Nuclear pairing

The particle-hole picture

- The lowest state – <u>ground state</u>- of a system of N=A fermions with an energy $E_0 = \sum_{i=1}^{A} \varepsilon_i$ $\quad |\psi_0\rangle = \prod_{i=1}^{A} \hat{a}_i^+ |0\rangle$

- <u>Fermi level</u>: the highest occupied state with energy ε_A

- <u>The expectation value of an operator O</u> in the ground state
$$\langle \Psi_0 | \hat{O} | \Psi_0 \rangle = \langle 0 | \hat{a}_A \cdots \hat{a}_1 \hat{O} \, \hat{a}_1^+ \cdots \hat{a}_A^+ | 0 \rangle$$

- Properties of ground state:
$$\hat{a}_i | \Psi_0 \rangle = 0, \quad i > A$$
$$\hat{a}_i^+ | \Psi_0 \rangle = 0, \quad i \le A$$

The simplest excited state

- Lift one particle from an occupied state into an unoccupied one: (one-particle/one-hole state)

$$\left|\Psi_{mi}\right\rangle = \hat{a}_m^+\hat{a}_i\left|\Psi_0\right\rangle, \quad m > A, \quad i \le A$$

$$E_{mi} - E_0 = \varepsilon_m - \varepsilon_i$$

- The next excitation is a two-particle/two-hole

$$\left|\Psi_{mnij}\right\rangle = \hat{a}_m^+\hat{a}_n^+\hat{a}_i\hat{a}_j\left|\Psi_0\right\rangle$$

$$E_{mnij} = \varepsilon_m + \varepsilon_n - \varepsilon_i - \varepsilon_j$$

Hamiltonian with two-body interaction in particle-number representation (2th quantization)

- A microscopic model that describes the structure of the nucleus in terms of the degree of freedom of the nucleons.

$$\hat{H} = \sum_{ij} t_{ij} \hat{a}_i^+ \hat{a}_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$

- An eigenstate of H:

$$|\Psi\rangle = \sum_{i_1 i_2, \cdots, i_A} c_{i_i, i_2, \cdots i_A} \hat{a}_{i_1}^+ \hat{a}_{i_2}^+ \cdots \hat{a}_{i_A}^+ |0\rangle$$

Hartree-Fock

- Single-particle Hamiltonian

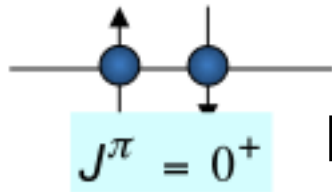$$\left(t + \Gamma \right) = t_{kl} + \sum_{j=1}^{A} \bar{v}_{kjlj}$$

    – h contains kinetic energy t and a self-consistent field Γ, which depends on the density of nucleus. It is a one-body field and averages over all two-body interactions.
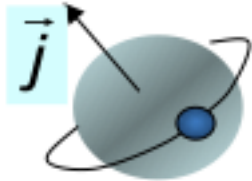
Reminder: Seniority symmetry/Pairing
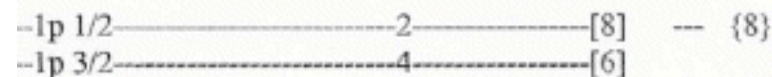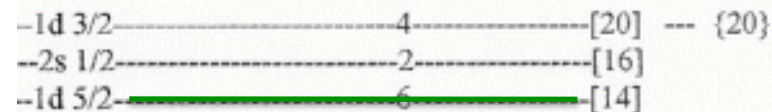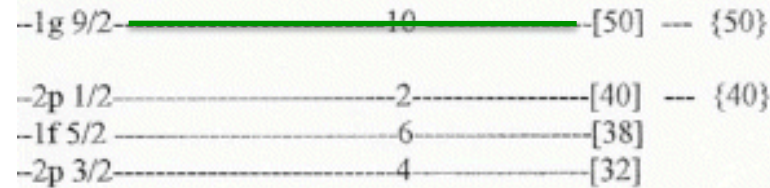
1943 Racah
1949 Goeppert-Mayer
1958 Nuclear BCS

$J^\pi = 0^+$

Even-even

$\vec{j}$

Odd-A
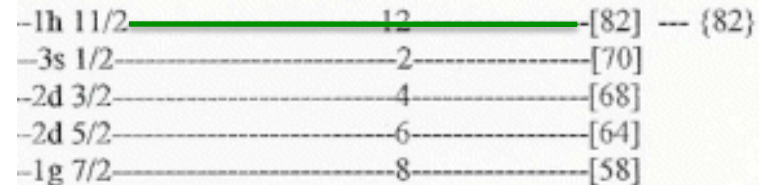
Mean field theories
➢ Single-particle model
  HO, WS…
➢ Hartree-Fock (density functional) approaches
  Skyrme force, boson exchange potentials
➢ Shell model
  Monopole

--1h 11/2	12	-[82]	--- {82}
--3s 1/2	2	-------[70]	
--2d 3/2	4	-------[68]	
--2d 5/2	6	-------[64]	
--1g 7/2	8	-------[58]	
--1g 9/2	10	-[50]	--- {50}
--2p 1/2	2	-[40]	--- {40}
--1f 5/2	6	-[38]	
--2p 3/2	4	-[32]	
--1f 7/2	8	-[28]	--- {28}
--1d 3/2	4	-[20]	--- {20}
--2s 1/2	2	-------[16]	
--1d 5/2	6	-[14]	
--1p 1/2	2	-------[8]	--- {8}
--1p 3/2	4	-------[6]	

http://www.nobelprize.org/nobel_prizes/physics/laureates/1963/mayer-lecture.pdf

Introduction to pairing

- In solid-state physics: A pair of electrons in metal with opposite spins and momentums close to Fermi surface interact with each other and make a pair. They have energy lower than Fermi surface which indicates that they are bound.

- In nuclear physics: A pair of nucleons with total spin I=0. This is a short range (large spatial overlap) nucleon-nucleons interaction.

- Experimental observations that require short range interaction in the model :
  - The energy gap
  - The level density
  - Odd-even mass effect
  - Moment of inertia
  - Deformation
  - The low-lying 2^+

Nilsson plus pairing Hamiltonian constitutes a minimal model for nuclear structure

Matematisk-fysiske Meddelelser
udgivet af
Det Kongelige Danske Videnskabernes Selskab
Bind 32, nr. 16

Mat. Fys. Medd. Dan.Vid. Selsk. 32, no. 16 (1961)

THE EFFECT OF PAIR CORRELATION ON
THE MOMENT OF INERTIA AND
THE COLLECTIVE GYROMAGNETIC RATIO
OF DEFORMED NUCLEI
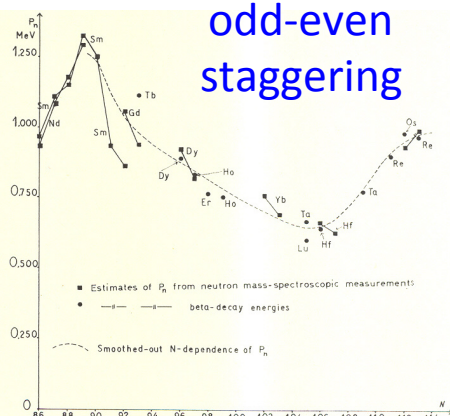
BY

S. G. NILSSON AND O. PRIOR

odd-even staggering

Fig. 1. The odd-even mass difference parameter P_n for neutrons in region I ($150 < A < 188$). The squares refer to mass-spectroscopic measurements by JOHNSON and BHANOT[25], while the circles refer to beta-decay energy data. The dashed curve represents averaged values used in the moment –of– inertia calculation.
Added in proof: Recently published more complete mass-spectroscopic measurements by BHANOT, JOHNSON and NIER[30] give 100–200 keV lower P_n-values in the region $N = 108$–112; see furthermore fig. 28.
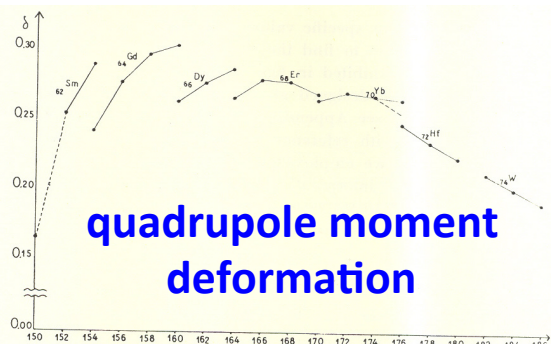
quadrupole moment deformation

Fig. 15. Values of the eccentricity parameter δ in region I used in the calculations. The values of δ are obtained by means of eq. (41) from the quadrupole moments given by ELBEK et. al.[19], assuming $R_z = 1.2 \times A^{1/3}$ f. Note that the dashed line ending at Yb176 represents a slight ad hoc correction of the Yb176 point. Such a correction is in line with the level diagram of ref. 15.
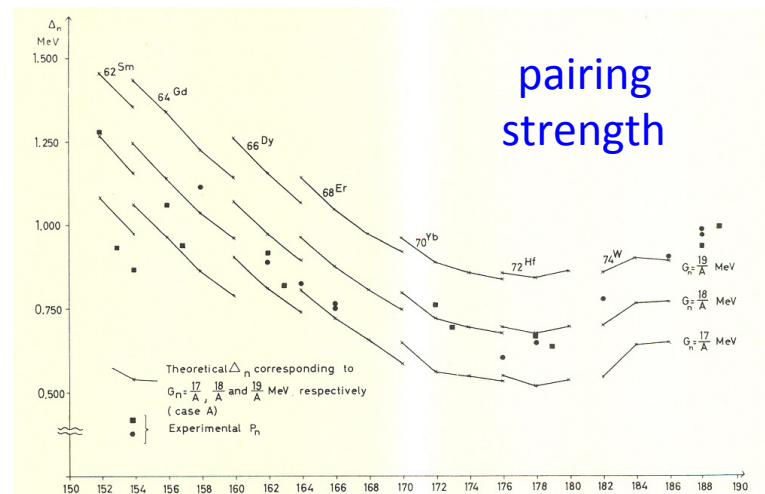
pairing strength

Fig. 7. The relation between values of Δ_n and G_n in region I obtained in the calculations. For details of the single-particle spectrum employed, denoted as "case A", see table I. The points exhibited for comparison refer to the P_n-values of fig. 1.
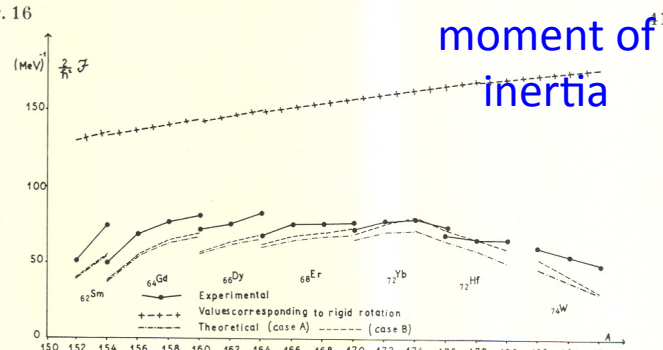
moment of inertia

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.

Belyaev: Mat. Fys. Medd. Dan. Vid. Selsk. 31 no. 11 (1959)
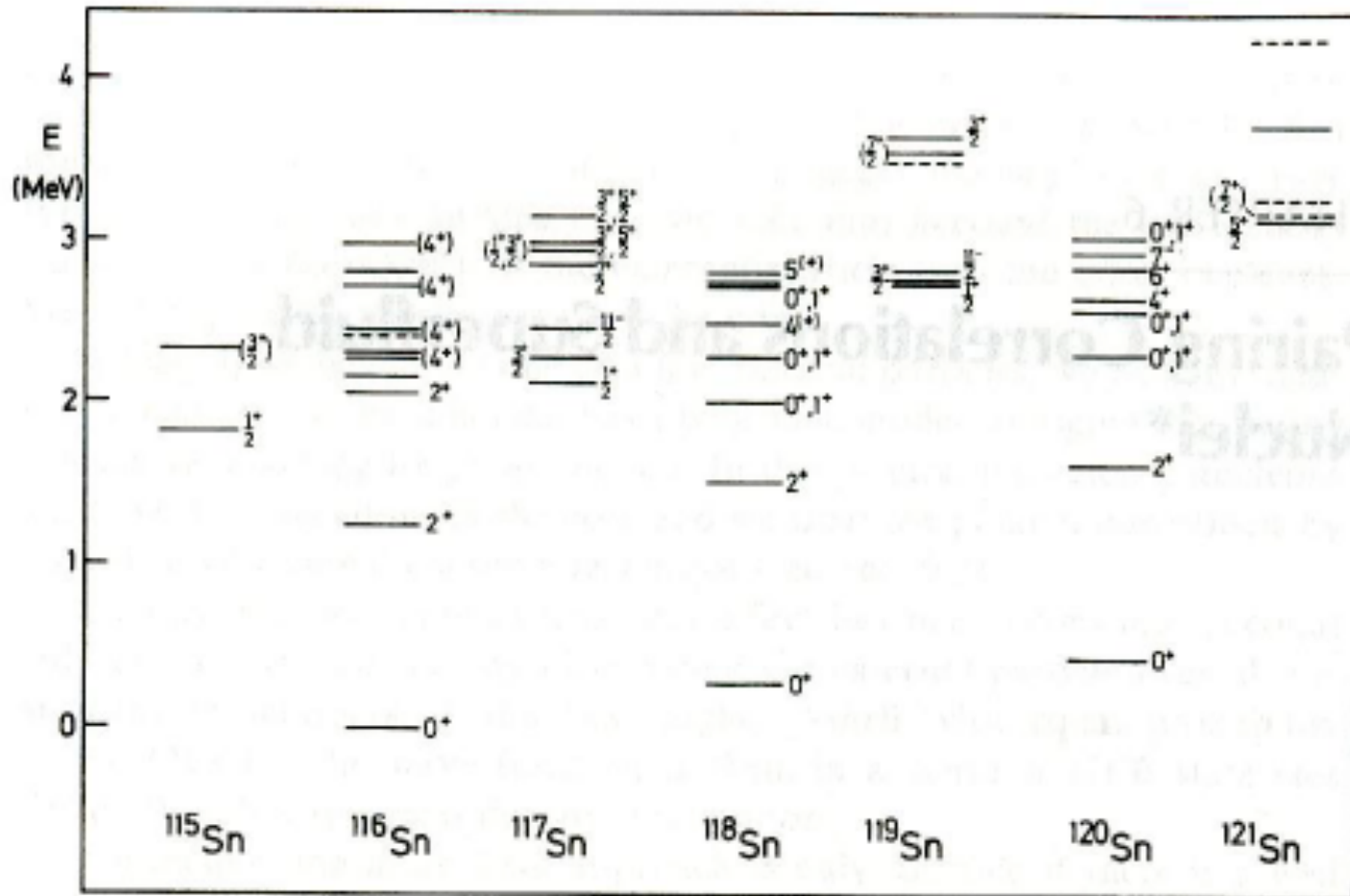
The energy gap due to pairing

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

Introduction to pairing

- To explain these phenomena we need to take into the account short range nucleon-nucleon interaction.

- The most effective pairing coupling is I=0

- They are similar to long range particle-hole interaction.

- No exact solution, it is an approximation by variational principle

The seniority model

The seniority model provides a simple model for pairing phenomena.
System: N fermions in a single j-shell.
Hamiltonian:

$$H = -G \sum_{m,m'>0} \hat{a}_m^\dagger \hat{a}_{-m}^\dagger \hat{a}_{-m'} \hat{a}_{m'}$$

$$= -G\hat{S}_+\hat{S}_-$$

where

$$\hat{S}_+ = \sum_{m>0} \hat{a}_m^\dagger \hat{a}_{-m}^\dagger \quad \text{and} \quad \hat{S}_- = \left(\hat{S}_+\right)^\dagger.$$

Rewrite Hamiltonian as

$$H = -G\left(\vec{S}\cdot\vec{S} - \hat{S}_0^2 + \hat{S}_0\right)$$

in terms of total quasi-spin

$$\vec{S} = \sum_{m>0} \vec{s}^{(m)}.$$

and total z-component of quasi spin

$$\hat{S}_0 = \sum_{m>0} \hat{s}_0^{(m)} = \frac{1}{2}(\hat{N} - \Omega).$$

Here, $\Omega = j + 1/2$ is the maximal number of pairs for a single j-shell. The eigenvalues S of total quasi-spin are

$$S = \frac{1}{2}|N - \Omega|, \ldots, \frac{1}{2}\Omega - 1, \frac{1}{2}\Omega.$$

Thus, the energies of the seniority model are

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

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:

- 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

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

Two-particle spectrum of pure pairing force: $J = 0$ ground state is separated from degenerate $J = 2, 4, 6, \ldots, 2j - 1$ levels.
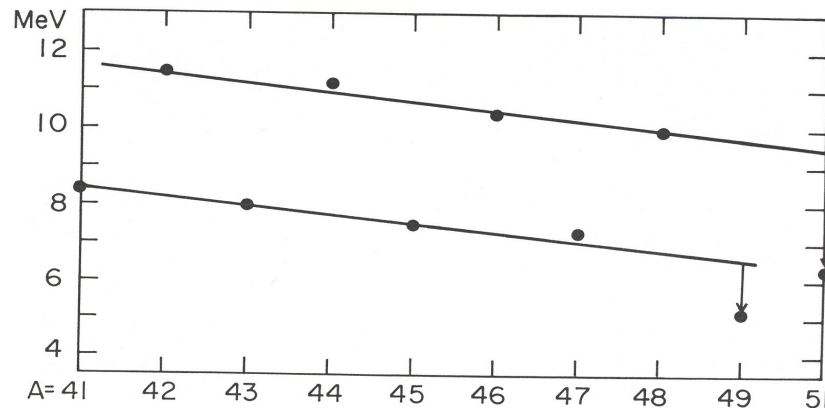
Seniority coupling and binding energy
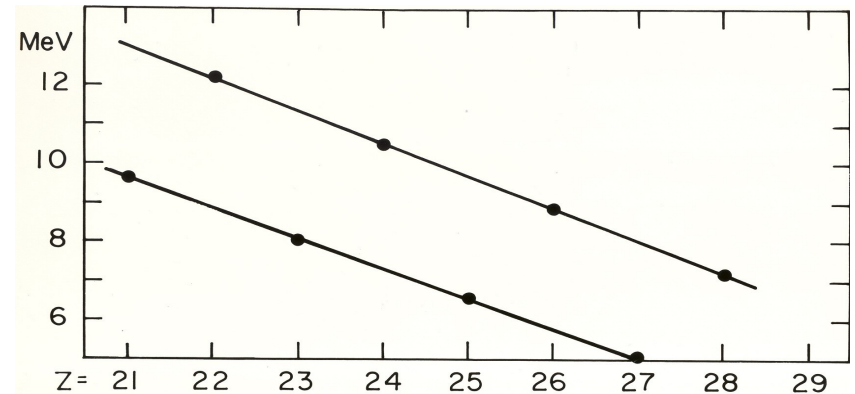
Semi-magic nuclei

$$\hat{V} = a + b\mathbf{t}_1 \cdot \mathbf{t}_2 + GP_0,$$

Binding energies of ground states in j^n configuration

$$E\left(j^n\right) = Cn + \frac{1}{2}n(n-1)\alpha + \left[\frac{1}{2}n\right]\beta$$
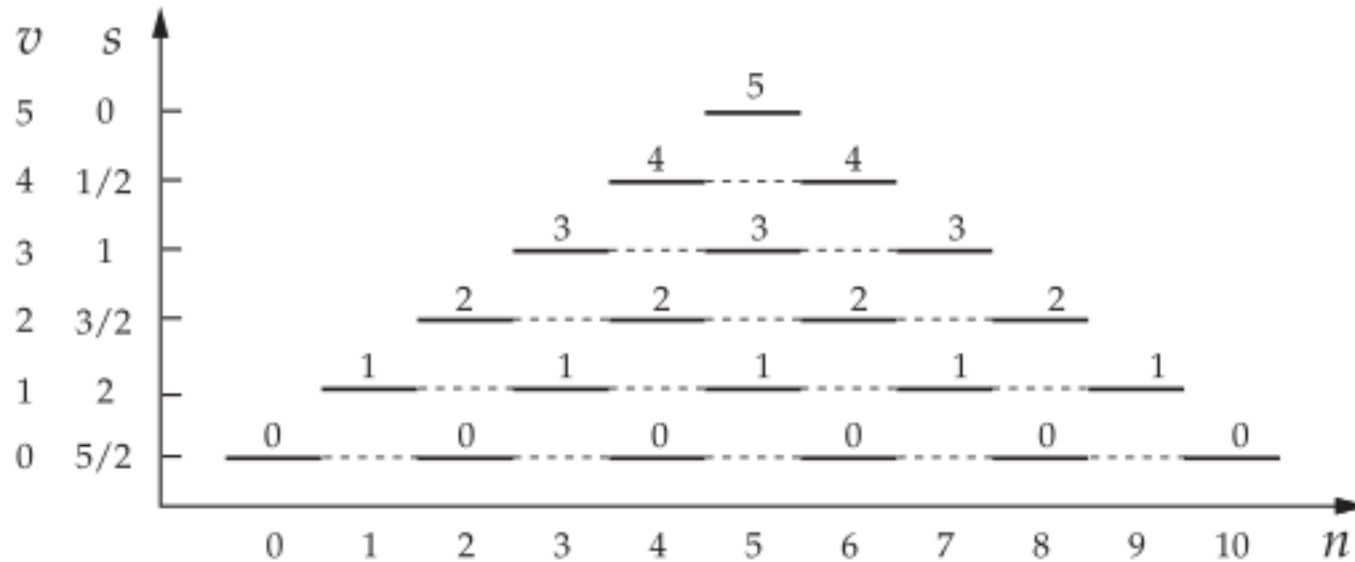

Neutron separation energies from Ca isotopes

Proton separation energies from N=28 isotones

I. Talmi, Simple models of complex nuclei (Harwood, Chur, Switzerland, 1993)

The spectrum with a pairing interaction

USp(10) irreps in the j=9/2 shell

v: Seniority
s: Quasispin

D. J. Rowe, M. J. Carvalho, and J. Repka, Rev. Mod. Phys. 84, 712 (2012).

Realistic interaction and monopole pairing

$(0f_{7/2})^2$ configuration

no interaction — $J=0$ pairing — realistic interaction
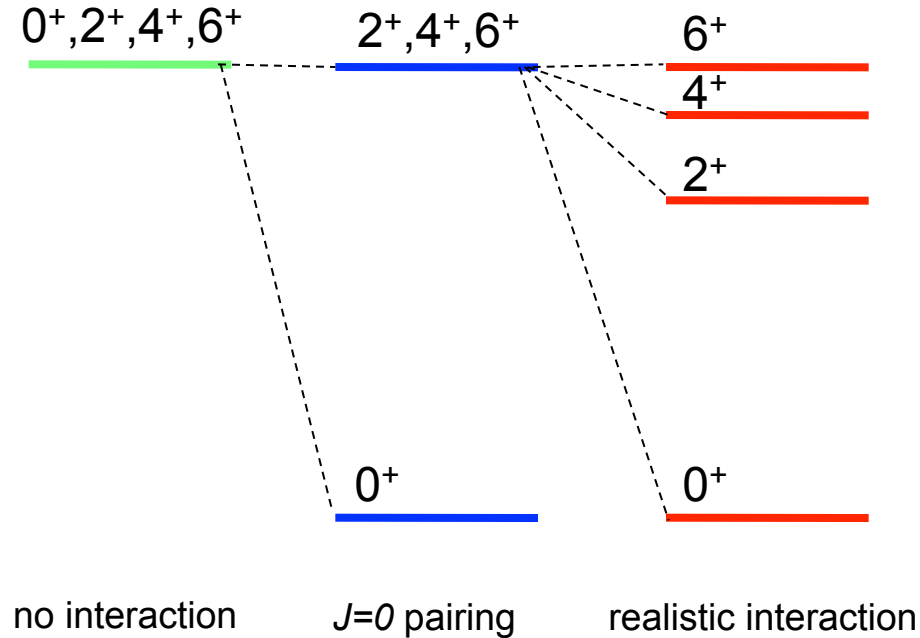
❖J=0 interactions are strongly attractive.
❖Seniority is conserved when j<9/2
❖Pairing interaction conserves seniority

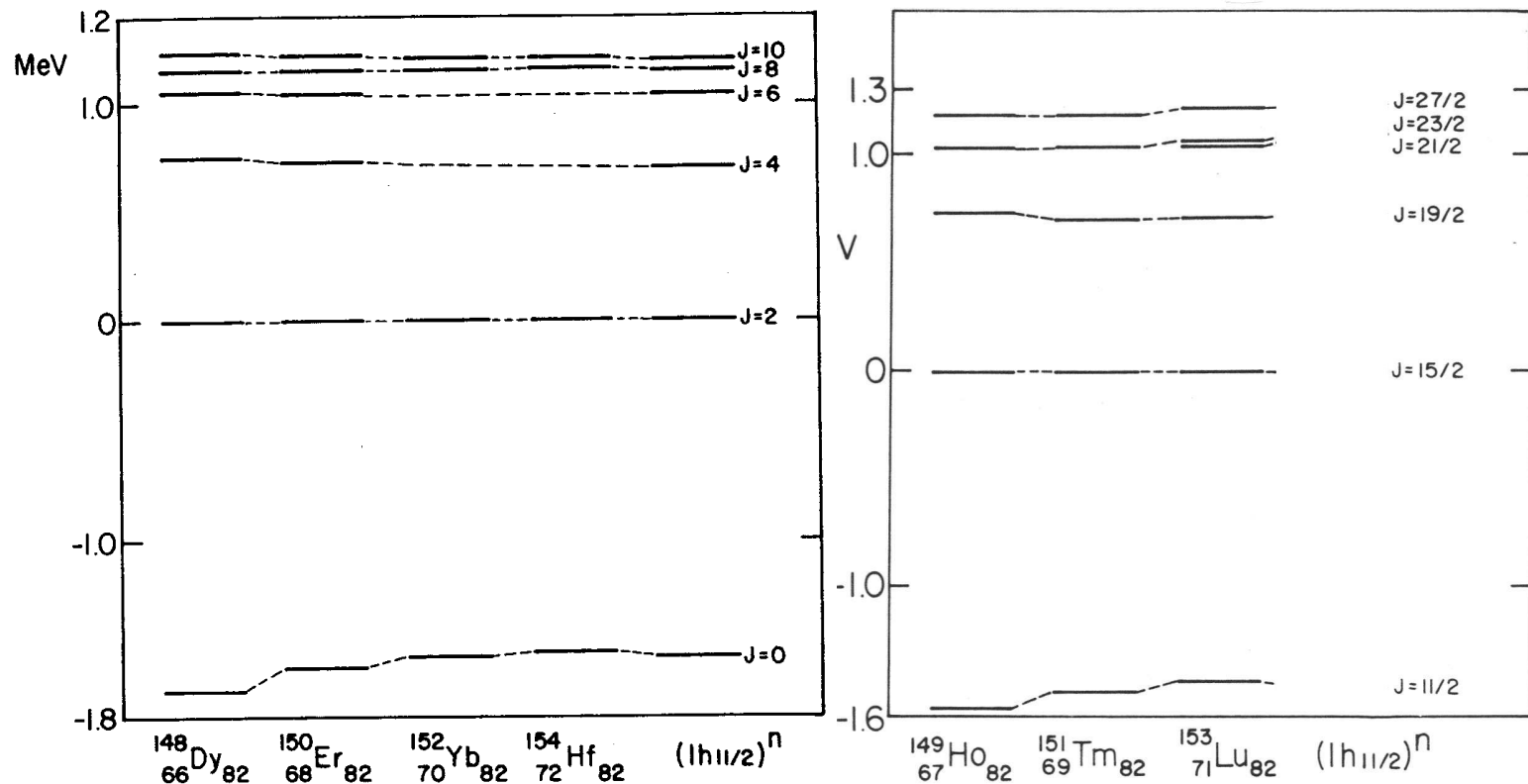$$\left\langle j^2 J M_J \left| \hat{V}_{\text{pairing}} \right| j^2 J M_J \right\rangle = \begin{cases} -\tfrac{1}{2}(2j+1)g_0, & J = 0 \\ 0, & J \neq 0 \end{cases}$$

Seniority coupling scheme with realistic interaction

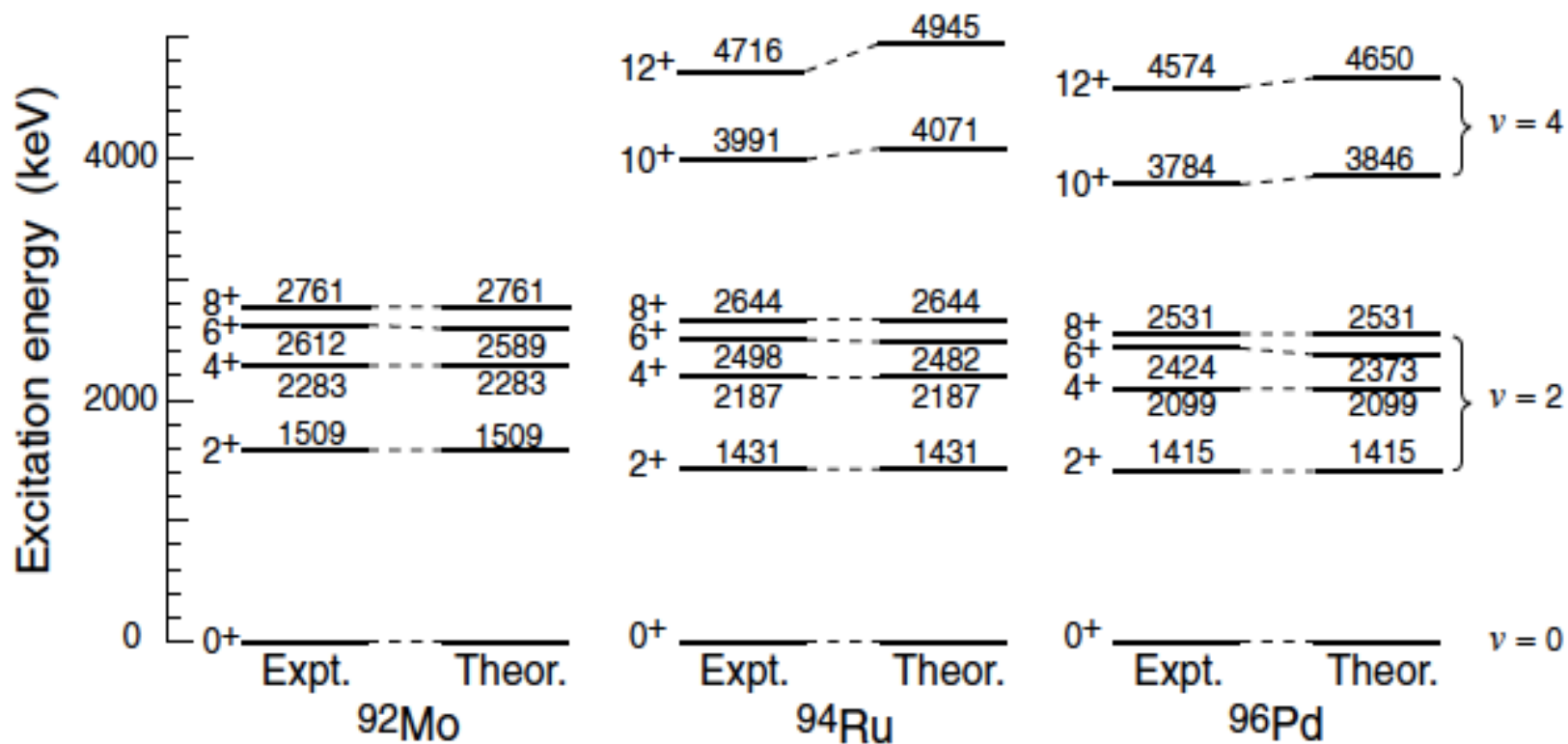$$|\text{g.s.}\rangle = |\nu = 0; J = 0\rangle = (P_j^+)^{n/2}|\Phi_0\rangle$$
$$|\nu = 2; JM\rangle = (P_j^+)^{(n-2)/2}A^+(j^2 JM)|\Phi_0\rangle$$

Energy levels of $0h_{11/2}$ protons in N=82 isotones

I. Talmi, Simple models of complex nuclei

Energy levels of $0g_{9/2}$ protons in N=50 isotones

D.J. Rowe and G. Rosensteel, Phys. Rev. Lett. **87** (2001) 172502

Conservation of seniority

the rotationally invariant interaction has to satisfy **[(2j − 3)/6]** linear constraints to conserve seniority.

$$j = 9/2 : 65v_2 - 315v_4 + 403v_6 - 153v_8 = 0$$

$$j = 11/2 : 1020v_2 - 3519v_4 - 637v_6 + 4403v_8 - 2541v_{10} = 0$$

$$j = 13/2 : 1615v_2 - 4275v_4 - 1456v_6 + 3196v_8 - 5145v_{10} - 4225v_{12} = 0$$

$j = 15/2$

$$1330V_2 - 2835V_4 - 1807V_6 + 612V_8$$
$$+ 3150V_{10} + 3175V_{12} - 3625V_{14} = 0,$$

and

$$77805V_2 - 169470V_4 - 85527V_6 - 4743V_8$$
$$+ 222768V_{10} + 168025V_{12} - 208858V_{14} = 0.$$

I. Talmi, Simple Models of Complex Nuclei
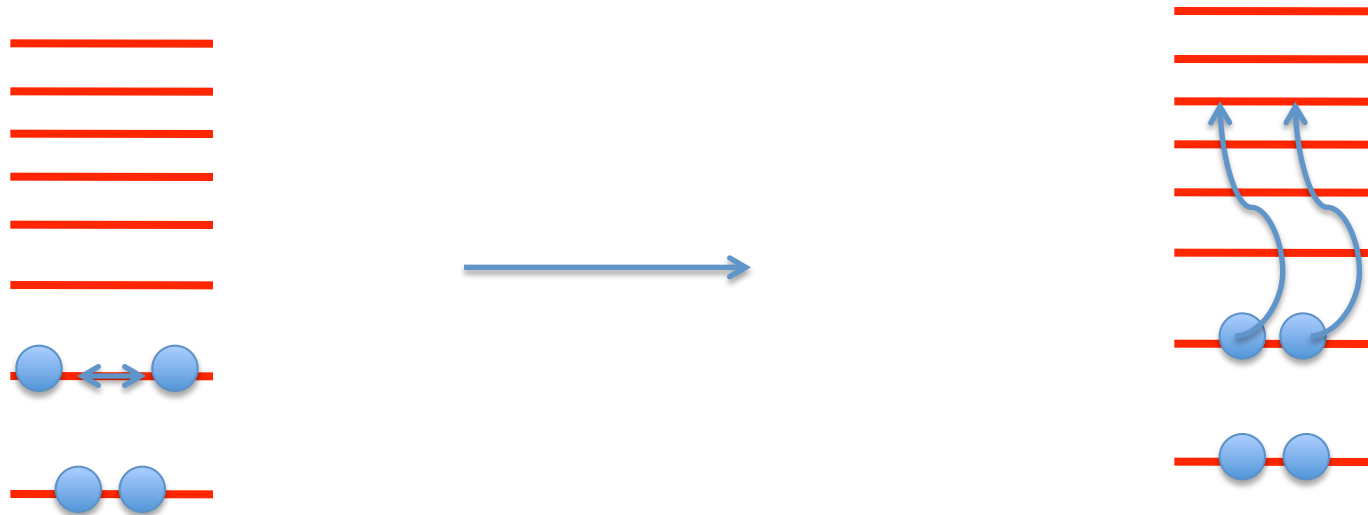*D.J. Rowe and G. Rosensteel, Phys. Rev. Lett. 87, 172501 (2001).*
P. Van Isacker and S. Heinze, Phys. Rev. Lett. 100, 052501 (2008).
CQ et al., PRC 82, 014304(2010)

The odd-even staggering revisited

What is the pairing correlation energy?

If one removes the self-energy, which may have been taken into account by the mean field, the binding energy of a single j system can be rewritten as

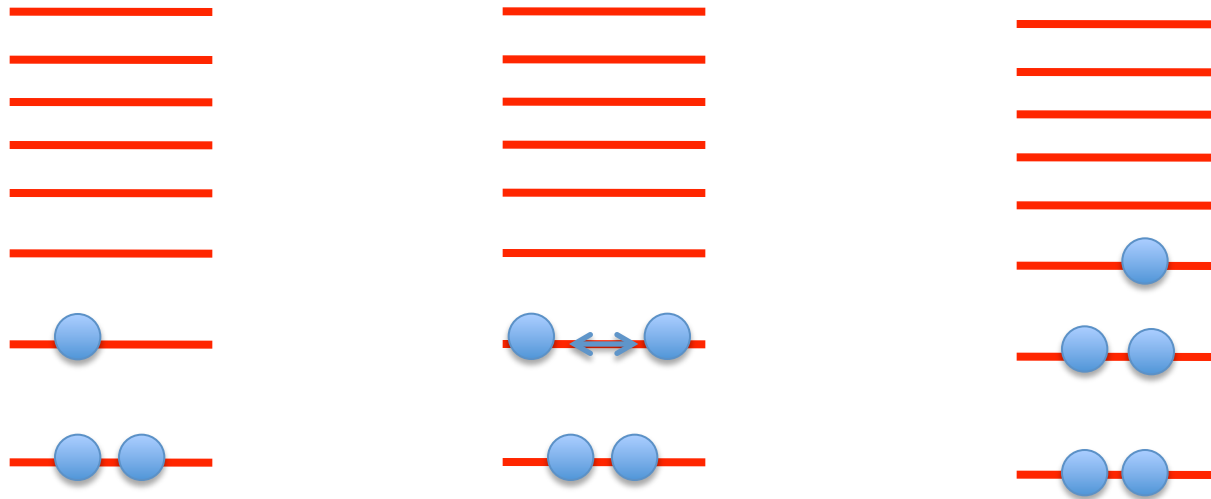$$E(j^n) = \frac{1}{4}n(n-1)G - \left[\frac{1}{2}n\right](j+1)G + \left[\frac{1}{2}n\right]G$$

A. Volya et al. / Physics Letters B 509 (2001) 37

$$E_{\text{corr}} = E - \sum_j \epsilon_j \overline{N}_j - \sum_j \frac{G_{jj}}{2\Omega_j - 1} \frac{\overline{N}_j(\overline{N}_j - 1)}{2},$$

OES may be attributed to:

- **Pairing correlation effect/pair energy**
- **Deformation effect/mean field effect**

$$\Delta_n = 1/2[2B(N,Z) - B(N+1,Z) - B(N-1,Z)]$$

A. Bohr, B. R. Mottelson, Nuclear structure, vol. 1, World Scientific, 1998.
W.Satula,J.Dobaczewski,W.Nazarewicz,Phys.Rev.Lett.81 (1998) 3599.
W. Friedman, G. Bertsch, E. Phys. J. A 41 (2009) 109.

Examples of OES formulae

$$\Delta^{(3)}(N) = -\frac{1}{2}\left[B(N-1,Z) + B(N+1,Z) - 2B(N,Z)\right]$$

$$= -\frac{1}{2}\left[S_n(N+1,Z) - S_n(N,Z)\right] \quad (1)$$

$$\Delta_C^{(3)}(N) = \frac{1}{2}\left[S_n(N,Z) - S_n(N-1,Z)\right]$$

$$= \frac{1}{2}\left[B(N,Z) + B(N-2,Z) - 2B(N-1,Z)\right]$$

$$= \frac{1}{2}\left[S_{2n}(N,Z) - 2S_n(N-1,Z)\right]$$

$$= \Lambda^{(3)}(N-1),$$

$$\Delta^{(4)}(N) = \frac{1}{4}\left[-B(N+1,Z) + 3B(N,Z) \right.$$

$$\left. - 3B(N-1,Z) + B(N-2,Z)\right]$$

$$= \frac{1}{2}\left[\Delta^{(3)}(N) + \Delta_C^{(3)}(N)\right].$$

$$\Delta^{(5)}(N) = \frac{1}{8}\left[B(N+2,Z) - 4B(N+1,Z) \right.$$

$$\left. + 6B(N,Z) - 4B(N-1,Z) + B(N-2,Z)\right]$$

$$= \frac{1}{4}\left[\Delta_C^{(3)}(N+2) + 2\Delta^{(3)}(N) + \Delta_C^{(3)}(N)\right].$$

$$\Delta_C^{(3)}$$

Examples of OES formulae

$$\Delta^{(3)}(N) = -\frac{1}{2}\left[B(N-1,Z) + B(N+1,Z) - 2B(N,Z)\right]$$

$$= -\frac{1}{2}\left[S_n(N+1,Z) - S_n(N,Z)\right] \quad (1)$$

$$\Delta_C^{(3)}(N) = \frac{1}{2}\left[S_n(N,Z) - S_n(N-1,Z)\right]$$

$$= \frac{1}{2}\left[B(N,Z) + B(N-2,Z) - 2B(N-1,Z)\right]$$

$$= \frac{1}{2}\left[S_{2n}(N,Z) - 2S_n(N-1,Z)\right]$$

$$= \Lambda^{(3)}(N-1),$$

$$\Delta^{(4)}(N) = \frac{1}{4}[-B(N+1,Z) + 3B(N,Z)$$

$$- 3B(N-1,Z) + B(N-2,Z)]$$

$$= \frac{1}{2}[\Delta^{(3)}(N) + \Delta_C^{(3)}(N)].$$

$$\Delta^{(5)}(N) = \frac{1}{8}[B(N+2,Z) - 4B(N+1,Z)$$

$$+ 6B(N,Z) - 4B(N-1,Z) + B(N-2,Z)]$$

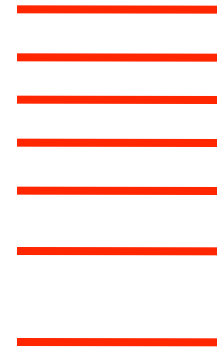$$= \frac{1}{4}[\Delta_C^{(3)}(N+2) + 2\Delta^{(3)}(N) + \Delta_C^{(3)}(N)].$$

Nobel-prize winning problem

For two particles in a non-degenerate system with a constant pairing, the energy can be evaluated through the well known relation,

$$G \sum_i \frac{2j_i + 1}{2\varepsilon_i - E_2} = 2. \qquad (10)$$

The corresponding wave function amplitudes are given by
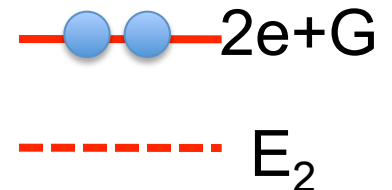
$$X_i = N_n \frac{2j + 1}{2\varepsilon_i - E_2} \qquad (11)$$

The correlation energy induced by the monopole pairing corresponds to the difference

$$\Delta = \varepsilon_\delta - \frac{1}{2} E_2, \qquad (12)$$

where δ denotes the lowest orbital. As the gap Δ increases the amplitude X_i becomes more dispersed, resulting in stronger two-particle correlation.

The Cooper Problem

Letters to the Editor

*P*UBLICATION *of brief reports of important discoveries in physics may be secured by addressing them to this department. The closing date for this department is five weeks prior to the date of issue. No proof will be sent to the authors. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents. Communications should not exceed 600 words in length and should be submitted in duplicate.*

Bound Electron Pairs in a Degenerate Fermi Gas*

LEON N. COOPER

Physics Department, University of Illinois, Urbana, Illinois

(Received September 21, 1956)

I T has been proposed that a metal would display superconducting properties at low temperatures if

$= (1/V) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2)]$ which satisfy periodic boundary conditions in a box of volume V, and where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of electron one and electron two. (One can use antisymmetric functions and obtain essentially the same results, but alternatively we can choose the electrons of opposite spin.) Defining relative and center-of-mass coordinates, $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$, $\mathbf{r} = (\mathbf{r}_2 - \mathbf{r}_1)$, $\mathbf{K} = (\mathbf{k}_1 + \mathbf{k}_2)$ and $\mathbf{k} = \frac{1}{2}(\mathbf{k}_2 - \mathbf{k}_1)$, and letting $\mathcal{E}_K + \epsilon_k = (\hbar^2/m)(\frac{1}{4}K^2 + k^2)$, the Schrödinger equation can be written
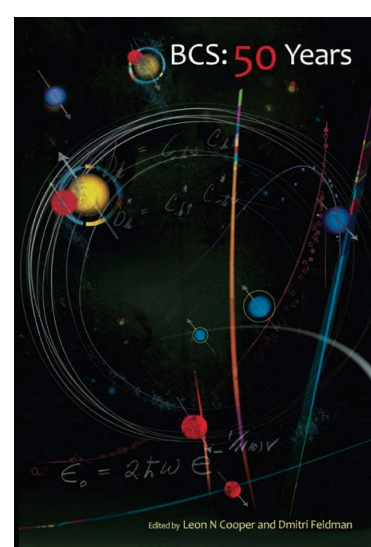
$$(\mathcal{E}_K + \epsilon_k - E)a_\mathbf{k} + \sum_{\mathbf{k}'} a_{\mathbf{k}'}(\mathbf{k}|H_1|\mathbf{k}') \times \delta(\mathbf{K} - \mathbf{K}')/\delta(0) = 0 \quad (1)$$

where

$$\Psi(\mathbf{R},\mathbf{r}) = (1/\sqrt{V})e^{i\mathbf{K}\cdot\mathbf{R}}\chi(\mathbf{r},K),$$
$$\chi(\mathbf{r},K) = \sum_\mathbf{k} (a_\mathbf{k}/\sqrt{V})e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2)$$

and

$$(\mathbf{k}|H_1|\mathbf{k}') = \left(\frac{1}{V}\int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}}H_1 e^{i\mathbf{k}'\cdot\mathbf{r}}\right)_{0 \text{ phonons}}.$$

A pair of electrons with an attractive interaction on top of an inert Fermi sea.

$$|\phi\rangle = \sum_{k>k_F} \frac{1}{2\varepsilon_k - E} c^+_{k\uparrow} c^+_{-k\downarrow} |FS\rangle, \quad \frac{1}{G} = \sum_{k>k_F} \frac{1}{2\varepsilon_k - E}$$

Theory of Superconductivity*

J. Bardeen, L. N. Cooper,† and J. R. Schrieffer‡
Department of Physics, University of Illinois, Urbana, Illinois
(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $(\hbar\omega)^2$, consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5kT_c$ at $T=0°K$ to zero at T_c. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

BCS: 50 Years

Edited by Leon N Cooper and Dmitri Feldman

$\epsilon_o = 2\hbar\omega \, \epsilon$
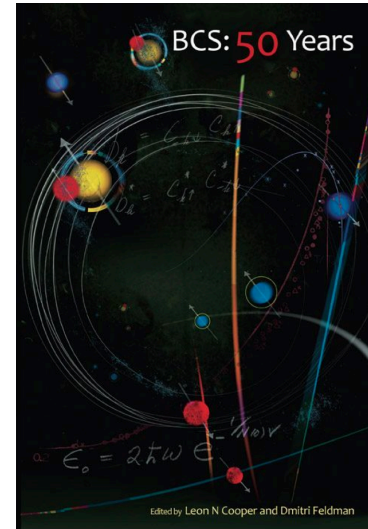
Possible Analogy between the Excitation Spectra of Nuclei and Those of the Superconducting Metallic State

A. Bohr, B. R. Mottelson, and D. Pines*

FIG. 1. Energies of first excited intrinsic states in deformed nuclei, as a function of the mass number. The experimental data may be found in *Nuclear Data Cards* [National Research Council, Washington, D. C.] and detailed references will be contained in reference 1 above. The solid line gives the energy $\delta/2$ given by Eq. (1), and represents the average distance between intrinsic levels in the odd-A nuclei (see reference 1).

The figure contains all the available data for nuclei with $150 < A < 190$ and $228 < A$. In these regions the nuclei are known to possess nonspherical equilibrium shapes, as evidenced especially by the occurrence of rotational spectra (see, e.g., reference 2). One other such region has also been identified around $A = 25$; in this latter region the available data on odd-A nuclei is still represented by Eq. (1), while the intrinsic excitations in the even-even nuclei in this region do not occur below 4 Mev.

We have not included in the figure the low lying $K=0$ states found in even-even nuclei around Ra and Th. These states appear to represent a collective odd-parity oscillation.

gap in e-e spectra
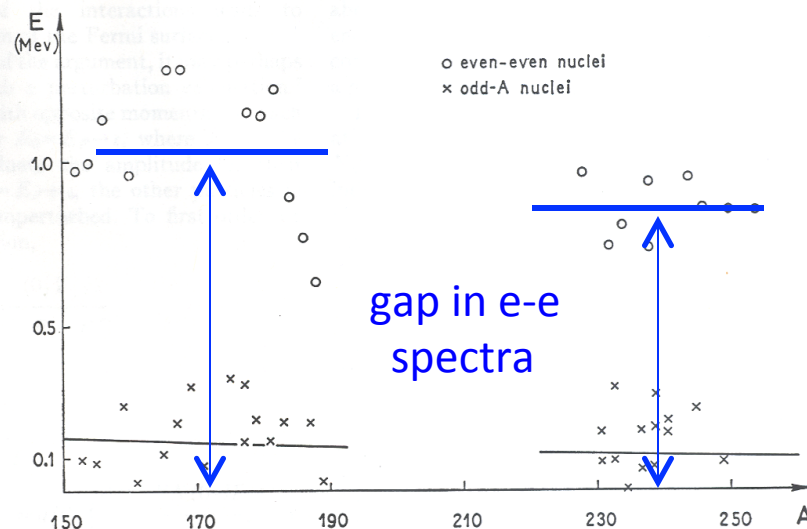
Pairing gap and the alpha formation
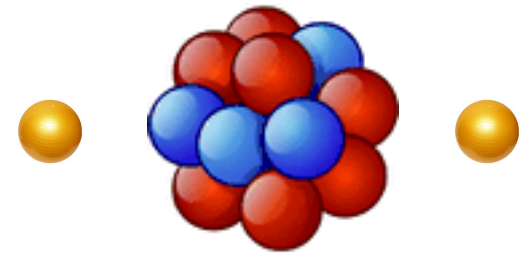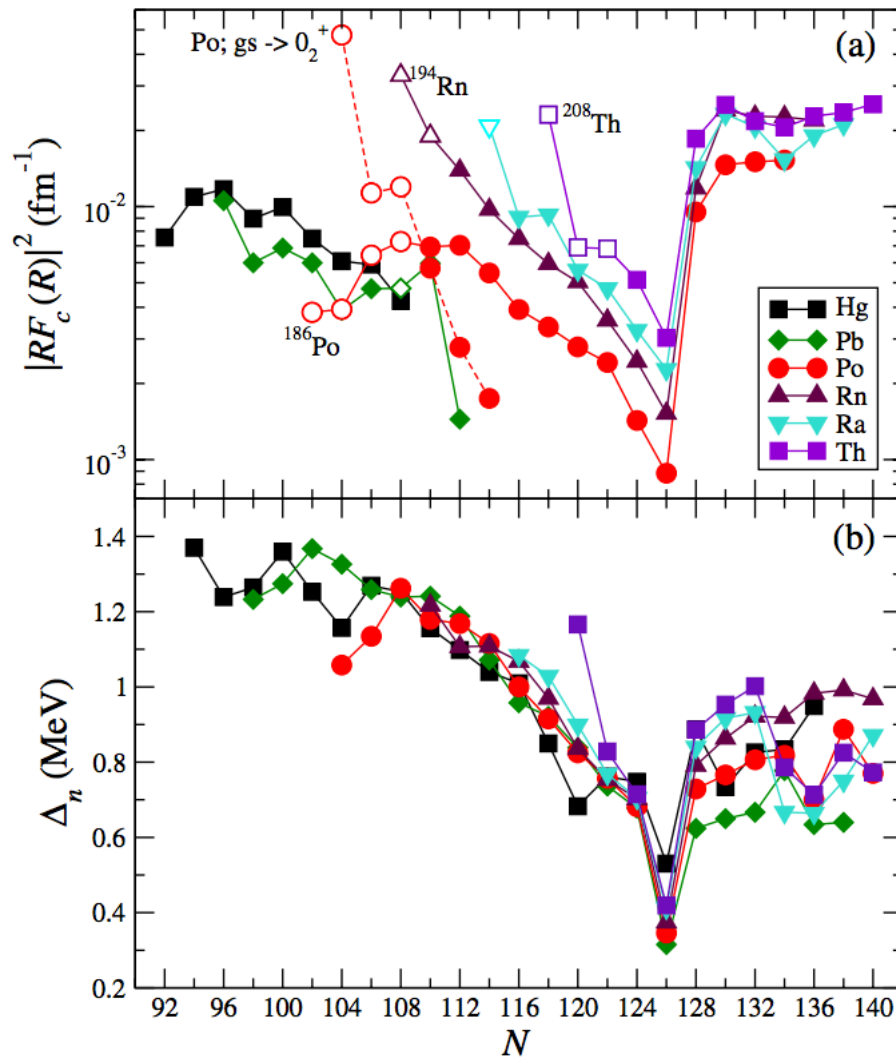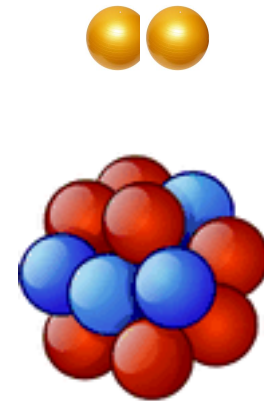

No Pairing

'Strong' pairing

OES in semi-magic nuclei and comparison with the HFB calculations
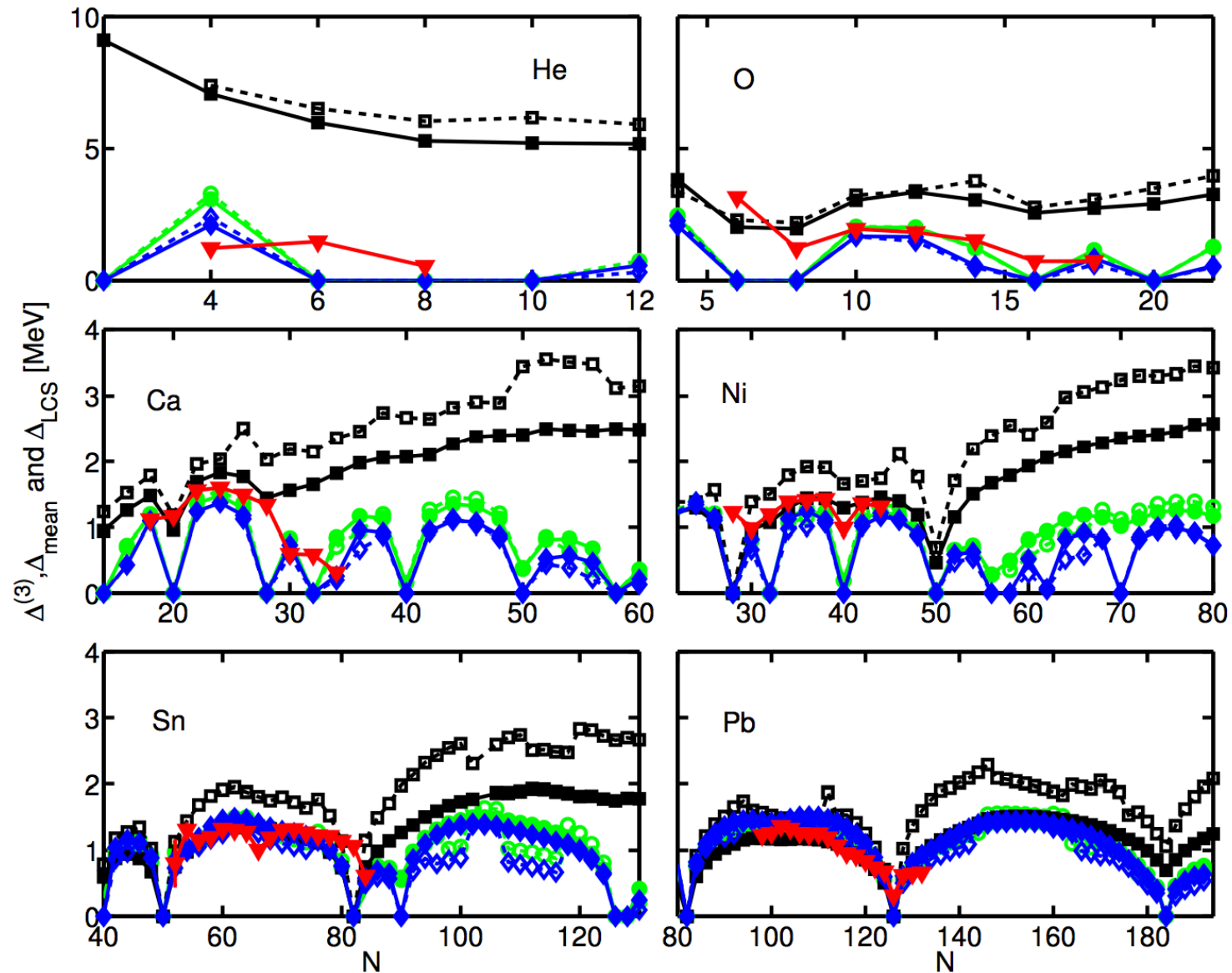
The BCS model

BCS model- BCS state

A many-body system is described by following Hamiltonian:

$$H = \sum_{k_1 k_2} t_{k_1 k_2} a^+_{k_1} a_{k_2} + \frac{1}{2} \sum_{k_1 k_2 k_3 k_4 <>0} v_{k_1 k_2 k_3 k_4} a^+_{k_1} a^+_{k_2} a_{k_4} a_{k_3}$$

In BCS model we speculate that ground state should be built up from pair creation operators $a^+_k a^+_{-k}$

This is the approximated solution: Trial wave function for even-even nuclei

$$|BCS\rangle = \prod_{k>0} \left(u_k + v_k a^+_k a^+_{\bar{k}} \right) |-\rangle$$

K are the single particle levels

u_k^2 and v_k^2 represent the probability that a certain pair state is not or is occupied.

$$\{k, -k\}$$

An example is a spherical basis

$$|k\rangle = |nljm\rangle,$$

$$Conjugate\ state : |\bar{k}\rangle = |nlj - m\rangle\ m > 0$$

BCS model- BCS state

Example: For Hartree-Fock states we would have:
$v_k=1$ and $u_k=0$ below Fermi level
$v_k=0$ and $u_k=1$ above Fermi level
However in BCS model states over Fermi level can be occupied (energetically favored)

u_k and v_k are variational parameters. We determine them in a way that the corresponding state has minimum energy.
Normalization of BCS state:

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

We require: $\boxed{u_k^2 + v_k^2 = 1}$

BCS model

Great disadvantage: Particle number is not conserved in BCS! BCS state is the superposition of different number of pairs.

$$\left|BCS\right\rangle \propto \left|-\right\rangle + \sum_{k>0}\frac{v_k}{u_k}a_k^+a_{-k}^+\left|-\right\rangle + \frac{1}{2}\sum_{kk'}\frac{v_kv_{k'}}{u_ku_{k'}}a_k^+a_{-k}^+a_{k'}^+a_{-k'}^+\left|-\right\rangle + \dots$$

$$N = \left\langle BCS\right|\hat{N}\left|BCS\right\rangle = 2\sum_{k>0}v_k^2$$

This is fit to the interpretation of v_k

BCS model

Hence, we need to restrict the variation by a supplementary condition. We define a parameter λ in the Hamiltonian to keep the expectation value of particle number to the desired particle number.

We add a term –λN to Hamiltonian:

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

We call this Lagrange multiplier λ as Fermi energy or chemical energy, since it describes the energy variation in the system by changing the particle number.

BCS model-Pure pairing force

Hamiltonian has a the form:

$$\sum_{k>0} \varepsilon_k a_k^+ a_k + \sum_{kk'>0} \left\langle k, \bar{k} \left| v \right| k', \bar{k}' \right\rangle a_k^+ a_{\bar{k}}^+ a_{\bar{k}'} a_{k'}$$

Single-particle part $v_{k\bar{k}k'\bar{k}'}$ Residual interaction acting on pairs of nucleons

In this model we assume a constant matrix elements – G (pure pairing force):

$$H = \sum_{k>0} \varepsilon_k a_k^+ a_k - G \sum_{kk'>0} a_k^+ a_{\bar{k}}^+ a_{\bar{k}'} a_{k'}$$

BCS model- Pure pairing force

Lets consider the Hamiltonian with the variational condition

$$H = \sum_{k>0} \varepsilon_k a_k^+ a_k - G \sum_{kk'>0} a_k^+ a_{\bar{k}}^+ a_{\bar{k}'} a_{k'}$$

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

The expectation value:

$$\langle BCS|\hat{H}'|BCS\rangle = 2\sum_{k>0}(\varepsilon_k^0 - \lambda)v_k^2 - \sum_{k>0}Gv_k^4 - G\underbrace{\left(\sum_{k>0}u_k v_k\right)}_{\Delta}^2 \qquad \boxed{\Delta = G\sum_{k>0}u_k v_k}$$

The matrix elements are:

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

$$\langle \mathrm{BCS}|\hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k'} \hat{a}_{k'}|\mathrm{BCS}\rangle = \begin{cases} u_k v_k u_{k'} v_{k'} & \text{for } k \neq k' \\ v_k^4 & \text{for } k = k' \end{cases}$$

BCS model- Pure pairing force

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

v_k determines the BCS wave function completely, we can express u_k in terms of v_k by the normalization condition

$$\delta \langle BCS | \hat{H}' | BCS \rangle = 0,$$

$$\left(\frac{\partial}{\partial v_k} + \frac{\partial u_k}{\partial v_k} \frac{\partial}{\partial u_k} \right) \langle BCS | H' | BCS \rangle = 0$$

BCS model-Pure pairing force

Finally the expectation value:

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

Differentiate this with respect to v_k:

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

Equations for different k are coupled by Δ

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

BCS model

We get for BCS equations the following:

$$\varepsilon_k = \varepsilon_k^0 - \lambda - \underbrace{G \cdot v_k^2}_{\text{often neglected}}$$

$$2\bar{\varepsilon}_k v_k u_k + \Delta(v_k^2 - u_k^2) = 0$$

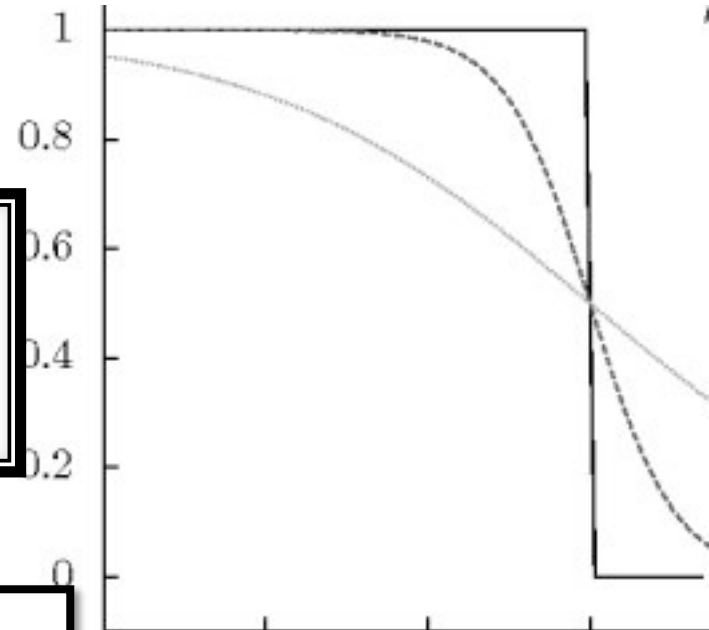The occupation probability (assume we know Δ):

$$v_k^2 = \frac{1}{2}\left(1 \pm \sqrt{1 - \frac{\Delta^2}{\varepsilon_k^2 + \Delta^2}}\right) = \frac{1}{2}\left(1 \pm \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}}\right)$$

Insert this into definition of gap we can get this iterative equation.

Gap equation:

$$\Delta = \frac{G}{2}\sum_{k>0}\frac{\Delta}{\sqrt{\varepsilon_k^2 + \Delta^2}}$$

Results of BCS model

- In the special case of a single j-shell all ε_k are equals so all v_k^2's are equals. From the particle-number condition we get

$$\left\langle BCS \middle| \hat{N} \middle| BCS \right\rangle = 2 \sum_{k>0} v_k^{\,2} = N \Rightarrow v_k = \sqrt{\frac{N}{2\Omega}}, u_k = \sqrt{1 - \frac{N}{2\Omega}}$$

$$\Delta = G \cdot \sqrt{\frac{N}{2}\left(\Omega - \frac{N}{2}\right)}$$

- The gap has a parabolic dependence on the number of particle in the shell. It is zero for empty or filled shells.

- For N=Ω: $$2\Delta = G \cdot \Omega$$

Ω is the number of pairs

Trivial solution

$$\Delta = 0$$

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

$$= 0 \quad (\epsilon_\nu > \lambda)$$

Superfluid solution

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

$$v_\nu^2 = \frac{1}{2}\left(1 + \frac{\epsilon_\nu - \lambda}{\sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}}\right) < 1$$
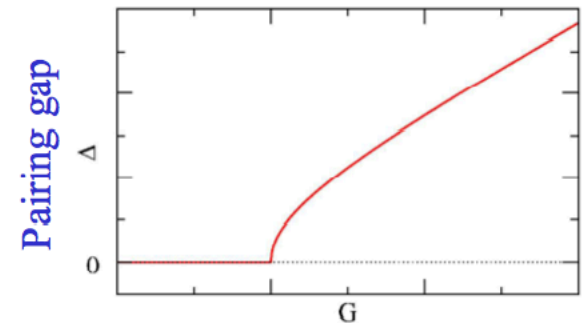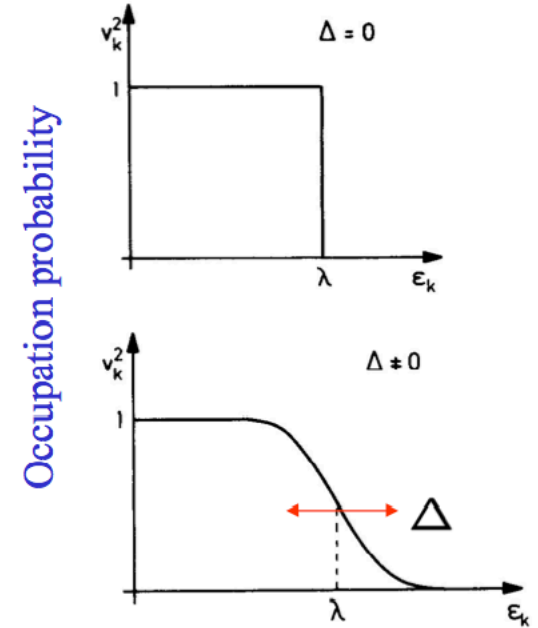
Norma-Superfulid phase transition

The BCS many-body wavefunction captured the essence of a new state of matter. It contained the important concept of "off diagonal long range order".

"that didn't conserve the number of electrons. It was a variable number of electrons and that had worried me, I remember. And so I decided, "Well, what I should do is multiply that wave function by a term involving e to minus the number of particles and — just like in the grand canonical ensemble in statistical mechanics — sort of extend that idea to the wave function in quantum mechanics.""

Other pairing models

Cautious: can be complicated.
Just for those who are interested.

Exact diagonalization

- Shell model calculations restricted to the v=0 subspace
- There are as many independent solutions as states in the v=0 space.
- **Valid for any forms of pairing.**

$$\langle \{s_j\}, \ldots N_j + 2, \ldots N_{j'} - 2, \ldots |$$
$$\times H | \{s_j\}, \ldots N_j, \ldots N_{j'}, \ldots \rangle$$
$$= \frac{G_{jj'}}{4} \big[(N_{j'} - s_{j'})(2\Omega_{j'} - s_{j'} - N_{j'} + 2)$$
$$\times (2\Omega_j - s_j - N_j)(N_j - s_j + 2) \big]^{1/2}.$$
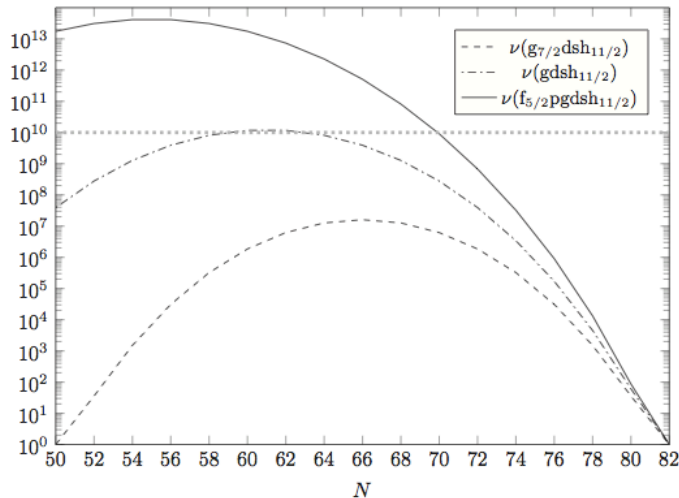
10^2 in seniority space
Easier to include many shells

Richardson's approach
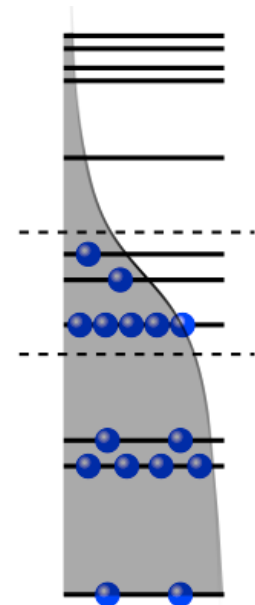
A RESTRICTED CLASS OF EXACT EIGENSTATES OF THE PAIRING-FORCE HAMILTONIAN *

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$$H_P = \sum_k \varepsilon_k n_k + g \sum_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$|\Psi\rangle = \prod_{\alpha=1}^{M} \Gamma^\dagger_\alpha |0\rangle, \quad \Gamma^\dagger_\alpha = \sum_k \frac{1}{2\varepsilon_k - E_\alpha} c^+_{k\uparrow} c^+_{-k\downarrow}$$

Richardson equation

$$1 + g \sum_{k=0} \frac{1}{2\varepsilon_k - E_\alpha} + 2g \sum_{\beta(\neq\alpha)=1}^{M} \frac{1}{E_\alpha - E_\beta} = 0, \quad E = \sum_{\alpha=1}^{M} E_\alpha$$

Richardson equation

• A set of *M* nonlinear coupled equations with *M* unknowns (E_α) and it is very difficult to solve.

• The pair energies are either real or complex conjugated pairs and do not have clear physical meaning.

• The wave function is not given directly

$$1 + g \sum_{k=0} \frac{1}{2\varepsilon_k - E_\alpha} + 2g \sum_{\beta(\neq\alpha)=1}^{M} \frac{1}{E_\alpha - E_\beta} = 0, \quad E = \sum_{\alpha=1}^{M} E_\alpha$$

For two pairs in a single-j shell

$$E_\alpha = -(\Omega - 1)g \pm i\sqrt{\Omega - 1}\,g$$

Hartree-Fock-Bogoliubov HFB

- A generalized single-particle picture which look for the most general product wave functions consisting of independent quasi-particles.

- A simple method of constructing the excited states of the nucleus as quasi-particle excitations

- Contain both long range interaction ph and short range interaction pp, unifies Hartree-Fock with BCS theory
  - HF gives rise to self-consistent field Γ which leads to deformation of ground state
  - BCS gives pairing correlations which the sum of Δ leads to a superfluid state.

- The basic idea of any quasi-particle concepts is to represent the ground state as vacuum with respect to quasi-particles. The basic idea in HFB is to use BCS state as vacuum.

$$\alpha_k |BCS\rangle = 0$$

Bogoliubov transformation

- Landau and Migdal defined the vacuum and the quasi-particles as exact eigenstates of many-body system, however, there is no simple relation between quasi-particle and "bare" particle
  - Bare particles are given by some basic creation/annihilation operator e.g. plane waves and HO sates
- Hence we use Bogoliubov quasi-particle: linear connection to the bare particles
  - Natural extension of BCS
  - Easy to handle
  - Not exact solution, only approximation

Bogoliubov transformation

A general linear transformation from the particle operator c_l and c_l^+ to the quasi-particle operator β_k^+ β_k (Hermitian conjugate)

Indices l and k run over whole configuration space

$$\beta_+^k = \sum^l \cap^{lk} c_+^l + \Lambda^{lk} c^l$$

$$\begin{pmatrix} \beta \\ \beta^+ \end{pmatrix} = \begin{pmatrix} U^+ & V^+ \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^+ \end{pmatrix} = W^+ \begin{pmatrix} c \\ c^+ \end{pmatrix}$$

The operators β_k^+ β_k should obey the fermion commutation relations so W should be unitary and we get some conditions on U and V

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

$$U^+ U + V^+ V = 1, \quad UU^+ + V^* V^T = 1$$

$$U^T V + V^T U = 0, \quad UV^+ + V^* U^T = 0$$

Also we can invert c_l^+ in terms of quasi-particle operators:

$$c_l^+ = \sum_k U_{lk}^* \beta_k^+ + V_{lk} \beta_k$$

Bogoliubov transformation

<u>Theorem of Bloch & Messiah</u>: The unitary matrix W can be decomposed as

$$W = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \overline{U} & \overline{V} \\ \overline{V} & \overline{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix}$$

Defines fully occupied levels i
Empty levels m and paired level p

$$\underbrace{\begin{matrix} c \rightarrow a \\ c^+ \rightarrow a^+ \end{matrix}}_{D} \quad \underset{\overrightarrow{\overline{U},\overline{V}}}{} \quad \underbrace{\left\{\begin{matrix} \alpha \rightarrow \beta \\ \alpha^+ \rightarrow \beta^+ \end{matrix}\right.}_{C}$$

$$\overline{U} = \begin{pmatrix} 0 & & & & & & & & & \\ & \ddots & & & & & & & & \\ & & 0 & & & & & & & \\ & & & u_1 & 0 & & & & & \\ & & & 0 & u_1 & & & & & \\ & & & & & \ddots & & & & \\ & & & & & & u_n & 0 & & \\ & & & & & & 0 & u_n & & \\ & & & & & & & & 1 & \\ & & & & & & & & & \ddots \\ & & & & & & & & & & 1 \end{pmatrix}$$

$$\overline{V} = \begin{pmatrix} 1 & & & & & & & & & \\ & \ddots & & & & & & & & \\ & & 1 & & & & & & & \\ & & & 0 & v_1 & & & & & \\ & & & v_1 & 0 & & & & & \\ & & & & & \ddots & & & & \\ & & & & & & 0 & v_n & & \\ & & & & & & v_n & 0 & & \\ & & & & & & & & 0 & \\ & & & & & & & & & \ddots \\ & & & & & & & & & & 0 \end{pmatrix}$$

Bogoliubov transformation

Meaning of this decomposition:

1. A unitary matrix D defines canonical basis, we still have particle picture

$$a_k^+ = \sum_l D_{lk} c_l^+$$

2. Application of Bogoliubov transformation (generate Bogoliubov quasi-particles)

$$\left.\begin{aligned}\alpha_p^+ &= u_p a_p^+ - v_p a_{\bar{p}} \\ \alpha_{\bar{p}}^+ &= u_p a_{\bar{p}}^+ + v_p a_p\end{aligned}\right\} (p,\bar{p}) \; paired \; levels \; 2 \times 2 \; boxe$$

$$Blocked \; levels : \begin{cases}\alpha_i^+ = a_i, & \alpha_m^+ = a_m^+ \\ \alpha_i = a_i^+, & \alpha_m = a_m\end{cases}$$

3. Application of unitary matrix C transform quasi-particle basis.

$$\beta_k^+ = \sum_{k'} C_{kk'} \alpha_{k'}^+$$

HFB-vacuum

- Ground state of the many-body system defines as vacuum with respect to quasi-particles.

$$\beta_k \underbrace{\left|\Phi\right\rangle}_{HFB-wf} = 0, \quad k = 1...M \qquad \underbrace{\left|\Phi\right\rangle}_{HFB-wf} = \prod_k \beta_k \left|-\right\rangle$$

- We start with bare vacuum and multiply by a product of annihilation operators β_k
  - Example GS of HF: the product runs over the annihilation operator of all hole states

$$\left|\Phi_{HF}\right\rangle = \prod_i \alpha_i \left|-\right\rangle = \prod_i a_i^+ \left|-\right\rangle$$

Derivation of the HFB equation

- Now we want to find U and V which defines the quasi-particle operators and the wave function Φ

- Many-body system Hamiltonian:

$$H = \sum_{k_1 k_2} t_{k_1 k_2} c_{k_1}^+ c_{k_2} + \frac{1}{2} \sum_{k_1 k_2 k_3 k_4 <>0} v_{k_1 k_2 k_3 k_4} c_{k_1}^+ c_{k_2}^+ c_{k_4} c_{k_3}$$

- We assume that Φ is the trial solution to this Hamiltonian and use variation principle.

- Again we need to constrain H with subsidiary condition to conserve number of particle N.

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

Derivation of HFB equations

- We have to vary the energy expectation value

$$\delta \frac{\langle \Phi | \hat{H}' | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0$$

- With respect to the matrices U and V this variation is not convenient.

- We use <u>Thouless theorem</u>: Let Φ be a single-particle state of HFB-type. Any other state Φ' that is not orthogonal to φ can be obtained via

$$\left| \Phi' \right\rangle = \left| \Phi \right\rangle + \left| \delta \Phi \right\rangle = \exp \left\{ \sum_{k<l} Z_{kl} \beta_l^+ \beta_k^+ \right\} \left| \Phi \right\rangle$$

Derivation of the HFB equations

Using quasi-particle representation for the Hamiltonian. Expand energy expectation value up to quadratic order for infinitesimal variations.

$$\hat{H}' = U + \hat{H}_{11} + \hat{H}_{20} + \hat{H}_{40} + \hat{H}_{31} + \hat{H}_{22}$$

The linear term in Z vanishes (require H^{20}=0)

Two indices H$_{ij}$ denote the number of creation and annihilation operators

$$\left. \frac{\partial}{\partial Z} \frac{\left\langle \Phi' \middle| \hat{H}' \middle| \Phi' \right\rangle}{\left\langle \Phi' \middle| \Phi' \right\rangle} \right|_{Z=0} = H_{20} = 0$$

- U is the energy of the BCS ground state with zero quasi-particle
- H$_{11}$ indicates the dependence of the energy of quasi-particle and quasi-hole excitation
- H$_{20}$ violates quasi-particle number conservation and even implies that the BCS state will not be true ground state
- Higher terms can be neglected

Derivation of HFB equation

- The requirement $H^{20}=0$ determines the first two transformations (U and V coefficients). The third transformation comes from diagonalization of H^{11}

This corresponds
to diagonalization of this super-matrix:
$$\begin{pmatrix} H_{11} & H_{20} \\ -H_{20}^* & -H_{11}^* \end{pmatrix}$$

- This yields the HFB equations in the space of the basis operators c_l and c_l^+:

$$H = W \begin{pmatrix} H_{11} & H_{20} \\ -H_{20}^* & -H_{11}^* \end{pmatrix} W^+ = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

$$h_{kl} = t_{kl} + \underbrace{\sum_{ij} \bar{v}_{kilj} \rho_{ij}}_{\Gamma_{kl}} - \lambda \qquad \Delta_{kl} = \frac{1}{2} \sum_{ij} \bar{v}_{klij} \kappa_{ij}$$

Result of HFB

- They are more or less like HF
- 2M-dimentional set of non-linear equations
- Difference with simple BCS: the coupling of the occupation numbers and the self-consistency problem
- HFB is capable to describe all phase transition within mean field approximation
- HFB calculation are valuable to compute bulk properties for nuclei such as masses, deformation, radii etc. across nuclear chart.