

Chapter 7

Mean field, BCS solution of pairing

The pairing interaction correlates pairs of nucleons moving in time reversal states (Cooper pairs) over lengths of the order of $\xi = \hbar v_F / E_{corr}$, much larger than nuclear dimensions (cf. e.g. [?]), in keeping with the fact that the associated two-nucleon correlation energy is $E_{corr} \approx 0.5\text{--}2$ MeV. The presence of these extended, strongly overlapping virtual objects, known as Cooper pairs, affect most of the properties of nuclei close to their ground state, as well as of their decay. This is a natural consequence of the fact that Cooper pair formation and their eventual condensation (also virtual), not only introduces a new energy length (pairing gap) over which the Fermi energy becomes blurred like in the case of an effective (quantal) temperature, but above all it changes the statistics of the associated degrees of freedom. An example of the central role pairing correlations have on the properties of atomic nuclei is provided by the exotic decay $^{223}\text{Ra} \rightarrow ^{209}\text{Pb} + ^{14}\text{C}$. The measured decay constant $\lambda = 4.3 \times 10^{-16}\text{s}^{-1}$, implies that the wavefunction describing the ground state of the superfluid nucleus ^{223}Ra has a component of amplitude of about 10^{-5} corresponding to a shape closely resembling ^{209}Pb in contact with ^{14}C . But this requirement can be fulfilled only if this exotic, strongly deformed system, is superfluid. In other words, if pairs of nucleons are correlated over distances of the order of 20 fm, sum of the Pb and C diameters [?].

7.0.1 Pairing correlations

Nuclear superfluidity can be studied at profit in terms of the mean field, BCS diagonalization of the pairing Hamiltonian [?], namely,

$$H = H_{sp} + V_p, \quad (7.1)$$

where

$$H_{sp} = \sum_{\nu} (\epsilon_{\nu} - \lambda) a_{\nu}^{\dagger} a_{\nu}, \quad (7.2)$$

while

$$V_p = -\Delta(P^{\dagger} + P) - \frac{\Delta^2}{G}, \quad (7.3)$$

and

$$\Delta = G\alpha_0, \quad (7.4)$$

is the pairing gap ($\Delta \approx 12 \text{ MeV}/\sqrt{A}$), $G (\approx 25 \text{ MeV}/A)$ being the pairing coupling constant [?], and

$$P^+ = \sum_{\nu>0} P_\nu^+ = \sum_{\nu>0} a_\nu^+ a_{\bar{\nu}}^+, \quad (7.5)$$

$$P = \sum_{\nu>0} a_{\bar{\nu}} a_\nu, \quad (7.6)$$

are the pair addition and pair removal operators, a_ν and a_ν^+ being single-particle creation and annihilation operators, $(\nu\bar{\nu})$ labeling pairs of time reversal states.

The BCS ground state wavefunction describing the most favorable configuration of pairs to profit from the pairing interaction, can be written in terms of the product of the occupancy probabilities h_ν for individual pairs,

$$|BCS\rangle = \Pi_\nu ((1 - h_\nu)^{1/2} + h_\nu^{1/2} a_\nu^+ a_{\bar{\nu}}^+) |0\rangle, \quad (7.7)$$

where $|0\rangle$ is the fermion vacuum.

Superfluidity is tantamount to the existence of a finite average value of the operators (7.5), (7.6) in this state, that is, to a finite value of the order parameter

$$\alpha_0 = \langle BCS | P^+ | BCS \rangle = \langle BCS | P | BCS \rangle^*, \quad (7.8)$$

which is equivalent to Cooper pair condensation. In fact, α_0 gives a measure of the number of correlated pairs in the BCS ground state. While the pairing gap (7.4) is an important quantity relating theory with experiment, α_0 provides the specific measure of superfluidity. In fact, the matrix elements of the pairing interaction may vanish for specific regions of space, or in the case of specific pairs of time reversal orbits, but this does not necessarily imply a vanishing of the order parameter α_0 , nor the obliteration of superfluidity.

In keeping with the fact that Cooper pair tunneling is proportional to $|\alpha_0|^2$, this quantity plays also the role of a ($L = 0$) two-nucleon transfer sum rule, sum rule which is essentially exhausted by the superfluid nuclear $|BCS\rangle$ ground state (see Fig. 3). Within the above context, one can posit that two-nucleon transfer reactions are the specific probes of pairing in nuclei.

7.0.2 Fluctuations

The BCS solution of the pairing Hamiltonian was recasted by Bogoliubov [?] and Valatin [?] in terms of quasiparticles,

$$\alpha_\nu^+ = U_\nu a_\nu^+ - V_\nu a_{\bar{\nu}}, \quad (7.9)$$

linear transformation inducing the rotation in (a^+, a) -space which diagonalizes the Hamiltonian (7.1).

The variational parameters U_ν, V_ν appearing in the above relation indicate that α_ν^+ acting on $|0\rangle$ creates a particle in the state $|\nu\rangle$ which is empty with a probability $U_\nu^2 \equiv (1 - h_\nu)$, and annihilates a particle in the time reversal state $|\bar{\nu}\rangle$ (creates a hole) which is occupied with probability $V_\nu^2 (\equiv h_\nu)$. Thus,

$$|BCS\rangle = \Pi_{\nu>0} (U_\nu + V_\nu a_\nu^+ a_{\bar{\nu}}^+) |0\rangle, \quad (7.10)$$

is the quasiparticle vacuum, as $|BCS\rangle \sim \Pi_\nu \alpha_\nu |0\rangle$, the order parameter being

$$\alpha_0 = \sum_{\nu>0} U_\nu V_\nu. \quad (7.11)$$

Making use of these results (see also App. (Chapter 7 derivation spectroscopic amplitudes)) we collect in Table 1 the spectroscopic amplitudes associated with the reactions $^{A+2}\text{Sn}(p,t)^A\text{Sn}$, for A in the interval 112-126, as well as the spectroscopic amplitudes of other pairing vibrational modes (see below as well as [?, ?]).

The BCS number and gap equations are,

$$N = 2 \sum_{\nu>0} V_\nu^2, \quad (7.12)$$

$$\frac{1}{G} = \sum_{\nu>0} \frac{1}{2E_\nu}, \quad (7.13)$$

where

$$V_\nu = \frac{1}{\sqrt{2}} \left(1 - \frac{\epsilon_\nu - \lambda}{\epsilon_\nu} \right)^{1/2}, \quad (7.14)$$

$$U_\nu = \frac{1}{\sqrt{2}} \left(1 + \frac{\epsilon_\nu - \lambda}{\epsilon_\nu} \right)^{1/2}, \quad (7.15)$$

while the quasiparticle energy is defined as

$$E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}. \quad (7.16)$$

7.0.3 Pairing rotations

The phase of the ground state BCS wavefunction may be chosen so that $U_\nu = |U_\nu| = U'_\nu$ is real and $V_\nu = V'_\nu e^{2i\phi}$ ($V'_\nu \equiv |V_\nu|$). Thus [?, ?, ?],

$$|BCS(\phi)\rangle_{\mathcal{K}} = \Pi_{\nu>0} (U'_\nu + V'_\nu e^{-2i\phi} a_\nu^+ a_{\bar{\nu}}^+) |0\rangle = \Pi_{\nu>0} (U'_\nu + V'_\nu a_\nu^+ a_{\bar{\nu}}^+) |0\rangle = |BCS(\phi=0)\rangle_{\mathcal{K}'}, \quad (7.17)$$

where $a_\nu^+ = e^{-i\phi} a_\nu^+$ and $a_{\bar{\nu}}^+ = e^{-i\phi} a_{\bar{\nu}}^+$. This is in keeping with the fact that a_ν^+ and $a_{\bar{\nu}}^+$ are single-particle creation operators which under gauge transformations (rotations in the 2D-gauge space of angle ϕ) induced by the operator $G(\phi) = e^{-i\hat{N}(\phi)}$ and connecting the intrinsic and the laboratory frames of reference \mathcal{K} and \mathcal{K}' respectively, behave according to $a_\nu^+ = \mathcal{G}(\phi) a_\nu^+ \mathcal{G}^{-1}(\phi) = e^{-i\phi} a_\nu^+$ and $a_{\bar{\nu}}^+ = \mathcal{G}(\phi) a_{\bar{\nu}}^+ \mathcal{G}^{-1}(\phi) = e^{-i\phi} a_{\bar{\nu}}^+$, a consequence of the fact that \hat{N} is the number operator and that $[\hat{N}, a_\nu^+] = a_\nu^+$.

The fact that the mean field ground state ($|BCS(\phi)\rangle_{\mathcal{K}}$) is a product of operators - one for each pair state - acting on the vacuum, implies that (7.17) represents an ensemble of ground state wavefunctions averaged over systems with $\dots N-2, N, N+2 \dots$ even number of particles. In fact, (7.17) can also be written in the form

$$\begin{aligned} |BCS\rangle_{\mathcal{K}} = & (\Pi_{\nu>0} U'_\nu) \left(1 + \dots + \frac{e^{-(N-2)i\phi}}{\left(\frac{N-2}{2}\right)!} \left(\sum_{\nu>0} c_\nu a_\nu^+ a_{\bar{\nu}}^+ \right)^{\frac{N-2}{2}} + \frac{e^{-Ni\phi}}{\left(\frac{N}{2}\right)!} \left(\sum_{\nu>0} c_\nu a_\nu^+ a_{\bar{\nu}}^+ \right)^{\frac{N}{2}} \right. \\ & \left. + \frac{e^{-(N+2)i\phi}}{\left(\frac{N+2}{2}\right)!} \left(\sum_{\nu>0} c_\nu a_\nu^+ a_{\bar{\nu}}^+ \right)^{\frac{N+2}{2}} + \dots \right) |0\rangle, \end{aligned} \quad (7.18)$$

where $c_\nu = V'_\nu / U'_\nu$.

Adjusting the Lagrange multiplier λ (chemical potential, see Eqs. (7.12-7.16)), one can ensure that the mean number of fermions (Eq. (7.12)) has the desired value N_0 .

Summing up, the BCS ground state is a wavepacket in the number of particles. In other words, it is a deformed state in gauge space defining a privileged orientation in this space, and thus an intrinsic coordinate system \mathcal{K}' [?, ?, ?]. The magnitude of this deformation is measured by α_0 .

7.0.4 Pairing vibrations

All the above arguments, point to a static picture of nuclear superfluidity which results from BCS theory. This is quite natural, as one is dealing with a mean field approximation. The situation is radically changed taking into account the interaction acting among the Cooper pairs (quasiparticles) which has been neglected until now, that is the term $-G(P^+ - \alpha_0)(P - \alpha_0)$ left out in the mean field (BCS) approximation leading to (7.3) [?, ?]. This interaction can essentially be written as (for details see e.g. [?] App. J)

$$H_{\text{residual}} = H'_p + H''_p, \quad (7.19)$$

where

$$H'_p = -\frac{G}{4} \left(\sum_{\nu>0} (U_\nu^2 - V_\nu^2)(P_\nu^+ + P_\nu) \right)^2, \quad (7.20)$$

and

$$H''_p = \frac{G}{4} \left(\sum_{\nu>0} (P^+ - P) \right)^2. \quad (7.21)$$

The term H'_p gives rise to vibrations of the pairing gap which (virtually) change particle number in ± 2 units. The energy of these pairing vibrations cannot be lower than 2Δ . They are, as a rule, little collective, corresponding essentially to almost pure two-quasiparticle excitations (see excited 0^+ states of Fig. 3).

The term H''_p leads to a solution of particular interest, displaying exactly zero energy, thus being degenerate with the ground state. The associated wavefunction is proportional to the particle number operator and thus to the gauge operator inducing an infinitesimal rotation in gauge space. The fluctuations associated with this zero frequency mode diverge, although the Hamiltonian defines a finite inertia. A proper inclusion of these fluctuations (of the orientation angle ϕ in gauge space) restores gauge invariance in the $|BCS(\phi)\rangle_{\mathcal{K}}$ state leading to states with fixed particle number

$$|N_0\rangle \sim \int_0^{2\pi} d\phi e^{iN_0\phi} |BCS(\phi)\rangle_{\mathcal{K}} \sim \left(\sum_{\nu>0} c_\nu a_\nu^+ a_\nu^+ \right)^{N_0/2} |0\rangle. \quad (7.22)$$

These are the members of the pairing rotational band, e.g. the ground states of the superfluid Sn-isotope nuclei. These states provide the nuclear embodiment of Schrieffer's ensemble of ground state wavefunctions which is at the basis of the BCS theory of superconductivity.

Summing up, while the correlations associated with H''_p lead to divergent fluctuations which eventually restore symmetry ($[H_{sp} + H''_p, \hat{N}] = 0$), H'_p gives essentially rise to non-collective particle number fluctuations, which are essentially pure two-quasiparticle states.

The situation is quite different in the case of normal systems, where pairing vibrations, namely the pair addition and pair removal modes [?, ?, ?], are strongly excited in two-particle transfer reactions (see Fig. 4). Let us elaborate on this point, making use

of the so called two-level model, in which the single-particle levels associated with occupied (empty) states are assumed to be degenerate and separated by an energy D . The parameter which measures the interplay between pairing correlations and shell effects is

$$x = \frac{2G\Omega}{D}, \quad (7.23)$$

where $G(\approx 25/A \text{ MeV})$ is the pairing coupling constant, while $\Omega = (2j+1)/2$ is the pair degeneracy of each of the two levels, assumed to be equal. Making use of the simple estimate of the spacing $D = 2/\rho$ between levels close to the Fermi energy in terms of the level density (for one type of nucleons, e.g. neutrons) $\rho = 3A/2\epsilon_F$ [?], one obtains $D = 4\epsilon_F/3A$ which for ^{120}Sn leads to $D \sim 0.4 \text{ MeV}$ (cf. e.g. [?] Ch. 2 and refs therein). Making use of the fact that the average pair degeneracy of the valence orbitals of ^{120}Sn is approximately 3, one obtains $x \approx 3$, implying that pairing effects overwhelm shell effects and the static (pairing rotational) view of Cooper pair condensation is operative.

On the other hand, in a closed shell system like, e.g., ^{208}Pb , $D \approx 3.4 \text{ MeV}$. Making use of the fact that the last occupied orbit in ^{206}Pb is a $p_{1/2}$ orbit, the first unoccupied being a $g_{9/2}$ level, one can use $\Omega = 5$ in calculating the value of x , which becomes $x = 0.35$. This value indicates that, in the present case, shell effects are dominant.

This does not mean that Cooper pairs are not present in the ground state of ^{208}Pb . It means that they break as soon as they are created as virtual states through ground state correlations. Testifying to this scenario is the fact that the expected $2p - 2h$ 0^+ state in ^{208}Pb at an energy of $2D \approx 6.8 \text{ MeV}$, is observed at 4.9 MeV . The difference between these two numbers corresponds almost exactly to the sum of the correlation energy of ^{208}Pb (gs) (0.640 MeV) and of ^{210}Pb (gs) (1.237 MeV). Thus, the first 0^+ excited state of ^{208}Pb corresponds to a two-phonons pairing vibrational state, product of the pair addition ($|^{210}\text{Pb}(gs)\rangle\rangle$) and of the pair removal ($|^{206}\text{Pb}(gs)\rangle\rangle$) modes of ($|^{208}\text{Pb}(gs)\rangle\rangle$).

In other words, we are in presence of an incipient attempt of condensation in terms of two correlated Cooper pairs, which, forced to be separated in two different nuclides by particle conservation, get together in the highly correlated two-phonon pairing vibrational state of ^{208}Pb . No surprise that its microscopic structure can also be, rather easily, calculated almost exactly, by diagonalizing a schematic pairing force $H_p = -GP^+P$, in the harmonic approximation (RPA). The two-nucleon transfer spectroscopic amplitudes associated with the reactions $^{206}\text{Pb}(t,p)^{208}\text{Pb}(gs)$, $^{206}\text{Pb}(^{18}\text{O},^{16}\text{O})^{208}\text{Pb}(gs)$, $^{48}\text{Ca}(t,p)^{50}\text{Ca}(gs)$, $^{10}\text{Be}(p,t)^8\text{Be}(gs)$ and $^9\text{Li}(p,t)^7\text{Li}(gs)$, and thus with the excitation (deexcitation) of pair addition and pair subtraction modes, are collected in Table 1. For details, cf. [?].

Properly adjusting G for a given value of particles N , one can make this excitation to coincide with twice the value given in Eq.(??). Also to correlate the ground state, by the amount needed to reproduce the odd-even staggering expressed by Eq.(??). This value is

$$G \approx \frac{25}{A} \text{ MeV}. \quad (7.24)$$

Making use of this value and of the empirical relation $\Delta = 12/\sqrt{A} \text{ MeV}$ one can write

$$\frac{\Delta^2}{G} \approx 5 \text{ MeV},$$

for the second term in Eq.(??). To be noted that this gain in binding energy, is partially compensated by and increase in single-particle energy associated with the first term

and due to the fractional occupation of the single-particle levels around the Fermi surface. The summed effect amounts to only about 1 MeV ($\approx \Delta$) of extra binding energy acquired by the even-even system due to pairing with respect to the odd-even system. This quantity, *which is very important to characterize the structure of a nucleus close to the ground state*, is still very small compared to the total binding energy of the system ($\approx A \times 8\text{MeV} \approx 1\text{GeV}$).

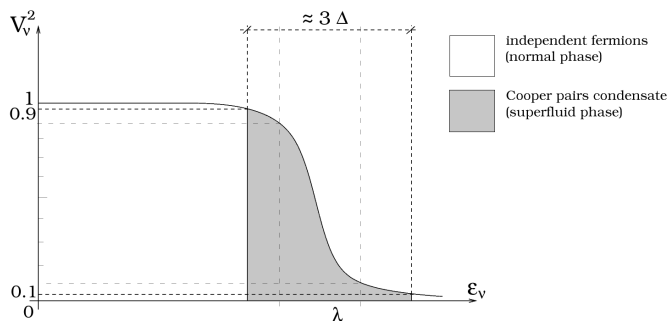


Figure 7.1: Schematic representation of the occupation of single particles of a non-interacting and of a superficial Fermi system, like e.g. nucleons.

In other words, a system of independent particles is affected only on a small region ($\approx 2\Delta$) around the Fermi energy as compared to this energy ($2\Delta/\lambda = 2\Delta/\varepsilon_F \approx 2 - 3\text{MeV}/36\text{MeV} \approx 0.1$). What is actually modified is the occupation of the single-particle levels around λ (cf. Fig. 7.1). For single-particle states fulfilling $|\varepsilon_v - \lambda| \gg 1.5\Delta$, the system retains the single-particle properties¹. For single-particle states such that $|\varepsilon_v - \lambda| \lesssim 1.5\Delta$, the occupancy of the levels are strongly modified and the system is composed of nucleons coupled to angular momentum $J = 0$ (singlet states, i.e. $S = 0$ and $L = 0$, $J = L + S$). These pairs are known as Cooper pairs, and behave like bosons (cf. App. A and Å, and Fig. 7.2). In nuclei, the number of Cooper pairs is small, typically 4 – 6². One would thus expect strong fluctuations of the associated pairing gap (cf. Ch. 10 and Ch. 13), fluctuations which may blur many of the sharp properties found in the case of infinite systems (bulk matter, thermodynamic limit).

Cooper pairs are strongly overlapping and, as befits bosons they occupy the same (lowest energy) state, known also as condensate (cf. Fig. 7.3). The only way to excite this condensate is by breaking a pair, that is, by providing the system with, at least, an energy of 2Δ . On the other hand, acting with an external field but providing an energy less than 2Δ , the condensed phase will not react, as the first quantal excited state has an energy of at least 2Δ .

In particular, if we set a deformed nucleus (cf. Sect. 2.1) into rotation ($\hbar\omega_{rot} < 2\Delta$) one would expect from the above picture the moment of inertia to be about $\frac{1}{2}\mathcal{I}_{rig}$, where \mathcal{I}_{rig} is the rigid (independent particle motion, situation in which the orbitals of

¹In connection with the discussion carried out after Eq. (100), we note that one can produce a particle-hole excitation based on the states with $|\varepsilon_v - \lambda| \gg 1.5\Delta$. Such an excitation would have an energy which is at least 3Δ , larger than that associated with the breaking of a Cooper pair.

²Making use of the BCS solution for a single j-shell, $\Delta = G\Omega/2$, $\Omega = j + 1/2$, for $N = \Omega$ (maximum value of Δ (cf. Ch. 12)). From the empirical values given in Eqs.(?) and (?), $\Omega = 2\Delta/G = (24/\sqrt{A} \text{ MeV})/(25/A \text{ MeV}) \approx \sqrt{A} \approx 10$ for medium heavy nuclei. Because $N = \Omega = 10$, one concludes that about ≈ 5 Cooper pairs participate in the nuclear pairing condensation.

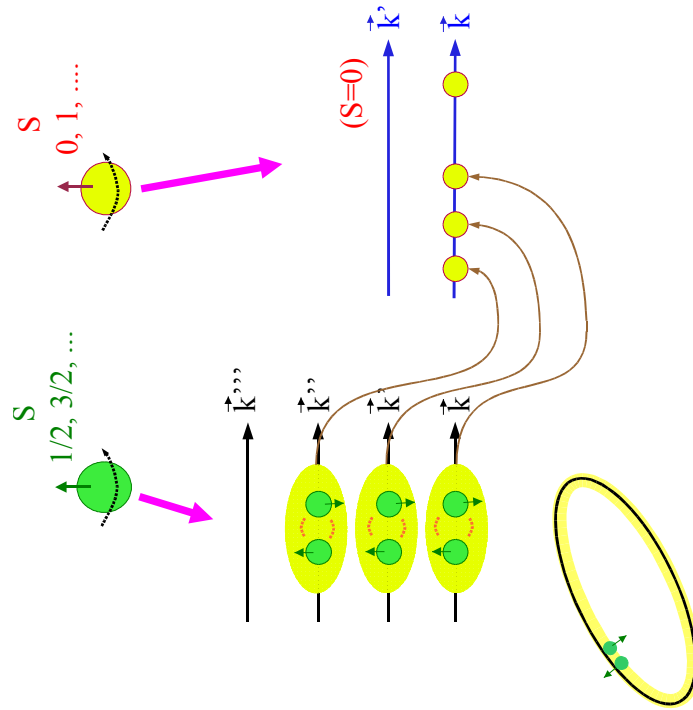


Figure 7.2: .

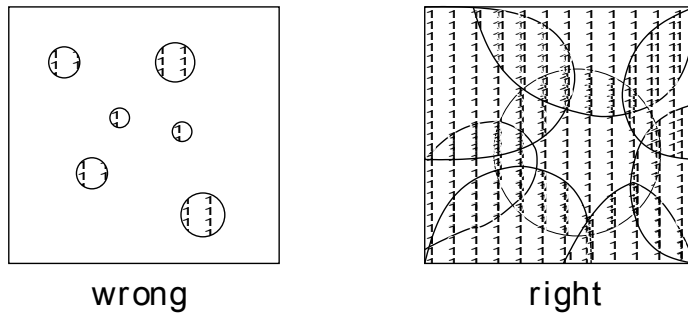


Figure 7.3: Schematic representation of the distribution of Cooper pairs (close dashed areas) in a superconducting (superfluid made out of fermions) system. To the left we display the so called Schafroth (independent) pair picture. To the right the (right) coherent picture, where Cooper pairs are strongly overlapping.

the nucleon are strongly anchored to the mean field) moment of inertia. This is because only the matter which is pushed directly by the walls will be set into motion, while the core which should be set into motion by "viscosity" will not react (cf. Fig. 7.4), as the system cannot be excited but by breaking a pair, thus by receiving at least an energy 2Δ .

From the energy difference between members of a rotational band, which can be accurately parametrized according to the relation (cf. Fig. ??)

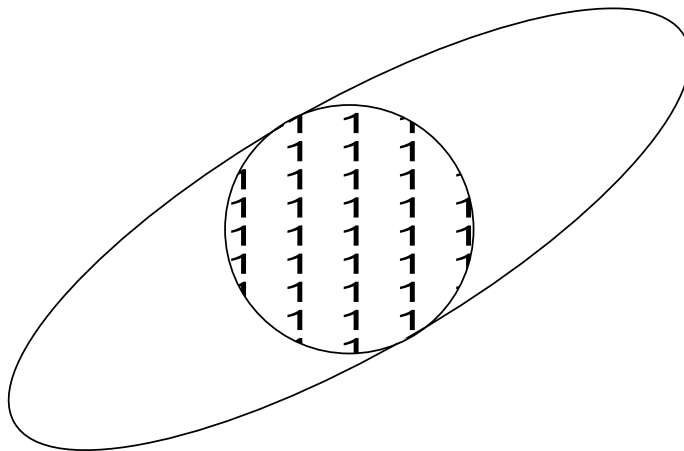


Figure 7.4: Schematic representation of the reaction to rotation of the superfluid matter filling a deformed nucleus.

$$\mathcal{E}_I = \frac{\hbar^2}{2\mathcal{I}} I(I+1), \quad (7.25)$$

one obtains a value of \mathcal{I} which, at low angular momenta, is as predicted by pairing theory, that is, about one half the rigid moment of inertia. In other words, the system can be viewed as a spheroidal container filled with a non-viscous fluid, that is, a superfluid. If one sets the nucleus into rotation, one would then expect to observe a phase transition from the superfluid phase to the normal phase at a rotational frequency in which $\hbar\omega_{rot}$ approximates the value 2Δ needed to break a Cooper pair (cf. Fig. 7.5). In fact, rotational bands have been observed, at very large values of the spin, displaying a rigid moment of inertia.

As we discuss below, the situation is however more subtle than just stated, and is associated with the fact that the nucleus is a zero-dimension superfluid (cf. Chapter 9), displaying strong quantal size effects (QSE), that is, a discrete single-particle spectrum close to the Fermi energy (cf. e.g. Fig. ??).

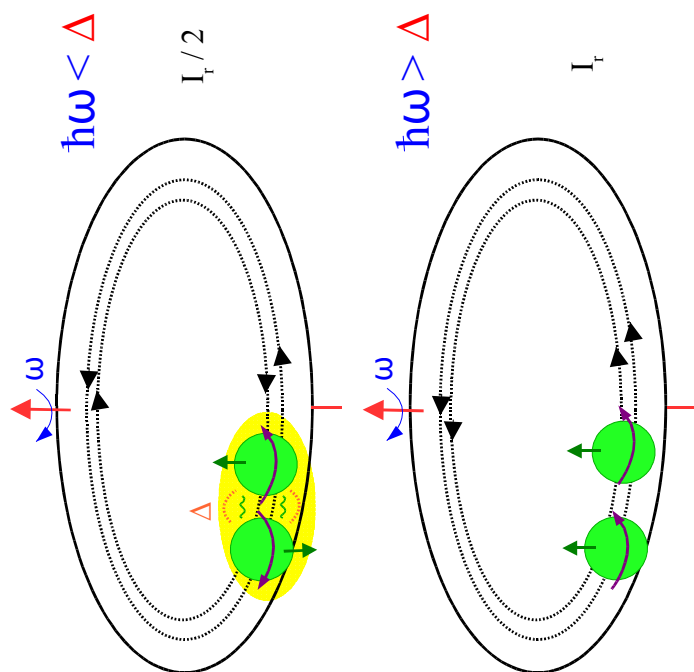


Figure 7.5: .