Mass Number Dependence of Nuclear Pairing.

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Abstract

Large scale Hartree-Fock-Bogoliubov (HFB) calculations with the finite-range Gogny force D1S have been performed in order to extract the corresponding theoretical average mass dependence of the nuclear gap values. Good agreement with experimental data from the three-point filter $\Delta^{(3)}(N)$ with $N$ odd has been found for both the neutron and proton gaps. The results of our study support earlier findings [W. Satu/suppress la, J. Dobaczewski, and W. Nazarewicz, Phys. Rev. Lett. 81 3599 (1998)] that the mass dependence of the gap is much weaker than the so far accepted $12A^{-1/2}$ MeV law.

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In recent years, the study of pairing properties in systems of condensed matter so small that the coherence length of the Cooper pairs becomes comparable with the size of the system has increased considerably. This is the case for ultra small superconducting metallic grains [1] but one also thinks that magnetically trapped fermionic atoms like $^6$Li can become superfluid at temperatures which may be reached experimentally in the near future [2]. A fermionic system of finite size where the superfluid properties have been studied experimentally and theoretically since decades is the atomic nucleus [3]. Very efficient mean field approaches have been developed in the past to account quantitatively for a great amount of experimental data. One of the most successfull models in this context is that developed by Gogny and collaborators.
with the use of a finite range effective interaction D1S [4,5]. However, the
global mass number (A) dependence of the gap has never been investigated in
a systematic way using this force. Such a study has now become particularly
timely because it has been observed [6] that the commonly accepted law for
the average gap parameter ($\Delta = 12A^{-1/2}$ MeV) strongly overestimates
the gap values in light nuclei. Empirical information concerning gap parameters
can be derived in principle from large-scale analysis of odd-even staggering
(OES) of nuclear binding energies. One should bear in mind, however, that
there are two basic physical mechanisms behind OES, namely: (i) an effect
of spontaneous breaking of spherical symmetry (Jahn-Teller mechanism [7] or
shape effect) and, (ii) the blocking of pair correlation by an unpaired fermion.
Determination of the pairing component of OES therefore requires a careful
deconvolution, at least to the extent possible, of both effects. Thus the aim
of this work is to demonstrate that the average gap parameters at the Fermi
surface deduced from large-scale unconstrained Gogny-HFB calculations are
consistent with component of OES deduced from empirical data according to
the method proposed in [6]. In particular, it will be shown that the theoretical
A dependence of the average gap is much weaker than $12/\sqrt{A}$ dependence
what is in coincidence with the experimental data analysis performed in [6].

The simplest way to quantify the OES of binding energies is to use the three-
point filter

$$\Delta^{(3)}(N) = \frac{\pi N}{2} [B(N - 1) + B(N + 1) - 2B(N)]$$  \hspace{1cm} (1)

where $\pi_N = (-1)^N$ is the number parity and $B(N)$ the (negative) binding
energy of the system of particle number $N$. Eq. (1) assumes proton number
$Z$ to be fixed and thus provides neutron OES. An expression appropriate for
proton OES can be obtained by replacing $N$ with $Z$ in Eq. (1) and by fixing
the neutron number $N$.

In nuclear structure studies, filter (1) is not considered as an appropriate
measure of the neutron or proton pairing gaps. This is mainly due to strong
symmetry energy [$B_{sym} \propto (N - Z)^2$] contributions. However, because sym-
metry energy is number-parity independent and rather weakly depends on
shell effects, its influence can be removed by using higher order filters like the
four-point formula:

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

Global analysis of empirical data using filter (2) leads to the commonly used es-
timate $\Delta = 12 A^{-1/2}$ MeV for the pairing gap [8]. This classical way of reason-
ing leading from formula (1) to (2) has its roots in the macroscopic-microscopic
model. It assumes [9] that the major contribution [apart from pairing] to (1) comes from the smooth liquid-drop component of the total energy (or more precisely from the symmetry energy term as mentioned above) while the shell-correction energy $\delta E_{\text{shell}}$ varies slowly enough with $N$ and $Z$ to neglect its contribution to (1) or (2). This assumption is, however, hardly acceptable because $\delta E_{\text{shell}}$ is by definition the difference between the strongly oscillating shell-energy, $E_{\text{sp}} = \sum_{\text{occup}} e_i$, and the smooth Strutinsky-smeared energy, $\tilde{E}_{\text{sp}}$. The single-particle (sp) shell-energy term, $E_{\text{sp}}$, gives rise to OES which is well recognized in metallic clusters [10]. In the extreme case of independent particles (fermions) filling two-fold Kramers-degenerated levels of a fixed, deformed potential well, the sp OES is $\Delta^{(3)}_{\text{sp}}(2n+1) \approx 0$ and $\Delta^{(3)}_{\text{sp}}(2n) \approx (e_{n+1} - e_n)/2$, where $e_n$ and $e_{n+1}$ stand for effective Nilsson levels at the Fermi energy [6].

In a previous study [6], it has been demonstrated, using self-consistent Skyrme-Hartree-Fock calculations, that the contribution to (1) due to the smooth Strutinsky energy, $\tilde{E}_{\text{sp}}$, nearly cancels out the contribution coming from the liquid-drop symmetry energy. Consequently, only $\Delta(N) \equiv \Delta^{(3)}(N = 2n + 1)$ can be considered as a probe of the pairing component of OES, while $\Delta^{(3)}(N = 2n)$ mixes both mean-field and pairing effects. Note, that filter (2) always mixes pairing and sp components whatever the number-parity is.

These ideas have recently been tested within a wide class of exactly solvable models invoking monopole pairing Hamiltonians [11,12]. Although these models do always oversimplify various properties of complex nuclei, these studies clearly indicate the correctness of the proposed method, particularly for weak and intermediate pairing correlations, which is by far the most commonly encountered situation in finite nuclei. In this case a consistency between the BCS (or HFB) pairing gap and the $\Delta^{(3)}(2n + 1)$ filter has been found as well.

We therefore think that $\Delta^{(3)}(N = 2n+1)$ is the best suited filter for the extraction of gap values from experimental data. One should be aware, however, that there is ongoing debate concerning detailed interpretation of $\Delta^{(3)}(N = 2n + 1)$ as well as higher order filters [$\Delta^{(5)}$] [13–15]. In particular, an effect of time-odd mean-field was intensively studied in Ref. [15]. This mean-field effect indeed enters directly empirical $\Delta^{(3)}(N = 2n + 1)$ [as well as $\Delta^{(4,5)}$] through odd-A nuclei and should, in principle, be removed explicitly. However, our knowledge concerning its magnitude is highly uncertain. For example, systematic Skyrme-Hartree-Fock calculations of Ref. [12] indicate attractiveness (repulsiveness) of this effect for SLy4 (SIII, SkM$^*$) respectively with average absolute magnitude of the order of 100keV in odd-A light nuclei.

Extensive HFB calculations have been performed in order to determine the ground state structure of nearly 400 even-even nuclei located in the neighborhood of those for which experimental pairing gaps have been extracted [6]. The D1S parameterization of the Gogny Force [4,5] has been employed throughout.
this work. Theoretical pairing gaps are then deduced from the pairing field obtained with this force in these nuclei, with the purpose of making comparisons with experimental gaps. It is of importance to point out that the calibration of the matrix elements of the Gogny force in the pairing channel has been based on OES in tin isotopes [4] and that the A dependence of the calculated pairing gaps is ultimately governed by self-consistency requirements of the HFB solutions.

According to the Bogoliubov theory [16], the quasiparticle states can be obtained from the iterative diagonalization of the HFB Hamiltonian

\[
H = \begin{pmatrix}
    h - \mu I & -\Delta \\
    -\Delta & -h + \mu I
\end{pmatrix},
\]

(3)

where \( h \) and \( \Delta \) are the matrices of the Hartree-Fock hamiltonian – the sum of the nucleon kinetic energy and average field – and of the pairing field in the HO basis, respectively, \( \mu \) represents the chemical potential ensuring conservation of nucleon numbers, and \( I \) is the unity matrix. Using time-reversal symmetry and appropriate phase conventions, \( h \) and \( \Delta \) can be taken as real symmetric matrices.

In order to derive from the HFB method theoretical quantities corresponding to empirical proton and neutron pairing gaps, the following technique is used. Single-particle energies \( \varepsilon_i \), pairing gaps \( \Delta_i \) and occupation probabilities \( v_i^2 \) analogous to those defined in BCS theory are first calculated. They can be derived by either diagonalizing the Hartree-Fock Hamiltonian \( h \), or expressing all relevant quantities in the canonical basis [17]. In the first case, the \( \varepsilon_i \) are taken as the eigenvalues of \( h \), and the \( \Delta_i \) and \( v_i^2 \) as the diagonal components of \( \Delta \) and of the one-body density matrix \( \rho \) once they are expressed in the Hartree-Fock representation. In the second case, the \( v_i^2 \) are the eigenvalues of \( \rho \), while the \( \Delta_i \) and \( \varepsilon_i \) are taken as the diagonal components of \( \Delta \) and \( h \) in the canonical basis. The two methods have been checked to yield very close single particle energies and practically identical values of the \( v_i^2 \) and \( \Delta_i \) [18]. In the present work, the first method has been employed, and we will assume that the above quantities have their usual physical meaning. When applied separately to each kind of nucleons, single particle quantities denoted \( \varepsilon_i^\pi, \Delta_i^\pi, v_i^\pi \) for protons, and \( \varepsilon_i^\nu, \Delta_i^\nu, v_i^\nu \) for neutrons can thus be derived for all nuclei under consideration.

Numbers representing the proton and neutron pairing gaps \( \Delta^\pi \) and \( \Delta^\nu \) in each nucleus have then been defined in two different ways. On the one hand, we define \( \Delta^\pi_{last} = \Delta^\pi_{i=Z} \) and \( \Delta^\nu_{last} = \Delta^\nu_{i=N} \), where \( i = Z \) (resp. \( i = N \)) is the \( Z \)th (resp. \( N \)th) proton (resp. neutron) state counted from the deepest one. On
the other hand, we define

\[ \Delta_{\text{aver}}^\pi = \sum_i u_i^{\pi 2} v_i^{\pi 2} \Delta_i^{\pi} / \sum_i u_i^{\pi 2} v_i^{\pi 2} \]  

(4)

and similarly for neutrons. In the second definition, the individual level gaps \( \Delta_i \) are averaged out around the Fermi surface, with weights equal to the pair correlation probability of the two nucleons on each level. The purpose of this averaging is to smear out the sometimes large fluctuations \( \approx 100 \text{ keV} \) obtained for the individual \( \Delta_i \)'s in the vicinity of the Fermi surface. The gaps derived from the two methods are both functions of the nucleus proton and neutron numbers \( Z \) and \( N \).

Finally, as in Ref. [6], proton (resp. neutron) pairing gaps averaged over \( N \) (resp. \( Z \)) are defined as

\[ \overline{\Delta_{\text{type}}^\pi}(Z) = \frac{1}{M} \sum_{N=N_1,N_2,...,N_M} \Delta_{\text{type}}^\pi(N,Z). \]  

(5)

where type is either last or aver. We have decided to compare experimental \( \Delta^{(3)} \)'s with the pairing gaps of Eq.(5) instead of theoretical \( \Delta^{(3)} \)'s because the D1S Gogny force has not been designed to reproduce masses of odd-even or odd-odd nuclei. Indeed, HFB calculations do not account for particle-vibration coupling (which is known to be responsible for a decrease of a few hundreds of keV of the odd-even or odd-odd nuclei masses) but correctly describe even-even nuclei pairing properties.

The theoretical gaps given by Eq.(5) are displayed in Figs. 1 and 2 together with the corresponding experimental data. It is important to mention here that even if theoretical calculations have been performed for even-even nuclei, we have deliberately plotted the gaps as function of the odd-\( Z \) (resp. odd-\( N \)) values (the same as those used in [6] to extract experimental data) from which the neighboring even-even nuclei studied theoretically have been selected.

In view of the great sensitivity of the gap with respect to all input parameters (force, effective mass, etc ...) there is an excellent overall agreement of the theoretical quantities with experiment. The \( A^{-1/3} \)-law in the fits of Figs. 1 and 2 has no particular deep theoretical fundation (see, however the remarks made in connection with Fig. 3) and other \( A \)-dependences can represent the average trend as well. This average behavior makes it however clear that the \( A \)-dependence of the gaps is much weaker than the \( \Delta = 12 A^{-1/2} \text{ MeV} \) law previously assumed. This finding is very satisfying as these theoretical results give further credit to the analysis of experimental data in [6] also concluding that the \( A \) dependence of the gap is weaker than the \( \Delta = 12 A^{-1/2} \text{ MeV} \) law.
For magic numbers, theoretical gaps go to zero, since there is no pairing. In this case, the $\Delta^{(3)}$ value deduced from experiment does not really describe a pairing effect, but rather an average of single-particle gaps around shell closures. Theoretical $\Delta$'s agree particularly well with experimental ones in mid-shell nuclei where experimental $\Delta^{(3)}$'s represent a genuine pairing effect. For these reasons, we did not include in the theoretical average, the nuclei having a magic number of protons or neutrons.

In Fig. 1, one notices that theoretical $\Delta_{\text{aver}}$ overestimate experimental data. One reason is the absence, in our calculations, of the Coulomb Interaction in the pairing field since it would require too much computing time. However, we have checked for a couple of nuclei that including it reduces the gap-values by 100 to 200 keV, depending on the nucleus proton number, thus improving the agreement with the experimental data.

Other sources of uncertainty may partly be accounted for through the effective force. This is likely to be the case for the recently debated influence of surface vibrations on nuclear pairing [19,20] which is claimed to give a sizeable contribution to nuclear superfluidity. Since, however, the gap values calculated from the D1S Gogny force are quite realistic (see Figs. 1 and 2), it is justified to assume that the Gogny force accounts for such effects at least on the average.

In view of the good agreement of experiment and theory found in Figs. 1 and 2, we further investigate the average trend of the theoretical Gogny-HFB gap values versus $A$. For this purpose, we define $\Delta_N$ for a given $N$ as an arithmetic average over several $Z$-values – taken in an interval so that the nucleus $(Z,N)$ belongs either to what we call the stability valley (SV) or the neutron rich region (NR) – of the theoretical $\Delta_{\text{aver}}$. Noticing that the relation [21] $Z_s = A/(1.98 + 0.0155A^{2/3})$ almost perfectly defines the most stable nuclei, the SV and NR are defined as the region $0.94Z_s \leq Z \leq 1.05Z_s$ and $Z \leq 0.94Z_s$, respectively. In order to further smoothen the curves, we also average the mean $\Delta_N$’s together with the $\Delta_{N \pm 1}$’s and $\Delta_{N \pm 2}$’s. The width $\Delta N = 8$ of this last average should be small enough not to affect significantly the mean trends. Finally, this procedure gives us the full black squares in Fig. 3. It is important to mention that for nuclei close to drip lines, the method used to solve the HFB equations does not allow us to include continuum effects. In order to test the validity of our results for such nuclei, we have checked that their pairing properties are stable with respect to a large increase of the harmonic oscillator basis. This test consists in introducing quite a different representation of unbound orbitals and therefore the observed stability indicates that our theoretical $\Delta$’s are not significantly sensitive to continuum effects.

From the obtained curve in Fig. 3(a), one again clearly sees that the old $\Delta = 12A^{-1/2}$ MeV law strongly overestimates the average trend, at least for small $A$. We also inserted our least square fit assuming a $\Delta_N = \alpha + \beta A^{-1/3}$ law.
Justification for this choice stems from the weak coupling approximation for the gap, i.e. \( \Delta \propto \exp(-1/G, \rho) \), where \( G \propto 1/A \) is the usual constant pairing matrix element and \( \rho \propto A(1 + cA^{-1/3}) \) the level density at the Fermi energy [3]. Indeed, performing a Taylor-expansion in powers of the small parameter \( c \) yields the above mentioned law for \( \Delta \). It is also worth mentioning that such a mass dependence of the pairing gap has also been obtained in ref. [22] (see also ref [23]). The best fit values for Fig. 3(a) are found to be \( \alpha = 0.3 \) and \( \beta = 3.1 \). Calculation indicate slightly different trends for \( \Delta_N \) in SV and NR regions. In particular for Fig. 3(b) we find \( \alpha = 0.35 \) and \( \beta = 2.6 \). The asymptotic value is rather close to the nuclear matter value \( \Delta_{nm} = 0.4 \) MeV obtained with the Gogny Force [24].

The fact that in Fig. 3(b) rather large \( \Delta_N \) values for large \( N \) are found is likely an indication of the increasing role of the neutron skin. Similar tendencies are obtained for the proton gaps (not shown). The different average trends seen in Figs. 2 and 3 (in particular for low \( N \) values) are due to the fact that in Fig. 2 all experimentally available data are taken into account irrelevant whether they correspond to stable or exotic nuclei whereas in Fig. 3 two regions have been sorted out. Our choice \( \Delta_N = \alpha + \beta A^{-1/3} \) is certainly not unique but the \( A^{-1/3} \) dependence, besides having some theoretical justification as explained above, yields overall the best results among the various choices we tried. For example, an improved fit with different parametrisation can be obtained in Fig. 3(a), but there is no point in making a separate fit for each figure.

The increase of the gap with decreasing size of the nucleus may eventually be a rather generic feature in meso- and nano-scopic systems. Indeed, also in small superconducting metallic grains and in thin superconducting films there seems to be a tendency for increasing gap-values as the size of the system is reduced [25]. Whether the physical origin of the effect is the same in all cases remains to be seen.

In summary we investigated the mass dependence of the average gap values for neutrons and protons in large scale HFB calculations with the Gogny D1S effective interaction. Very good agreement with the experimental filter \( \Delta^{(3)}(N = 2n + 1) \) is found. This indicator was advocated previously [6] for its capability to eliminate spurious mean field components from the gap values in an optimal way. The present theoretical study therefore supports the much weaker dependence of the gap, advanced in [6], than the so far accepted \( \Delta = 12A^{-1/2} \) MeV law. The agreement between experimental and theoretical size dependence of \( \Delta \) is a non trivial fact and this study may open similar investigations in other finite superfluid or superconducting systems.

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Fig. 1. Comparison between experimental and theoretical proton pairing gaps plotted as functions of the proton number $Z$. Squares represent experimental gaps extracted with the filter $\Delta^{(3)}$. Stars and circles are the corresponding theoretical values $\Delta_{\text{last}}$ and $\Delta_{\text{aver}}$ defined in the text. The shaded area represents the gap limits between which the experimental data are found before average. The lower curve corresponds to a least square fit on experimental data imposing an $A^{-1/3}$ law.
Fig. 2. Same as Fig.1 for neutrons.
Fig. 3. Theoretical gaps for neutrons in the SV and NR regions. Note that zero gap values at magic numbers are included but lifted to finite values after averaging.