Mean-field Based Approaches to Pairing Correlations in Atomic Nuclei

M. Anguiano, J.L. Egido, L.M. Robledo

Departamento de Física Teórica, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Abstract

The evolution of the pairing correlations from closed shell to midshell nuclei is analyzed in the Sn isotopes with the Finite Range Density Dependent Gogny force. As theoretical approaches we use the Hartree-Fock-Bogoliubov, the Lipkin-Nogami, their particle number projected counterparts and the full variation after particle number projection method. We find that whereas all approaches succeed rather well in the description of the total energy they differ significantly in the pairing correlation content of the wave functions. The description of the evolution from the weak to the strong pairing regime is also approach dependent, specially at shell closure.

Key words: Z= 50 isotopes, pairing correlations, Gogny interaction, Hartree-Fock-Bogoliubov, Lipkin-Nogami, particle number projection.

PACS: 21.10.Re, 21.10.Ky, 21.60.Ev, 21.60.Jz, 27.70.+q, 27.80.+w

Pairing correlations play an important role in the understanding of nuclear phenomena. Observables like moments of inertia, level densities and energies of the lowest-lying excited states, to mention a few, are strongly influenced by these correlations. In spite of their relevance pairing correlations are still not well understood. On the experimental side, because the pairing energy itself is not an observable, it is not easy to extract relevant information from the data (at high angular momentum, for example, we have gapless superconductivity). On the theoretical side, the basic problem is the mean field approximation to the pairing field which is not as effective as it is with the deformation (Hartree-Fock) field.

Recently, new experimental techniques have made possible to access regions far away from the stability line allowing to study, among others, very exotic

---

1 Present address: Dipartamento di Fisica, Universita di Lecce, 73100 Lecce, Italy.
systems where pairing correlations play a key role to make the nuclei bound [1]. The experimental studies of N=Z nuclei also provide useful information on the proton-neutron pairing, see for example reference [2]. It seems therefore timely to study the pairing correlations with a force able to provide both binding and pairing energies. In the past there have been several theoretical approaches to the nuclear pairing problem most of them using schematic or separable forces with little predictive power. From a more fundamental point of view effective forces should be used in these studies. The most popular of the density dependent forces, the Skyrme forces, in general use a different force for the particle-particle than for the particle-hole channel and so do, in general, the relativistic approaches. The only density dependent force which has a selfcontained pairing force, because of its finite range, is the Gogny force [3]. This property of the Gogny force makes it unique to study different theoretical approaches because the renormalization of the force is, in principle, not needed due to its selfcontainedness. The purpose of this letter is to investigate the pairing correlations in different mean-field based approaches along different pairing regimes using the finite range density dependent Gogny interaction.

The simplest microscopic approach to describe the nuclear many-body system is the Hartree-Fock (HF) theory. The HF wave function is an antisymmetrized product of single particle wave functions determined in a variational way. The particles move independently in the HF orbitals determined selfconsistently excluding thereby any particle-particle correlation besides the ones considered in the common mean-field potential. The basic and oldest approach to include particle-particle correlations, i.e., pairing correlations, is the BCS approach [4]. This is still a mean field approach, where the wave function is a product of quasiparticle operators $\beta_k$, i.e., $|\text{BCS}\rangle \propto \prod \beta_k | - \rangle$, given by the Bogoliubov-Valatin transformation

$$
\beta^+_k = u_k a^+_k - v_k a_k, \quad \beta^-_k = u_k a^-_k + v_k a_k
$$

with $a_k, a^+_k$ the annihilation and creator particle operators in the Hartree-Fock basis and $\tilde{k}$ the time reversal orbital to $k$. The coefficients $u_k, v_k$ are determined by the Ritz variational principle. Since the Ansatz of Eq. (1) mixes creation and annihilation operators the wave function $|\text{BCS}\rangle$ is not an eigenstate of the particle number operator. The variational equation is therefore

$$
\frac{\delta}{\delta \Phi} \langle \Phi | \hat{H} | \Phi \rangle - \lambda \frac{\delta}{\delta \Phi} \langle \Phi | \hat{N} | \Phi \rangle = 0,
$$

with $|\Phi\rangle = |\text{BCS}\rangle$ and $\lambda$ the Lagrange multiplier determined under the constraint that the BCS wave function has on the average the particle number $N$. In spite of its simplicity and success the BCS approach lacks selfconsistency in the sense that the HF and the pairing fields are not treated on the same footing, i.e., first the HF orbitals are calculated and then their occupancies around
the Fermi surface determined by the BCS equations. The theory which remedies this drawback is the Hartree-Fock-Bogoliubov (HFB) approach. This is again a mean field approach, with wave function $|\text{HFB}\rangle = \prod \alpha_k |\text{−}\rangle$, and with quasiparticle operators $\alpha_k$ determined by the generalized Bogoliubov transformation

$$\alpha_k = \sum U_{lk} c_l + V_{lk} c_l^\dagger.$$  (3)

where $c_l, c_l^\dagger$ are the annihilation and creator particle operators in a suitable basis. In this case the variational parameters are the matrices $U, V$ which are determined by minimization of Eq. (2) but now with $|\Phi\rangle = |\text{HFB}\rangle$. The mean field approaches (HF, BCS, HFB) have been widely used over the years with simple separable forces, effective forces and relativistic ones, to describe many nuclear properties and provide the backbone to theories beyond mean field as the Random-Phase-Approximation (RPA) or the Generator Coordinate Method (GCM).

The success of the mean field approaches is based on their ability to deal with single particle motion as well as with the collective motion associated with symmetries. The collective degrees of freedom are incorporated in the variational Hilbert space by the spontaneous symmetry breaking mechanism. The wave functions of this enlarged Hilbert space are not eigenstates of the symmetry operators and are usually constrained to obey the symmetries on the average. For most symmetries the mean field approach is very satisfactory, for instance, for the rotational motion associated to the angular momentum, see Ref. [5] for a thorough discussion. In the case of pairing correlations, in which we are interested in this letter, the crucial quantities are the number of correlated pairs and the level density around the Fermi surface. If these quantities are small, and in nuclei they usually are, mean field theories are not enough and one should do something better.

The semi-classic recipe of solving the BCS and HFB equations with a constraint on the particle number operator can be derived as the first order result of a full quantum-mechanical expansion (the Kamlah expansion) [6] of the particle number projected quantities in terms of unprojected ones. The second order in this expansion takes into account the particle number fluctuations and might cure some of the deficiencies of the first order approximation. However, full calculations up to second order are rather cumbersome [23,8,9] and most second order calculations have been done using the Lipkin-Nogami (LN) recipe proposed in Refs. [10–12]. The original formulation of the LN method was for a simple separable pairing interaction but it has been recently extended to

---

2 Continuous symmetries, as rotations in any space: coordinate space, gauge space of particle number operator, etc as well as discrete symmetries, e.g. spatial parity.
non-separable ones [13] and density dependent finite range forces [14,15]. The variational equations of the LN method are given by

$$\frac{\delta}{\delta \Phi} (\hat{H} - h_2 (\Delta \hat{N})^2) - h_1 \frac{\delta}{\delta \Phi} (\hat{N}) = 0,$$

(4)

with $h_1$ and $h_2$ given by

$$h_1 = \frac{\langle \hat{N} \hat{H} \rangle - \langle \hat{H} \rangle \langle \Delta \hat{N} \rangle^2}{\langle \langle \Delta \hat{N} \rangle^2 \rangle},$$

(5)

$$h_2 = \frac{\langle \langle \hat{H} - \langle \hat{H} \rangle \rangle (\Delta \hat{N})^2 \rangle - \langle \hat{H} \Delta \hat{N} \rangle \langle \langle \Delta \hat{N} \rangle^3 \rangle / \langle \langle \Delta \hat{N} \rangle^2 \rangle}{\langle \langle \Delta \hat{N} \rangle^4 \rangle - \langle \langle \Delta \hat{N} \rangle^2 \rangle^2 - \langle \langle \Delta \hat{N} \rangle^3 \rangle^2 / \langle \langle \Delta \hat{N} \rangle^2 \rangle}.$$

(6)

with $\Delta \hat{N} = \hat{N} - \langle \hat{N} \rangle$ and $\langle \hat{O} \rangle \equiv \langle \Phi | \hat{O} | \Phi \rangle$ for any operator $\hat{O}$. In the LN approach the $h_2$ parameter is not varied, contrary to what a variational method would require, but only updated in each iteration of the minimization process. In this respect the LN approach is not a fully variational method and its success not quite well understood.

In a mean field based approach, the ideal treatment of pairing correlations in nuclei is particle number projection (PNP) before the variation [16]. This theory is rather complicated and up to now has been mainly applied to separable forces [17] or in small configuration spaces [18]. Only recently [19] an exact particle number projection has been performed with finite range forces, the Gogny forces, and large configuration spaces. Let $| \Phi \rangle$ be a product wave function of the HFB type, i.e. a particle number symmetry violating wave function. We can generate an eigenstate $| \Psi_N \rangle$ of the particle number by the projection technique [5]

$$| \Psi_N \rangle = \hat{P}_N | \Phi \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{i(N-\langle N \rangle)\phi} | \Phi \rangle.$$  

(7)

The particle number projected energy is given by

$$E_{proj}^N = \frac{\langle \Psi_N | \hat{H} | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle} = \int_0^{2\pi} d\phi e^{-i\phi N} \langle \Phi | \hat{H} e^{i\phi N} | \Phi \rangle = \int_0^{2\pi} d\phi y(\phi) E(\phi).$$  

(8)

with

$$y(\phi) = \frac{\langle \Phi | \hat{H} e^{i\phi N} | \Phi \rangle}{\langle \Phi | e^{i\phi(N-\langle N \rangle)} | \Phi \rangle}, \quad E(\phi) = \frac{\langle \Phi | \hat{H} e^{i\phi N} | \Phi \rangle}{\langle \Phi | e^{i\phi N} | \Phi \rangle}. $$  

(9)
One should distinguish the projection after variation method (PAV) from the variation after projection method (VAP). In the PAV approach the wave function $|\Phi\rangle$ is determined by solving Eqs. (2) with $|\Phi\rangle$ a HFB wave function and with this wave function one can calculate the projected energy with Eq. (8). In the VAP approach the wave function $|\Phi\rangle$ is determined minimizing the projected energy, Eq. (8). Obviously the VAP method provides a much better approach. In our case all the variational equations are solved by the Conjugate Gradient Method [20].

As mentioned above we want to investigate the pairing correlations in different mean-field based approaches using the Gogny interaction in the numerical applications. For this purpose we investigate some properties of the Sn isotopes ($Z = 50$) from the $N = 50$ shell closure to the $N = 82$ one. The aim is to study the evolution of the pairing characteristics from the weak pairing regime (around the shell closure) to the strong pairing regime (midshell) to investigate the quality of the different approaches. We have studied the ground state properties of the Sn isotopes in the HF, HFB, and LN approaches. We have also performed projected calculations of the ‘after variation’ type, the PAV and the PLN (Projected LN). In the PAV (PLN) method the intrinsic wave function $|\Phi\rangle$ is determined by the HFB (LN) equations, afterwards a particle number projection on this wave function is performed allowing the calculation of projected expectation values. Furthermore we have performed the VAP calculation. We think that this comparison is important because the studies performed so far were done with separable forces, mostly the monopole pairing. The calculations have been performed with a triaxial code and with $N_0=11$ oscillator shells. Furthermore the D1 parametrization of the Gogny force has been used [3]. To prevent the appearance of divergences associated with the negligence of the exchange terms in the particle number projected calculations [19], all calculations have been performed including all exchange terms of the forces, and all terms have been calculated without any approximation [21]. In the density dependent term of the Gogny force we have used the projected density prescription, see [19] for more details.

To investigate the pairing correlations we should look for a quantity which can be defined in all approaches. In BCS theory with monopole pairing usually the gap parameter has been used. This quantity is strongly related with the particle-particle correlation energy used in the HFB approach,

$$E_{pp} = -\frac{1}{2} Tr \left( \Delta \kappa^* \right),$$

with $\Delta_{kl} = \frac{1}{2} \sum_{mn} \tilde{v}_{klmn} \kappa_{mn}$ and $\kappa_{mn} = \langle \Phi | c_n c_m | \Phi \rangle$ and $v$, in our case, the Gogny and Coulomb interactions. We would like to remind that the density dependent part of the Gogny force does not contribute to the pairing field. In the LN approach we keep the same definition, that means, the contribution
of the $-\hbar^2 < (\Delta N)^2 >$ term to $E_{pp}$ is not considered, this contribution is added to the HF energy. The equivalent expression in the PNP case is (cf Eqs.(8-9)):

$$E_{pp} = 2\pi \int_0^{2\pi} d\phi y(\phi) E_{pp}(\phi) = -\frac{1}{2} \int_0^{2\pi} d\phi y(\phi) Tr \left( \Delta_{kl}^{10}(\phi) \kappa_{kl}^{01}(\phi) \right)$$  \hspace{1cm} (11)

with $\Delta_{kl}^{10}(\phi) = \frac{1}{2} \sum_{mn} \bar{v}_{klmn} \kappa_{mn}^{10}(\phi)$, and

$$\kappa_{kl}^{10}(\phi) = \frac{\langle \Phi | c_k c_l e^{i\phi N} | \Phi \rangle}{\langle \Phi | e^{i\phi N} | \Phi \rangle}, \quad \kappa_{kl}^{01}(\phi) = \frac{\langle \Phi | c_k^\dagger c_l^\dagger e^{i\phi N} | \Phi \rangle}{\langle \Phi | e^{i\phi N} | \Phi \rangle}. \hspace{1cm} (12)$$

Fig. 1. Left panel: The particle-particle correlation energy $E_{pp}$ for the Sn isotopes in different approaches, for neutrons (protons) on the top (bottom). Right panel: The particle number fluctuation in the HFB, LN and the intrinsic wave function of the VAP approaches. Symbols and conventions are given in the left panel.

In the left panel of Fig. 1 we present $E_{pp}$ for the Sn isotopes in the five approaches mentioned above, calculated via Eq. (10) for non-projected theories and Eq. (11) for projected theories. Curves on the top (bottom) of the left panel correspond to the neutron (proton) pairing correlations. The common wisdom about the general behavior of pairing correlations along a shell is that they behave as a semicircle: at shell closure there are not pairing correlations, as we keep adding particles the pairing correlations increase until midshell where they reach the maximum value. From this point on they decrease up to the point where the next shell closure is reached. This wisdom is mainly
based on the mean field approach (BCS and HFB). As a matter of fact the neutron pairing energy in the HFB approach resembles very much this pattern. Qualitatively the behavior of the neutron $E_{pp}$ in the five approximations is similar: they increase from both shell closures towards midshell, up to $N=58$ and $N=74$ where a kind of plateau develops from $A=110$ up to 122. Quantitatively, however, we find three distinctive behaviors corresponding to the three different intrinsic wave functions, the HFB and PAV approaches, the LN and PLN and finally the VAP one. Both, HFB and PAV, give no pairing correlations at the shell closures and display a kind of two hump behavior as a function of the mass number. The LN and PLN approaches, on the other hand, provide non-zero correlation energy at the shell closures (the LN overestimate the VAP result) and display a one hump behavior. The VAP approach, finally, provides the largest correlation energies, showing an even more pronounced two hump structure, and giving non-zero correlations at the shell closures.

If we exclude the VAP results we find a clear trend in the other approximations as a function of the mass number: At the shell closures and in their nearest vicinity there are large differences in the results for the different approaches. As we move to the middle of the major shell the four approximations provide results rather close to each other. Finally, around the middle of the major shell the dispersion in the results of the different approaches get larger. This peculiar behavior might be related, as we shall see later, with the number of subshells involved in the pairing mechanism. A remarkable point is the behavior of the LN (and the PLN to a lesser extend) neutron correlation energies at the shell closures. We observe that the value of $E_{pp}$ at the shell closures, i.e. $N=50$ and $N=82$, is not the extrapolation of the neighboring values, as it is the case for the HFB, PAV and VAP approaches. As we shall see later on this behavior is probably related with a degradation of the LN solution.

The proton correlation energies are depicted in the lower part of the same panel. The HFB and PAV energies, as expected are zero for all $N$ values (we have a major shell closure at $Z=50$) while the LN, PLN and VAP are not. They are not as large as the neutron ones, but the important point is that they are different from zero, i.e., these theories are able to gather a certain correlation energy from the so-called dynamical pairing. Interestingly the projected versions of the HFB (for neutrons) and LN (for neutrons and protons) approaches provide smaller particle-particle correlations than the unprojected ones. We also find that the reduction produced in the LN case for protons is large (about 30 % ) as compared with the one for neutrons or the HFB case (5 % ). This result seems to indicate that the LN approach in the closed shell regime overestimates the pairing correlations (cf. [22]).

A quantity that plays an important role in the approximate particle number projection methods is the fluctuation of the particle number operator. This quantity provides a measure on the degree of symmetry breaking in the cor-
responding wave function. This obviously only applies to symmetry breaking wave functions like BCS or HFB but not to symmetry conserving ones like HF or PNP wave functions. HFB or BCS wave functions with large $<(\Delta \hat{N})^2>$ are expected to have large pairing (gauge deformation) correlation energies. In the right panel of Fig. 1 the fluctuations of the particle number operator are shown. In the projected approaches the intrinsic wave functions are used in the calculations, consequently only the HFB, LN, and VAP approaches are shown. Symbols and conventions are the same as in the left panel. As expected the overall behavior is similar to the $E_{pp}$ in the corresponding approaches. It is interesting that, though the intrinsic wave functions of the VAP and PAV approaches have similar “deformation”, in the gauge space associated to the particle number operator, for many isotopes, the projection is much more effective producing larger $E_{pp}$ in the case of the VAP than in the PAV one.

Fig. 2. Upper part: The energy difference between the binding energy in the HF approach and the other theoretical approaches as a function of the mass number. Lower part: Same as upper part but constraining the HF solutions to spherical shapes.

Another way to measure the pairing correlations in a given approach is to look for the energy gain obtained by going from the HF (no pairing correlations allowed) to the respective approach (pairing correlations allowed). In this way we may define

$$\Delta E_G = E_{HF} - E_{\text{approach}}$$

(13)
where $E_{HF}$ and $E_{\text{approach}}$ are the total binding energies in the HF theory and in the corresponding approach. In this case approach stands for any of the HFB, PAV, LN, PLN and VAP approaches. Obviously, $\Delta E_G$ is a measure of the energy gain when particle-particle correlations are allowed.

In the upper part of Fig. 2 we display $\Delta E_G$ for the different approximations. The largest energy gain is provided by the VAP method followed by the PLN one. Interestingly, at variance with the $E_{pp}$ case, the PAV approach provides binding energies very similar to the LN one. In particular, it is surprising that, at the shell closures ($A = 100$ and 132), the LN approach provides both, binding energies very close to the HF ones and, at the same time, larger particle-particle correlation energies than the VAP method, see Fig. 1. These results could be interpreted again as a degradation of the LN approach in the very weak pairing regime. The PLN results on the contrary become closer to the VAP ones.

On the base of general arguments one would expect larger similarity between the bulk behavior of $E_{pp}$ and $\Delta E_G$ than the one found. A close look at the different solutions reveals that while in all approaches (with the exception of the HF one) all nuclei under study remain spherical, in the HF one some nuclei get deformed due to the absence of pairing correlations. That means in the upper panel of Fig. 2 some deformation effects are present and the comparison of $\Delta E_G$ with $E_{pp}$ is not as obvious as if these effects would not be there. To eliminate deformation effects we have performed spherical HF calculations. The quantities $\Delta E_G$ evaluated with the spherical binding energies are displayed in the lower panel of Fig. 2. As expected, since the HF energies are now smaller -we restrict ourselves to spherical shapes- we obtain larger values for $\Delta E_G$. As before PAV and LN values are close to each other and more interestingly the two hump structure found in Fig. 2 is recovered. We observe that, with the exceptions of the shell closures, the different curves behave more similar one to each other than they do in the particle-particle energy of Fig. 1.

To study the origin of the two hump structure we shall investigate the fractional harmonic oscillator shell occupancy, defined by

$$\nu(n, l, j) = \frac{1}{2j + 1} \sum_{m=-j}^{j} \langle \Phi | c_{nljm}^{\dagger} c_{nljm} | \Phi \rangle.$$  (14)

In the left part of Fig. 3 we represent the occupancies of the pairing active shells in the HFB approximation (for the other approaches the conclusions do not change). As expected at $N = 50$ the shells are empty and at $N = 82$ filled (the small deviations from zero and one are due to the fact that in the spherical HFB the quantum number $n$ is not conserved) and in between a smooth filling of the shells takes place. This smooth filling may give rise to
divergences in the PNP approaches when the occupancies $v_k^2$ take the value 0.5 and the exchange terms have been neglected [19] in the calculations. The largest pairing correlations are expected from the big shells and at half shell occupancy. Accordingly, we expect a maximum around $A = 108 - 110$ from the $d_{5/2}$ and $g_{7/2}$ orbitals and another one around $A = 124 - 126$ stemming from the $h_{11/2}$ orbit. Looking at the right panel of Fig. 3, where we have plotted separately the contribution to the total pairing energy of positive (HFB n+) and negative (HFB n-) parity shells, we find the expected behavior. The deep in the pairing energy around $A = 116$ is due to the fact that the gain in pairing of the small shells $s_{1/2}$ and $d_{3/2}$, which are being filled around this mass number, does not compensate the loss of pairing due to the higher occupancy of the $d_{5/2}$ and $g_{7/2}$ shells. A possible explanation of the fact that the HFB, LN, PAV and PLN give values for $E_{pp}$ with a larger dispersion around the major midshell than at the beginning or at the end of the shell, might be that in the first case one has to deal with five open subshells while in the second one only with one or two.

![Fig. 3. Left panel: Occupancies of the active orbitals in the HFB approach as a function of the mass number. Right panel: The neutron particle-particle correlation energy in the HFB approximation for positive and negative parity.](image)

Taking into account these results we may understand somewhat better the relation between $\Delta E_G$ and $E_{pp}$. The total energy in a given approach can be written as $E_{\text{approach}} = E_{HF}(\varphi_{\text{approach}}) + E_{pp}$, where $E_{HF}(\varphi_{\text{approach}})$ represents the kinetic energy and the contribution of the Hartree-Fock field to the energy calculated with the wave function $\varphi_{\text{approach}}$. This expression is also valid for the projected energy (PLN, PAV and VAP), see Eq. (B-1) of reference [19]. Substitution of $E_{\text{approach}}$ in Eq. (13) provides $\Delta E_G = E_{HF} - E_{HF}(\varphi_{\text{approach}}) - E_{pp}$. The quantity $|E_{HF} - E_{HF}(\varphi_{\text{approach}})|$ represents the loss of energy due to the readjustment of the plain HF occupancies caused by the pairing field. Looking at Fig. 3, we find that near the shell closures the occupancies, independently of the approach, are either zero or one, i.e., the HF occupancies are not very different from the ones of the corresponding approach and we do not expect large differences between $\Delta E_G$ and $E_{pp}$. As we move from closed

\[3 \text{ In the LN case we have to add the term } -\hbar_2 < (\Delta \hat{N})^2 >.\]
shells towards midshell the fractional occupancies increase deviating from the plain HF ones. The largest deviations between $\Delta E_G$ and $E_{pp}$ are expected, therefore, in the middle of the shell. A close look at Figs. 1 and 2 confirms these expectations. An interesting point is the inversion of the HFB (LN) and PAV (PLN) curves in Fig. 2 as compared with Fig. 1. The HFB (LN) line is below the PAV (PLN) in Fig. 2 at variance with Fig. 1 because the projected occupancies (PAV or PLN) are closer to the plain HF, i.e., smaller $|E_{HF} - E_{HF}(\phi_{\text{approach}})|$, than the unprojected ones (HFB or LN).

The HFB, PAV, LN and PLN approaches are approximations to the full variation after projection method. It would be interesting to see how much the different approximations deviate from the full VAP method which they try to emulate. In the upper part of Fig. 4 we plot the difference of the binding energies calculated in the different approaches and the VAP one. In the HFB case we find on the average deviations of about 2.6 MeV with the exception of the nuclei in the neighborhood of the shell closures and around $A = 116$ where we get larger values. These results are in qualitative agreement with the Kamland expansion, according to which the larger the deformation in the gauge space associated with the symmetry operator the better the expansion will be. In the right panel of Fig. 1 we have represented the fluctuations for the particle number operator, which give a measure of the gauge deformation as a function of the mass number. We find a qualitative correlation between $<(\Delta N)^2>$ and the goodness of the HFB approach. We find that for those mass numbers where $<(\Delta N)^2>$ has large values the HFB approach gets closer to the VAP method. The PAV results provide, on the average, an additional lowering of about 0.75 MeV. This approximation is rather uniform as a function of the mass number and only the two or three nuclei close to the shell closures deviate more from the average. The LN values are on the average about 1.7 MeV higher than the VAP and as the other approximations they differ at most from the VAP at the shell closures. However, in the LN only the $N = 50$ and $N = 82$ isotopes deviate strongly from the VAP values. A quantitative change is provided by the PLN. Its binding energies differ over a wide range by only about 0.75 MeV from the VAP, and even in the worst cases, for $N = 50$ and $N = 82$, the deviations is only about 1.25 MeV.

The discussion of the upper part of Fig. 4 does not give us information on the content of the wave functions, it tells us only about the ability of the different approaches to reproduce the binding energy of the VAP method which they try to emulate. Since the total energy is the sum of several terms, there is no guarantee that each term reproduces with the same quality the corresponding term in the VAP approach. To gain more insight into the wave function we have plotted in the lower panel of Fig. 4 the difference between the particle-particle correlation energy of the HFB, PAV, LN and PLN approaches and the VAP method. Let us first concentrate on the neutron parts. The first observation is that these quantities show a stronger dependence on the mass
number than the binding energies. The HFB and PAV results are close to each other, though the HFB ones get closer to the VAP than the PAV, contrary to what happened with the total energies. Furthermore they approach the VAP results best around \( A = 116 \), also at variance with the binding energy results. The LN and PLN results also behave similar, they approximate best the VAP results in the region around \( A = 116 \) and at the shell closures, though the good agreement at the shell closures could be fortuitous as we shall see below. Furthermore, the LN results get closer to the VAP than the PLN. These features of the LN and PLN are also the contrary to what we obtained for the total energies.

In the lower panel of Fig. 4, we see the discontinuities in the LN and PLN approaches at \( A=102 \) and \( A=130 \), already commented in reference to Fig. 1. This behavior could be associated with a failure of the LN expansion at the phase transitions. As a matter of fact in reference \([9]\) it has been shown that large changes in the \( h_2 \) parameter are associated with the breakdown of the second order expansion of the projected energy. On the left hand side of Fig. 5 we have plotted the \( h_2 \) parameters as a function of the mass number. As one can see the neutron \( h_2 \) parameter is rather constant and small from \( A=106 \)
up to $A=126$, then it rises to the large shell closure value of 0.6. For protons we find large and rather constant $h_2$ values (the small dip around $A=110$ has to do with the small bump at the same place in $<(\Delta N)^2>$, see Fig. 1). From this plot we conclude that the origin of the discontinuity is the fast change in $h_2$, which itself is caused by the breakdown of the expansion at second order. The overshooting of $E_{pp}$ in the LN approach at $A = 100$ and $A = 132$ is caused by the term $-h_2(\Delta N)^2$, in Eq. (4): The large $h_2$ value makes that term very big leading to an exaggerated scattering of neutrons pairs across the Fermi surface. This overshooting is equivalent to the behavior found in the two-level pairing model where the LN energy, in the weak pairing regime, is deeper than the exact one[23]. Concerning the proton particle-particle correlation energies we observe that the LN and PLN, as expected, stay rather constant with the mass number. The overshooting of the LN approach does not appear in this case, probably, because of the Coulomb antipairing effect [21].

![Fig. 5. Left panel: The $h_2$ coefficient of the LN approach as a function of the mass number. Right panel: The energy difference between the binding energy of the HFB, PAV, LN or PLN approach and the VAP one, for the solutions with no proton pairing correlation, as a function of the mass number.](image)

In the calculations we have chosen spherical nuclei in order to separate deformation effects from pairing effects, though in our triaxial codes one may get solutions with very small deformations. Now we would like to furthermore separate proton and neutron pairing effects. The comparison of the HFB and PAV binding energies with the VAP results for the Sn isotopes (proton closed shell) is not very fair because no proton pairing is obtained in the HFB and PAV approximations whereas this is not the case for VAP. The comparison of the LN and PLN approaches is not fair either because, as we have seen, for closed shells the LN expansion is not a good one. That means, the results for the proton channel may overshadow the results of the neutron channel. The comparison will be more equitable for ordinary nuclei (proton and neutron shells open) where the HFB approach will provide pairing in both channels and the LN one will perform better. In order to disentangle the different contributions in the Sn isotopes we have also performed VAP and LN calculations with the
additional constraint that no proton pairing is allowed. In this way the proton channel is treated in the same way in all approximations, i.e., the wave function is always of the HF type. In the right panel of Fig. 5 we display the difference of the binding energy in the HFB, PAV, LN or PLN approach and the VAP one, the LN (PLN) and VAP energies calculated with the mentioned constraint. In the HFB, PAV, LN and PLN approaches, with the exception of the shell closures at N=50 and N=82, we are able to reproduce the VAP results, on the average, within 1, 0.2, ±0.2 and 0.15 MeV, respectively. The projected versions PAV and PLN provide smoother approximations, i.e., less isotope dependence, than the unprojected ones. The LN approach provides in some cases slightly deeper energies than the VAP one. In the shell closures we find deviations of about 2 MeV in the HFB, PAV and LN approaches, only the PLN reproduces the total binding energy within 0.6 MeV. Looking at this figures one would be tempted to say that the weak pairing regime in the ground state of atomic nuclei only take place for closed shell nuclei. We may now return to the question on the quality of the LN and PLN approaches in the weak pairing regime. Let us compare the LN and PLN results of the right panel of Fig. 5 from $A = 106$ to $A = 124$, only strong pairing regime, with the corresponding ones in the upper panel of Fig. 4, weak (strong) pairing regime in the proton (neutron) channel. We find a certain degradation of the LN approach in the weak pairing regime, Fig. 4, since it deviates too much from the VAP as compared with Fig. 4. The PLN approach, on the other hand, provides rather reasonable results in the weak proton pairing regime.

Concerning to the neutron pairing energies $E_{pp}$ in the VAP approximation, they are almost unchanged by the fact that proton pairing correlations are not allowed. Therefore, the difference in the neutron pairing energies in the HFB (PAV) and the VAP one is still given by the bottom panel of Fig. 4.

In conclusion, we have investigated the behavior of the pairing correlations along a major shell in the variation after projection method plus four approximations to it with the effective Gogny force. If we look at the total binding energies we find that the best approximation to the VAP is provided by the PLN, followed by the LN or PAV and HFB. The PAV results being surprisingly good in midshell. The crucial test of the goodness of the approaches is provided by the shell closures and their nearest neighbors. There, only the PLN provides a reasonable approximation to the VAP method. For the other isotopes, all approaches are rather uniform and the quality of a given approach is almost independent of the mass number. We predict that the best approximations will be obtained for doubly open shell nuclei. We also show that the weak pairing regime in the ground state of atomic nuclei is limited to the nearest neighborhood of closed shells. The isotope dependence of the binding

---

4 This can easily be done by restricting the proton intrinsic variational wave function to be of the HF (not HFB!) type.

5 Excited states, specially high-spin ones, are explicitly excluded.
energies is smoother in the PAV and PLN approaches than in the HFB and LN ones, indicating that this behavior is caused by admixture of wrong particle number components in the wave function of the HFB and LN approaches. On the other hand, if we look at the wave function content, on the pairing correlation energies for example, we find that the results are strongly approach dependent and, in general, less uniform than the ones for binding energies. The ability of the different approximations to reproduce the particle-particle correlation energy of the VAP approach is worse than the one to reproduce the total binding energy. The last statement is obvious from the variational point of view. Specifically, we have found that mean field based theories like HFB are able to provide the total binding energies of doubly open shell nuclei up to 2 MeV (1 MeV per channel) of the VAP approach. For the LN, PAV and PLN theories the accuracy is much better (0.2 MeV per channel). However, the predictions for the pairing correlation energy in the HFB or PAV (LN or PLN) approach are about 3 MeV (2 MeV) away from the VAP approach, which corresponds to a 20 per cent (15 per cent) accuracy. Consequently, properties strongly dependent on the pairing correlations, like moments of inertia, level densities or excitation energies of the excited states, among others, may not be well described in non-VAP theories in spite of providing high accuracy in the total binding energy as compared with the VAP prediction.

We would like to remark, lastly, that these conclusions are based on the mean field theories most widely used in nuclear structure calculations. In principle one should compare these approaches, even the VAP one, with theories beyond mean field, which explicitly take into account additional pairing fluctuations.

Acknowledgements

This work was supported in part by DGI, Ministerio de Ciencia y Tecnologia, Spain, under Project BFM2001-0184.

References

[1] G.F. Bertsch and H. Esbensen, Ann. Phys. (N.Y.) 209(1991)327
[2] D. Rudolph et al, Phys. Rev. Lett. 86 (1996) 376
[3] J. Dechargé and D. Gogny, Phy. Rev. C 21(1980) 1568
[4] J. Bardeen,L.N. Cooper and J.R. Schrieffer, Phys. Rev. 108 (1957) 1175.
[5] P. Ring and P. Schuck, The Nuclear Many Body Problem (Springer-Verlag, Berlin, 1980).
[6] A. Kamlah, Z. Phys. 216, 52 (1968).
[7] D.C. Zheng, D.W.L. Sprung, H. Flocard, Phys. Rev. C 46 (1992) 1335.
[8] H. Flocard and N. Onishi, Ann. Phys. 254 (1997) 275.
[9] A. Valor, J. L. Egido and L. M. Robledo, Nucl. Phys. A 671 (2000) 189.
[10] H.J. Lipkin, Ann. Phys. (NY) 12 (1960) 425.
[11] Y. Nogami, Phys. Rev. B 134 (1964) 313.
[12] J. F. Goodfellow and Y. Nogami, Can. Jour. Phys. 44 (1966) 1321.
[13] P.-G. Reinhard et al, Phys. Rev. C 53 (1996) 2776.
[14] A. Valor, J.L. Egido and L. M. Robledo, Phys. Lett. B 392 (1997) 249.
[15] A. Valor, J. L. Egido and L. M. Robledo, Nucl. Phys. A 665 (2000) 46.
[16] K. Dietrich, H. J. Mang and J. H. Pradal, Phys. Rev. 135 (1964) B22.
[17] J. L. Egido and P. Ring, Nucl. Phys. A 383 (1982) 189; Nucl. Phys. A 388 (1982) 19.
[18] K. W. Schmid and F. Gruemmer, Rep. Prog. Phys. 50 (1987) 731.
[19] M. Anguiano, J.L. Egido and L. M. Robledo, Nucl. Phys. A 696 (2001) 467.
[20] J.L. Egido, J. Lessing, V. Martin and L.M. Robledo, Nucl. Phys. A 594 (1995) 70.
[21] M. Anguiano, J.L. Egido and L.M. Robledo, Nucl. Phys. A 683 (2001) 227.
[22] J. Dobaczewski and W. Nazarewicz, Phys. Rev. C 47 (1993) 2418.
[23] D. C. Zhen, D. W. L. Sprung and H. Flocard, Phys. Rev. C 46 (1992) 1355.