just the Clebsch-Gordan coefficients:

$$\mathfrak{T}_{j_1 m_1} \mathfrak{R}_{j_2 m_2} = \sum_{j(m)} C^{jm}_{j_1 m_1 j_2 m_2} \left\{ \mathfrak{T}_{j_1} \otimes \mathfrak{R}_{j_2} \right\}_{jm}$$

The inverse relation is

$$\left\{ \mathfrak{T}_{j_1} \otimes \mathfrak{u}_{j_2} \right\}_{jm} = \sum_{m_1 m_2} C^{jm}_{j_1 m_1 j_2 m_2} \mathfrak{T}_{j_1 m_1} \mathfrak{N}_{j_2 m_2}.$$

The wave function of two-particle system

- The Wigner 3*jm* symbol and Clebsch-Gordan (CG) coefficients:
  The Wigner 3*jm* symbols are usually used instead of the CG coefficients. These symbols possess simpler symmetry properties. The 3*jm* symbols are related to the CG coefficient by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_j+m_3+2j_1} \frac{1}{\sqrt{2j_3+1}} C^{j_3 m_3}_{j_1 -m_1 j_2 -m_2}$$

  The inverse relation is

$$C^{j_3 m_3}_{j_1 m_1 j_2 m_2} = (-1)^{j_1-j_2+m_3} \sqrt{2j_3+1} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}$$

- Symmetries in the CG coefficients:

$$C^{c\gamma}_{abb\beta} = (-1)^{a+b-c} C^{c\gamma}_{b\beta a\alpha} = (-1)^{a-\alpha}\sqrt{\frac{2c+1}{2b+1}} C^{b-\beta}_{a\alpha c-\gamma} = (-1)^{a-\alpha}\sqrt{\frac{2c+1}{2b+1}} C^{b\beta}_{c\gamma a-\alpha}$$

$$= (-1)^{b+\beta}\sqrt{\frac{2c+1}{2a+1}} C^{a-\alpha}_{c-\gamma b\beta} = (-1)^{b+\beta}\sqrt{\frac{2c+1}{2a+1}} C^{a\alpha}_{b-\beta c\gamma}$$

$$C^{c\gamma}_{a\alpha b\beta} = (-1)^{a+b-c} C^{c-\gamma}_{a-\alpha b-\beta}$$

The wave function of two-particle system

- Symmetries in the $3jm$ symbols:
  Permutations of columns

$$
\begin{pmatrix} a & b \\ \alpha & \beta \end{pmatrix} = \begin{pmatrix} b & c & a \\ \beta & \gamma & \alpha \end{pmatrix} = \begin{pmatrix} c & a & b \\ \gamma & \alpha & \beta \end{pmatrix} = (-1)^{a+b+c} \begin{pmatrix} a & c & b \\ \alpha & \gamma & \beta \end{pmatrix}
$$
$$
= (-1)^{a+b+c} \begin{pmatrix} b & a & c \\ \beta & \alpha & \gamma \end{pmatrix} = (-1)^{a+b+c} \begin{pmatrix} c & b & a \\ \gamma & \beta & \alpha \end{pmatrix}
$$

  Change of signs of momentum projections

$$
\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = (-1)^{a+b+c} \begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix}
$$

The wave function of two-particle system

- The two-body interaction in J-coupled form:
  Making use of the following relation,

$$|\alpha\beta\rangle = c^\dagger_\alpha c^\dagger_\beta |0\rangle = \sum_{JM} C^{JM}_{j_a m_\alpha j_b m_\beta} \left[\mathcal{N}_{ab}(J)\right]^{-1} |ab; JM\rangle$$

one can rewrite the two-body interaction as follows

$$\begin{aligned} V &= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|V|\gamma\delta\rangle c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \\ &= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \left[\mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J')\right]^{-1} C^{JM}_{j_a m_\alpha j_b m_\beta} C^{J'M'}_{j_c m_\gamma j_d m_\delta} \langle ab; JM|V|cd; J'M'\rangle c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \end{aligned}$$

Converting the annihilation operators into spherical tensors yields

$$c_\delta c_\gamma = (-1)^{j_d - m_\delta} \tilde{c}_{-\delta} (-1)^{j_c - m_\gamma} \tilde{c}_{-\gamma} = (-1)^{j_c + j_d - (m_\gamma + m_\delta) + 1} \tilde{c}_{-\gamma} \tilde{c}_{-\delta}$$

By summing over the $m_{\alpha,\beta,\gamma,\delta}$, we obtain

$$\begin{aligned} V = \tfrac{1}{4} \textstyle\sum_{abcd;JMJ'M'} \left[\mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J')\right]^{-1} \langle ab; JM|V|cd; J'M'\rangle \\ \times \left[c^\dagger_a c^\dagger_b\right]_{JM} (-1)^{J'+M'+1} \left[\tilde{c}_c \tilde{c}_d\right]_{J', -M'} \end{aligned}$$

The wave function of two-particle system

Considering the fact that the two-body interaction V is a scalar with rank $\lambda = 0$, thus,

$$\left\langle ab; JM|V|cd; J'M'\right\rangle \equiv \delta_{JJ'}\delta_{MM'}\langle ab; J|V|cd; J\rangle$$

The resulting expression for V is

$$\begin{aligned} V &= -\frac{1}{4}\sum_J\sum_{abcd}[\mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J)]^{-1}\langle ab; J|V|cd; J\rangle\sum_M(-1)^{J+M}\left[c_a^\dagger c_b^\dagger\right]_{JM}[\tilde{c}_c\tilde{c}_d]_{J,-M} \\ &= -\frac{1}{4}\sum_J\sum_{abcd}[\mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J)]^{-1}\sqrt{2J+1}\langle ab; J|V|cd; J\rangle\left[\left[c_a^\dagger c_b^\dagger\right]_J[\tilde{c}_c\tilde{c}_d]_J\right]_{00} \end{aligned}$$

where the following relation is used

$$C^{00}_{JMJ-M} = \frac{(-1)^{J-M}}{\sqrt{2J+1}}.$$

The wave function of two-particle system

The unnormalized two-body matrix element is defined as

$$\langle ab; J|V|cd; J\rangle_{\rm unnorm} = \sum_{\substack{m_\alpha m_\beta \\ m_\gamma m_\delta}} \langle j_a m_\alpha j_b m_\beta|JM\rangle\langle j_c m_\gamma j_d m_\delta|JM\rangle \bar{v}_{\alpha\beta\gamma\delta}.$$

The normalized two-body matrix element is defined as

$$\begin{aligned}\langle ab; J|V|cd; J\rangle &= \mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J) \sum_{\substack{m_\alpha m_\beta \\ m_\gamma m_\delta}} \langle j_a m_\alpha j_b m_\beta|JM\rangle\langle j_c m_\gamma j_d m_\delta|JM\rangle \bar{v}_{\alpha\beta\gamma\delta} \\ &= \mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J) \cdot \langle ab; J|V|cd; J\rangle_{\rm unnorm}.\end{aligned}$$

From J-coupled two-body matrix element to the m-scheme one

$$\begin{aligned}\bar{v}_{\alpha\beta\gamma\delta} &= \sum_{JM} [\mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J)]^{-1} \langle j_a m_\alpha j_b m_\beta|JM\rangle\langle j_c m_\gamma j_d m_\delta|JM\rangle \langle ab; J|V|cd; J\rangle \\ &= \sum_{JM} \langle j_a m_\alpha j_b m_\beta|JM\rangle\langle j_c m_\gamma j_d m_\delta|JM\rangle \cdot \langle ab; J|V|cd; J\rangle_{\rm unnorm}.\end{aligned}$$

The two-particle system with a pure pairing force

Considering the two-particle system with $T = 1$ (nn or pp) in a single j-shell ($\delta_{ab} = 1$, only even J nonzero). The normalization factor becomes,

$$\mathcal{N}_{ab}(J) = \frac{1}{\sqrt{2}}\delta_{J,\mathrm{even}}.$$

The two-body interaction is simplified as (a, b, c, d are restricted to the same quantum number nlj)

$$\begin{aligned} V &= -\frac{1}{4}\sum_J \sum_{abcd} \left[\mathcal{N}_{ab}(J)\mathcal{N}_{cd}(J)\right]^{-1} \sqrt{2J+1}\langle ab; J|V|cd; J\rangle \left[\left[c_a^\dagger c_b^\dagger\right]_J [\tilde{c}_c\tilde{c}_d]_J\right]_{00} \\ &= -\frac{1}{2}\sum_J \sqrt{2J+1}\langle jj; J|V|jj; J\rangle \left[\left[c_j^\dagger c_j^\dagger\right]_J \left[\tilde{c}_j\tilde{c}_j\right]_J\right]_{00} \end{aligned}$$

If only the $J = 0$ component is considered, one finds

$$\begin{aligned} V_{J=0} &= -\frac{1}{2}\langle jj; 0|V|jj; 0\rangle \left[c_j^\dagger c_j^\dagger\right]_0 \left[\tilde{c}_j\tilde{c}_j\right]_0 \\ &= -\frac{1}{2}\langle jj; 0|V|jj; 0\rangle \sum_{mm'} C^{00}_{jmjm'} c^\dagger_{jm} c^\dagger_{jm'} \sum_{m'' m'''} C^{00}_{jm'' jm'''} \tilde{c}_{jm''} \tilde{c}_{jm'''} \\ &= -\frac{1}{2}\langle jj; 0|V|jj; 0\rangle \sum_m (-1)^{j-m}\frac{1}{\sqrt{2j+1}} c^\dagger_{jm} c^\dagger_{j-m} \sum_{m'} (-1)^{j-m'}\frac{1}{\sqrt{2j+1}} \tilde{c}_{jm'} \tilde{c}_{j-m'} \end{aligned}$$

The two-particle system with a pure pairing force

In terms of the spherical tensor operators

$$\tilde{c}^{\dagger}_{jm} = (-1)^{j+m} c^{\dagger}_{j-m}, \quad \tilde{c}_{j-m} = (-1)^{j-m} c_{jm}$$

one finds

$$\begin{aligned} V_{J=0} &= \frac{1}{2} \langle jj;0|V|jj;0\rangle \frac{1}{2j+1} \sum_{mm'} c^{\dagger}_{jm} \tilde{c}^{\dagger}_{jm} \tilde{c}_{jm'} c_{jm'} \\ &= 2\langle jj;0|V|jj;0\rangle \frac{1}{2j+1} \sum_{m,m'>0} c^{\dagger}_{jm} \tilde{c}^{\dagger}_{jm} \tilde{c}_{jm'} c_{jm'} \\ &\equiv -G \sum_{m,m'>0} c^{\dagger}_{jm} \tilde{c}^{\dagger}_{jm} \tilde{c}_{jm'} c_{jm'} . \end{aligned}$$

where we have defined the constant G as

$$G = -\frac{2}{2j+1} \langle jj;0|V|jj;0\rangle,$$

which is the so-called pairing strength and has to be positive so that the pairing interaction $V_{J=0}$ is attractive.

Pairing in the degenerate single-j model

The two-particle system in single-j

Considering two particles in a single j-shell with only a pairing interaction:

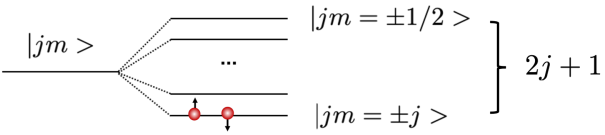


Figure: The single-j shell with the single-particle energy $\varepsilon_j = 0$.

- Hamiltonian:

$$H = -G \sum_{m,m'>0} c^\dagger_{jm} \tilde{c}^\dagger_{jm} \tilde{c}_{jm'} c_{jm'} .$$

- Expanding the wave function of the two-particle in terms of the two-particle basis constructed as

$$|\Psi(1,2)\rangle = \sum_{m>0} c_m |\Phi_m(1,2)\rangle, \quad |\Phi_m(1,2)\rangle = A^\dagger_{jm}|0\rangle = c^\dagger_{jm}\tilde{c}^\dagger_{jm}|0\rangle,$$

where $m = 1/2, 3/2, \cdots, j$ with the dimension $\Omega = j + 1/2$.

The two-particle system in single-j

Considering two particles in a single j-shell with only a pairing interaction:

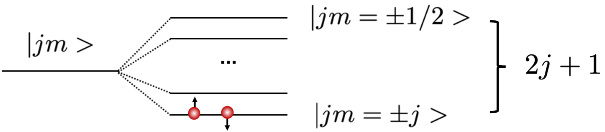


Figure: The single-j shell with the single-particle energy $\varepsilon_j = 0$.

- The eigenvalue problem:

$$HC = EC$$

with the matrix element is determined by

$$\begin{aligned} H_{mm'} &= \langle \Phi_m(1,2)|H|\Phi'_m(1,2)\rangle \\ &= \langle \Phi_m(1,2)| - G \sum_{m_1 m_2 > 0} c^\dagger_{jm_1} \tilde{c}^\dagger_{jm_1} \tilde{c}_{jm_2} c_{jm_2} |\Phi'_m(1,2)\rangle \\ &= -G \sum_{m_1, m_2 > 0} \langle 0|\tilde{c}_{jm} c_{jm} c^\dagger_{jm_1} \tilde{c}^\dagger_{jm_1} \tilde{c}_{jm_2} c_{jm_2} c^\dagger_{jm'} \tilde{c}^\dagger_{jm'} |0\rangle = -G. \end{aligned}$$

The two-particle system in single-j

Considering two particles in a single j-shell with only a pairing interaction:

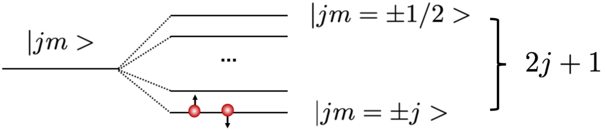


Figure: The single-j shell with the single-particle energy $\varepsilon_j = 0$.

- The Hamiltonian matrix is a $\Omega \times \Omega$ matrix,

$$H = -G \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}$$

The characteristic determinant is

$$(-G\Omega - E)(-E)^{\Omega-1} = 0$$

from which one finds the eigenvalues

$$E_1 = -\Omega G, \quad E_i = 0 \text{ for } i = 2, 3, \cdots, \Omega$$

The two-particle system in single-j

Considering two particles in a single j-shell with only a pairing interaction:

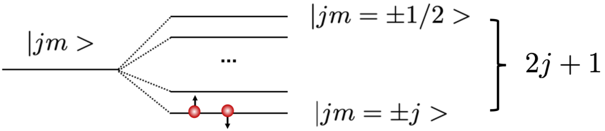


Figure: The single-j shell with the single-particle energy $\varepsilon_j = 0$.

- The wave function of the first (lowest-energy) state

$$\Psi_1 = \frac{1}{\sqrt{\Omega}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

In occupation number representation

$$|\Psi_1\rangle = \frac{1}{\sqrt{\Omega}} \sum_{m>0} A^\dagger_{jm}|0\rangle = \frac{1}{\sqrt{2}} \sum_m \frac{(-1)^{j+m}}{\sqrt{2j+1}} c^\dagger_{jm} c^\dagger_{j,-m}|0\rangle = -\frac{1}{\sqrt{2}} \left[c^\dagger_j c^\dagger_j\right]_{00} |0\rangle.$$

The seniority model

Considering N fermions in a single j-shell:

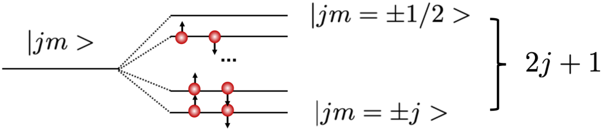


Figure: The single-j shell with the single-particle energy $\varepsilon_j = 0$.

- Hamiltonian:

$$H = -G \sum_{m,m'>0} c^\dagger_{jm} \tilde{c}^\dagger_{jm} \tilde{c}_{jm'} c_{jm'}$$
$$= -G \hat{S}_+ \hat{S}_-$$

We define a quasi-spin operator

$$\hat{S}_+ \equiv \sum_{m>0} S^{(m)}_+ = \sum_{m>0} c^\dagger_{jm} \tilde{c}^\dagger_{jm} \text{ and } \hat{S}_- = \left(\hat{S}_+\right)^\dagger$$

and

$$S^{(m)}_+ = c^+_m \tilde{c}^+_m, \quad S^{(m)}_- = \tilde{c}_m c_m, \quad S^{(m)}_0 = \frac{1}{2}\left(c^+_m c_m + \tilde{c}^+_m \tilde{c}_m - 1\right)$$

where $\tilde{c}^+_m \tilde{c}_m = c^+_{-m} c_{-m}$.

The seniority model

Considering N fermions in a single j-shell:

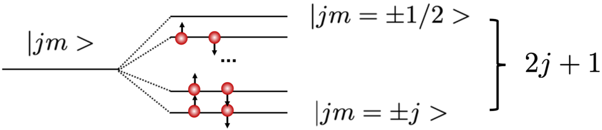


Figure: The single-j shell with the single-particle energy $\varepsilon_j = 0$.

Commutation relations

$$\left[S_+^{(m)}, S_-^{(m)}\right] = 2S_0^{(m)},$$
$$\left[S_0^{(m)}, S_\pm^{(m)}\right] = \pm S_\pm^{(m)}$$

The seniority model

- Define total quasi-spin operator: $\vec{S} = \sum_{m>0} \vec{S}^{(m)}$

$$
\begin{aligned}
H &= -G\hat{S}_+\hat{S}_- \\
&= -G\left[(\hat{S}_x + i\hat{S}_y)(\hat{S}_x - i\hat{S}_y)\right] \\
&= -G\left(\vec{S}^2 - S_0^2 + S_0\right)
\end{aligned}
$$

where we used the relation $[\hat{S}_x, \hat{S}_y] = i\hat{S}_0$, and

$$
S_0 = \frac{1}{2}\sum_{m>0}\left(c_m^+ c_m + c_{-m}^+ c_{-m} - 1\right) = \frac{1}{2}(\widehat{N} - \Omega),
$$

with $\Omega = j + 1/2$.

- The energy:

$$
E = -G\left[S(S+1) - \frac{1}{4}(N-\Omega)^2 + \frac{1}{2}(N-\Omega)\right].
$$

The seniority model

- Introducing the *seniority* quantum number (辛弱数) s in terms of the total "quasi-spin" quantum number S, (think about it: why defined in this way?)

$$S = (\Omega - s)/2,$$

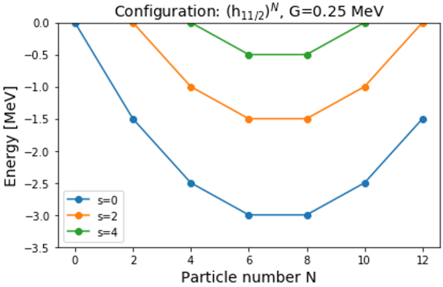
where the *seniority* quantum number s is ($s \leq \Omega$)

$$s = \begin{cases} 0, 2, 4, \cdots, & N = \text{even} \\ 1, 3, 5, \cdots, & N = odd \end{cases}$$

The seniority model

Alternatively, one uses the seniority quantum number $s = \Omega - 2S$

$$E(s, N) = -\frac{G}{4}\left[s^2 - 2s(\Omega+1) + 2N(\Omega+1) - N^2\right]$$



Note: $E(s=0, N=2) = -G\Omega$.

- s counts number of unpaired nucleons.
- ground state has minimal seniority $s = 0$ (or maximal quasi spin $S = \Omega/2$)
- for fixed N, excitations depend only on seniority quantum number
- $E(N, s=2) - E(N, s=0) = G\Omega$, independent on N.

The BCS theory

The BCS wave function

- The wave function of an even-even nucleus is represented as

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

where u_k and v_k represent variational parameters.

- The product runs only over half the configuration space, as indicated by $k > 0$. For each state $k > 0$ there exists a "conjugate" state $\bar{k} < 0$ and the states $\{k, \bar{k}\}$ generate the whole single-particle space. In a spherical basis ($m > 0$),

$$|k\rangle = |nljm\rangle_{CS} = |nljm\rangle_{BCS},$$
$$|\bar{k}\rangle = |-k\rangle = \hat{T}|k\rangle = (-1)^{j-m}|nlj-m\rangle_{CS} = |nlj-m\rangle_{BCS},$$

- The v_k^2 and u_k^2 represent the probability that a certain pair state $(k, \bar{k})$ is or is not occupied, which has to be determined in such a way that the corresponding energy has a minimum (variational principle).

The BCS wave function

- The norm of the BCS wave function is given by

$$\langle \mathrm{BCS} \mid \mathrm{BCS} \rangle = \left\langle 0 \left| \prod_{k>0}^{\infty} (u_k + v_k \hat{a}_{-k} \hat{a}_k) \prod_{k'>0}^{\infty} \left(u_{k'} + v_{k'} \hat{a}^\dagger_{k'} \hat{a}^\dagger_{-k'} \right) \right| 0 \right\rangle$$

The terms in parentheses all commute for different indices, so only the product of two such terms with the same index needs to be considered:

$$\begin{aligned}(u_k + v_k \hat{a}_{-k} \hat{a}_k) & \left(u_k + v_k \hat{a}^\dagger_k \hat{a}^\dagger_{-k} \right) \\ &= u_k^2 + u_k v_k \left(\hat{a}^\dagger_k \hat{a}^\dagger_{-k} + \hat{a}_{-k} \hat{a}_k \right) + v_k^2 \hat{a}_{-k} \hat{a}_k \hat{a}^\dagger_k \hat{a}^\dagger_{-k}\end{aligned}$$

The norm is

$$\langle \mathrm{BCS} \mid \mathrm{BCS} \rangle = \prod_{k>0}^{\infty} \left(u_k^2 + v_k^2 \right)$$

and for normalization we must require

$$u_k^2 + v_k^2 = 1.$$

The BCS wave function

- The BCS wave function can be written as

$$
\begin{aligned}
|\mathrm{BCS}\rangle &\propto |0\rangle + \sum_{k>0} \frac{v_k}{u_k} a^+_k a^+_{\bar{k}} |0\rangle + \frac{1}{2} \sum_{kk'>0} \frac{v_k v_{k'}}{u_k u_{k'}} a^+_k a^+_{\bar{k}} a^+_{k'} a^+_{\bar{k}'} |0\rangle + \cdots \\
&\propto |0\rangle + A^\dagger |0\rangle + \frac{1}{2} (A^\dagger)^2 |0\rangle + \cdots \\
&\propto \exp(A^\dagger)|0\rangle,
\end{aligned}
$$

where the generalized pairing operator is defined as

$$
A^\dagger \equiv \sum_{k>0} \frac{v_k}{u_k} a^+_k a^+_{\bar{k}}.
$$

- In solid state physics, where $N \simeq 10^{23}$, the violation of particle number has no influence on any physical quantity.
- In nuclei, however, the violation of the invariance corresponding to the particle number in many cases gives rise to serious errors.

The BCS equation

- We assume that a many-body system is described by the Hamiltonian

$$
\begin{aligned}
H &= \sum_{k_1 k_2 \gtrless 0} t_{k_1 k_2} a^+_{k_1} a_{k_2} + \frac{1}{4} \sum_{\substack{k_1 k_2 k_3 k_4 \\ \gtrless 0}} \bar{v}_{k_1 k_2 k_3 k_4} a^+_{k_1} a^+_{k_2} a_{k_4} a_{k_3} \\
&= \sum_{k \gtrless 0} \varepsilon^0_k a^+_k a_k - G \sum_{kk' > 0} \hat{a}^\dagger_k \hat{a}^\dagger_{-k} \hat{a}_{-k'} \hat{a}_{k'}, \quad G > 0
\end{aligned}
$$

- A Lagrange multiplier (subsidiary condition)

$$
\left\langle \mathrm{BCS} \middle| \hat{N} \middle| \mathrm{BCS} \right\rangle = N
$$

where $\hat{N}$ is the particle-number operator

$$
\hat{N} = \sum_{k \gtrless 0} a^\dagger_k a_k = \sum_{k > 0} \left(a^\dagger_k a_k + a^\dagger_{-k} a_{-k} \right)
$$

It can be shown that

$$
\boxed{\langle \mathrm{BCS} | \hat{N} | \mathrm{BCS} \rangle = 2 \sum_{k>0} v^2_k .}
$$

The BCS equation

- The expectation value of the pure single-particle part

$$\langle \mathrm{BCS}| \sum_{k \gtrless 0} \varepsilon_k^0 a_k^+ a_k |\mathrm{BCS}\rangle = 2 \sum_{k>0} \varepsilon_k^0 v_k^2.$$

- The expectation value of the residual interaction term

$$\begin{aligned}
&\langle \mathrm{BCS}| - G \sum_{kk'>0} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k'} \hat{a}_{k'} |\mathrm{BCS}\rangle \\
&= -G \sum_{\substack{kk'>0 \\ k\neq k'}} u_k v_k u_{k'} v_{k'} - G \sum_{k>0} v_k^2 \\
&= -G \left(\sum_{k>0} u_k v_k \right)^2 - G \sum_{k>0} v_k^4
\end{aligned}$$

- The expectation value of the total Hamiltonian becomes

$$\langle \mathrm{BCS}|\hat{H} - \lambda \hat{N}|\mathrm{BCS}\rangle = 2 \sum_{k>0} \left(\varepsilon_k^0 - \lambda \right) v_k^2 - G \left(\sum_{k>0} u_k v_k \right)^2 - G \sum_{k>0} v_k^4$$

The BCS equation

Homework: please derive the following relations:

$$\left\langle \mathrm{BCS} \left| \hat{a}_k^\dagger \hat{a}_k \right| \mathrm{BCS} \right\rangle = v_k^2$$

$$\left\langle \mathrm{BCS} \left| \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k'} \hat{a}_{k'} \right| \mathrm{BCS} \right\rangle = \begin{cases} u_k v_k u_{k'} v_{k'} & \text{for } k \neq k' \\ v_k^2 & \text{for } k = k' \end{cases}$$

The BCS equation

- The variational principle:

$$\frac{\partial}{\partial v_k}\left\langle \mathrm{BCS}\left|\sum_k\left(\varepsilon_k^0-\lambda\right)\hat{a}_k^\dagger\hat{a}_k - G\sum_{kk'>0}\hat{a}_k^\dagger\hat{a}_{-k}^\dagger\hat{a}_{-k'}\hat{a}_{k'}\right|\mathrm{BCS}\right\rangle = 0$$

The u_k depend on the v_k via the normalization $u_k^2+v_k^2=1$, which yields

$$u_k\,\mathrm{d}u_k + v_k\,\mathrm{d}v_k = 0$$

or

$$\frac{\partial}{\partial v_k} = \left.\frac{\partial}{\partial v_k}\right|_{u_k} - \frac{v_k}{u_k}\left.\frac{\partial}{\partial u_k}\right|_{v_k}.$$

The BCS equation

- The variational principle:

$$4\left(\varepsilon_k^0-\lambda\right)v_k-2G\left(\sum_{k'>0}u_{k'}v_{k'}\right)u_k-4Gv_k^3$$
$$-\frac{v_k}{u_k}\left[-2G\left(\sum_{k'>0}u_{k'}v_{k'}\right)\right]=0$$

All the equations for the different values of k are coupled through the term

$$\Delta=G\sum_{k'>0}u_{k'}v_{k'}$$

We proceed by assuming for the moment that Δ is known, deriving an explicit form for v_k and u_k, and then using the definition of Δ as a supplementary condition. If we abbreviate to

$$\varepsilon_k=\varepsilon_k^0-\lambda-Gv_k^2$$

reduces to

$$2\varepsilon_k v_k u_k+\Delta\left(v_k^2-u_k^2\right)=0$$

Squaring this equation allows us to replace u_k^2 by v_k^2, one finds

$$\boxed{v_k^2=\frac{1}{2}\left(1-\frac{\varepsilon_k}{\sqrt{\varepsilon_k^2+\Delta^2}}\right)},\quad \boxed{u_k^2=\frac{1}{2}\left(1+\frac{\varepsilon_k}{\sqrt{\varepsilon_k^2+\Delta^2}}\right)}$$

The BCS energy gap equation

- Substituting the u_k, v_k, one finds the energy gap equation:

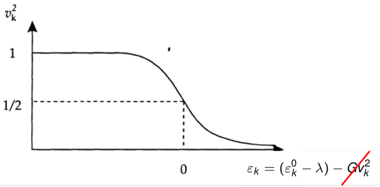
$$\Delta = G \sum_{k>0} u_k v_k = \frac{G}{2} \sum_{k>0} \frac{\Delta}{\sqrt{\varepsilon_k^2 + \Delta^2}}, \quad \varepsilon_k = (\varepsilon_k^0 - \lambda) - G v_k^2$$

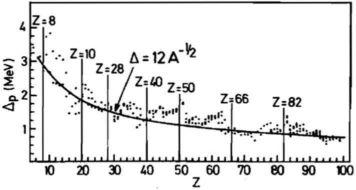
It can be solved iteratively using the known values of G and the single-particle energies ε_k^0. The other parameter λ then follows from simultaneously fulfilling the condition for the total particle number,

$$\sum_{k>0} 2 v_k^2 = N$$

To do this the term $-G v_k^2$ in the definition of the ε_k has to be neglected. This is usually done with the argument that it corresponds only to a renormalization of the single-particle energies.

The BCS energy gap equation





- The levels with $\varepsilon_k \approx 0$, i.e., those near the Fermi energy, will contribute most in the gap equation.
- Since proton and neutron Fermi energies are quite different, the gap equation is written separately for the proton and neutron energy-level schemes and there will also be separate strengths $G_{\rm p}$ and $G_{\rm n}$, gap parameters

$$G_{\rm p} \approx 17 \mathrm{MeV}/A \quad , \quad G_{\rm n} \approx 25 \mathrm{MeV}/A$$

- In many studies the pairing gaps are taken as the prescribed parameter, which simplifies the calculations considerably. It is also still a controversial question, whether for a deformed nucleus the pairing strength or gap depend on deformation.

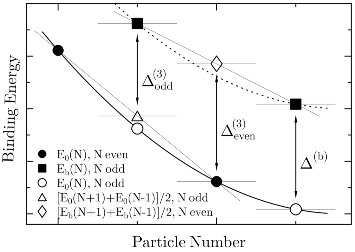
The pairing gap and odd-even mass difference

The pairing gap can be approximately determined by the odd-even mass difference:

$$\begin{aligned}\Delta_q^{(3)}(N_0) &= \frac{(-1)^{N_0}}{2}\left[E(N_0+1)-2E(N_0)+E(N_0-1)\right]\\ &= \frac{(-1)^{N_0}}{2}\left[\left.\frac{\partial^2 E_0}{\partial N^2}\right|_{N_0}+\frac{1}{12}\left.\frac{\partial^4 E_0}{\partial N^4}\right|_{N_0}+\cdots+D(N_0+1)-2D(N_0)+D(N_0-1)\right]\\ &\approx \frac{(-1)^{N_0}}{2}\left[D(N_0+1)-2D(N_0)+D(N_0-1)\right].\end{aligned}$$

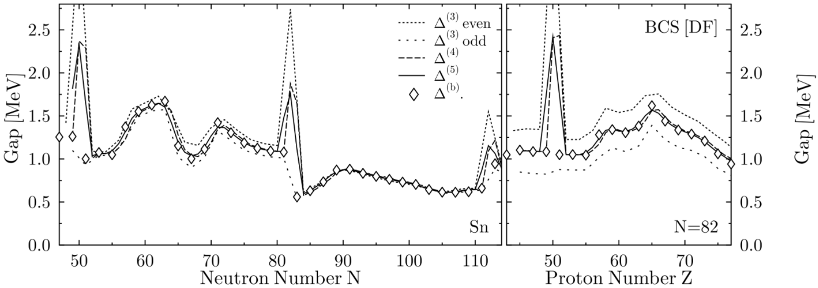
where D is defined as

$$D=\begin{cases}0, & \text{even proton and neutron number}\\ \Delta_\mathrm{n}, & \text{odd neutron number,}\\ \Delta_\mathrm{p}, & \text{odd proton number.}\end{cases}$$



M. Bender et al., EPJA8, 59 (2000)

The pairing gap and odd-even mass difference



M. Bender et al., Pairing gaps from nuclear mean-field models, EPJA8, 59 (2000)