Pairing schemes for HFB calculations of nuclei

T. Duguet*, K. Bennaceur† and P. Bonche**

*NSCL and Department of Physics and Astronomy, Michigan State University, East-Lansing, MI 48824, USA
†IPNL, CNRS-IN2P3 / Université Claude Bernard Lyon 1, 69622 Villeurbanne Cedex, France
**SPhT, CEA Saclay, 91191 Gif sur Yvette Cedex, France

Abstract. Several pairing schemes currently used to describe superfluid nuclei through Hartree-Fock-Bogolyubov (HFB) calculations are briefly reviewed. We put a particular emphasis on the regularization recipes used in connection with zero-range forces and on the density dependence which usually complement their definition. Regarding the chosen regularization process, the goal is not only to identify the impact it may or may not have on pairing properties of nuclei through spherical 1D HFB calculations but also to assess its tractability for systematic axial 2D and 3D mean-field and beyond-mean-field calculations.

1. INTRODUCTION

It has been known for a long time that the structure of the nucleus depends significantly on its superfluid nature. Indeed, pairing constitutes the main part of the residual interaction beyond the Hartree-Fock (HF) approximation and has a strong influence on most low-energy properties of the system [1]. This encompasses masses, separation energies, deformation, individual excitation spectra and collective excitation modes such as rotation or vibration. The role of pairing correlations is particularly emphasized when going toward the neutron drip-line because of the proximity of the Fermi surface to the single-particle continuum. Indeed, the scattering of virtual pairs into the continuum gives rise to a variety of new phenomena in ground and excited states of nuclei [2].

Despite its major role, our knowledge of the pairing force and of the nature of pairing correlations in nuclei is rather poor. The importance of resolving the range of the interaction, the nature and characteristics of its density dependence (in particular the isovector and low-density parts) have to be clarified [2, 3, 4, 5]. Also, the impact of the Coulomb force [6] and of the three-body force [7, 8] on pairing properties of nuclei is not well understood. Last but not least, particularly puzzling is the situation regarding beyond-mean-field effects. Screening effects due to density and spin fluctuations are known to strongly decrease the pairing gap in infinite neutron matter, both for singlet and triplet pairing [9, 10, 11, 12, 13]. Whether one can extend this result to finite nuclei is still an open question. In particular, the induced interaction and off-shell self-energy effects due to the exchange of surface vibrations between time-reversed states seems to increase the pairing gap in finite nuclei compared to that generated by the bare force only [14, 15]. In addition, the influence of the restoration of particle-number and pairing vibrations in even and odd nuclei still has to be characterized through systematic calculations.

In the present paper, we discuss results of spherical 1D Hartree-Fock-Bogolyubov (HFB) calculations using currently popular pairing schemes. This set of results constitutes a preview of a more extensive study [16]. Our goal at this stage is not to discuss their relevance in terms of reproduction of experimental data but rather to clarify their theoretical content to make such an ultimate comparison meaningful. Also, their tractability for systematic 2D and 3D mean-field and beyond-mean-field calculations is addressed. In section 2, we briefly outline the characteristics of the different pairing schemes. Results are displayed in section 3. Conclusions are given in section 4.

2. EXISTING PAIRING SCHEMES

To treat pairing, one needs to specify the many-body technique used and the appropriate interaction to insert into the calculation at the chosen level of approximation. The latter depends both on the situation and the system. In the
present case, we concentrate on a (self-consistent) mean-field description of finite nuclei using the HFB method [1]. Within such a framework, we compare pairing schemes differing not only by their analytical structure but also from the point of view of the motivation for their adjustment/definition. Phenomenological forces adjusted in the context of Density Functional Theory (DFT) and supposedly renormalizing all possible correlations through HFB calculations are compared to a microscopic vertex equivalent to the bare nucleon-nucleon force. The latter scheme is motivated by perturbative methods showing unambiguously that the interaction to be used in the particle-particle (p-p) channel at lowest order in irreducible vertices (i.e. well-defined mean-field theory) is the bare nucleon-nucleon (NN) force [17, 18, 19, 20]. At the next order, the irreducible pairing vertex involves the so-called polarization diagrams.

Until recently, only phenomenological pairing forces such as the Gogny force [21] or (Density-Dependent) Delta Interactions ((DD)DIs) [3, 4, 22, 23] have been used in mean-field and configuration mixing calculations [1]. Although successful in describing low-energy nuclear structure over the known mass table, they lack a clear link to the bare interaction. This feature strongly limits the reliability of their analytical structure such as their possible density dependence. Also, their direct fit to nuclear data through mean-field calculations makes probable the re-normalization of beyond-mean-field effects. This is a significant limitation if, and only if, one wants to go explicitly beyond that level of approximation. Finally, their fits performed onto very limited sets of nuclei around stability make their extrapolated use toward the drip-lines unsafe.

Let us now concentrate on DDDIs. The corresponding ansatz read as:

\[ D(\vec{r}_1, \vec{r}_2) = \frac{1}{2} \frac{P_\sigma}{\rho_0(\vec{r})} f(\vec{r}_1) \delta(\vec{r}_1 - \vec{r}_2) \, , \]

(1)

where \( P_\sigma \) is the spin-exchange operator, \( \rho_0(\vec{r}) \) is the local scalar-isoscalar part of the density matrix and \( f(\vec{r}_1) \) is the density-dependent form-factor. In the present case, we consider, "surface-type" (\( \rho_\sigma = \rho_{\text{sat}} \), where \( \rho_{\text{sat}} \) is the saturation density of symmetric nuclear matter) and "half-volume/half-surface type" (\( \rho_\sigma = 2\rho_{\text{sat}} \)) DDDI. It is worth noting that recent analysis of asymptotic matter and pair densities of exotic nuclei [4], the evolution of the pairing gap toward the neutron drip-line [24], moment of inertia of transfermium isotopes [3] and the average behavior of the odd-even mass differences over the mass table [25] have recently shown that an optimal compatibility between experimental data and results of HFB calculations was obtained for a DDDI between surface and volume.

When using DDDI to describe pairing, one needs to regularize the theory which otherwise diverges [29]. There are several phenomenological ways to do so. One scheme used in connection with the two-basis method to solve HFB equations consists of limiting the sum in the calculation of the pairing-field matrix elements to single-particle states whose energies lie inside a (smoothed) window \( \lambda - 5 \leq \epsilon_m \leq \lambda + 5 \) around the Fermi energy [26]. Another popular scheme used when solving the HFB problem in coordinate space consists of calculating the densities by limiting the integrals performed in the quasi-particle basis to states with \( E_{qp} < E_F = 60 \text{ MeV} \) [27, 28] \(^1\). It is only recently that the regularization of the pairing problem could be understood microscopically [29, 30]. The idea is to identify the divergences stemming from the use of a local gap and to regularize them through a well-defined renormalization procedure. This complements the DDDI with an effective coupling constant \( g_{\text{eff}}(\vec{r}) \) expressed in terms of an energy cut-off which has to be taken sufficiently far away from the Fermi energy to ensure that observable are independent of its value \(^2\). Note that \( g_{\text{eff}}(\vec{r}) \) comes in addition to the genuine density-dependent form factor \( f(\vec{r}) \).

In an attempt to describe pairing in the \( ^1S_0 \) channel starting from the bare NN interaction, a tractable form of the latter for HFB calculations of finite nuclei was proposed recently [31]. BCS pairing properties provided in infinite matter by AV18 [32] were reproduced very accurately. An effective version of the interaction (FR) was then introduced through a recast of the gap equation into a fully equivalent pairing problem. Resumming high energy pair scattering into the effective vertex provided the latter with a factor \( 2v_m^2 \), where \( v_m^2 \) denotes usual BCS occupation numbers. Such a factor acts as a microscopic regularizer and makes zero-range approximations meaningful. Thus, a zero-range (ZFR) approximating in infinite matter the same gaps at the Fermi surface as the bare force was defined [31].

Beyond the regularization factor, the recast of the pairing problem provides the effective pairing forces FR and ZFR with a density dependence of the form [31]:

\[ f_{(Z)FR}(\vec{r}) = A_{(Z)FR} + B_{(Z)FR} \ln \rho_0(\vec{r}) + C_{(Z)FR} [\ln \rho_0(\vec{r})]^2 \, , \]

(2)

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1 It is in fact in the so-called "single-particle equivalent spectrum" which allows the separation between particles and holes [28].

2 This parameter will be taken as the canonical basis size \( E_{\text{max}} \) in section 3 and in Fig. 1 when we test the convergence properties of the different methods.
where $\rho_q(\vec{r})$ is the local density of nucleons of isospin $q$. The isovector character of such density dependence is different from the one introduced for usual phenomenological DDDI. The coefficients entering the functional $f_{ZFR}(\vec{r})$ differ from those used for FR. The surface-enhanced character of phenomenologically optimized DDDI [3, 4, 24, 25] was derived in Ref. [31] and shown to be, to a large extent, a way of re-normalizing the range of the interaction. It was also shown that usual DDDIs miss the low-density behavior of the effective pairing force. This feature was briefly discussed along with the first published results of 3D HFB calculations with FR and ZFR [33].

For the present study, we select/define a set of 6 representative pairing schemes whose characteristics are summarized in Table 1. They combined the different possibilities discussed previously regarding the range, density dependences and regularization schemes. ULB is a commonly used surface-peaked interaction adjusted on superdeformed bands of medium mass nuclei [23]. DFTS, DFTM and RDFTM were adjusted in a similar fashion as was done in Ref. [34] by asking for the average neutron gap in $^{120}$Sn to be $<\Delta_n(120\text{Sn})>_c = \sum_{\lambda>0} \kappa_n^\lambda \kappa_{\lambda\min}^n / \sum_{\lambda>0} \kappa_{\lambda\min}^n = 1.245$ MeV. The definition of (Z)FR, free from any adjustment in finite nuclei, has already been discussed. The Gogny force is listed for completeness only.

### Table 1. Pairing schemes currently used in HFB calculations of finite nuclei.

| Name     | Range  | Regularization scheme | Density form factor | Type of density |
|----------|--------|------------------------|---------------------|-----------------|
| ULB      | zero   | phenomen. $\lambda - 5 \leq \epsilon_m \leq \lambda + 5$ | $\rho_c = \rho_{sat}$ | $\rho_0(\vec{r})$ |
| DFTS     | zero   | phenomen. $E_{gap} \leq 60$ MeV | $\rho_c = \rho_{sat}$ | $\rho_0(\vec{r})$ |
| DFTM     | zero   | phenomen. $E_{gap} \leq 60$ MeV | $\rho_c = 2\rho_{sat}$ | $\rho_0(\vec{r})$ |
| RDFTM    | zero   | micro. $g_{sat}(\vec{r})$ | $\rho_c = 2\rho_{sat}$ | $\rho_0(\vec{r})$ |
| ZFR§     | zero   | micro. $2\nu_1^2$ | Surface enhanced + rising at low dens | $\rho_q(\vec{r})$ |
| FR$^\dagger$ | finite | | | |
| Gogny§   | finite | | | |

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### 3. RESULTS

We perform 1D spherical HFB calculations of tin even-even isotopes’ ground-states. The HFB equations are solved using the two-basis method [26]. The Sly5 Skyrme force [35] is used in the p-h channel. The calculations are redone for each pairing scheme listed in Table 1, except for the Gogny force. By keeping the same force in the p-h channel, the pairing vertices are probed and compared in a consistent manner, including the self-consistent coupling between the two channels. Of course, properties of the force in the p-h channel have an impact on the results. In that respect, it is worth noting that the considered DDDI were adjusted together with the SLy5 (SLy4 for ULB) parameterization in the p-h channel whose isoscalar effective mass is $m^*/m = 0.7$. Also, ZFR and FR were defined once for all without any reference to finite nuclei and are insensitive to the effective mass used as far as their parameters values are concerned [31].

The binding energy $E_{tot}$ is displayed in Fig. 1 for $^{120}$Sn and $^{170}$Sn as a function of the energy $E_{max}$ of the highest HF single-particle state included in the calculation. For both nuclei, $E_{tot}$ converges significantly faster for the finite range force FR than for DDDI, regularized either microscopically (RDFTM and ZFR) or phenomenologically (DFT) §. If we look at an accuracy of 10 keV, $E_{tot}(^{120}$Sn) is converged around $E_{max} = 10$ MeV for FR whereas one has to go up to around $+80 MeV$ for ZFR and RDFTM. The explicit (smooth) cut-off at $E_c = 60$ MeV for DFTM makes necessary to go even slightly higher whereas ULB converges to much better accuracy for $E_{max} \approx +5$ MeV thanks to its very

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§ The staggering behavior of $E_{tot}$ as a function of $E_{max}$ for RDFTM seems to be due to a combined effect of the sharp cut-off $E_c$ used in the corresponding regularization method and of the discretization of the continuum we perform when solving the HFB equations. By treating the continuum exactly as was done in Refs. [29, 30], such a staggering should disappear.
FIGURE 1. Left panel: binding energy of $^{120}\text{Sn}$ as a function of the energy $E_{\text{max}}$ of the highest single-particle state included in the canonical basis. Right Panel: same as left panel for $^{170}\text{Sn}$ (vertical scales are different).

small active window around the Fermi level $^4$. It is important to notice, however, that both microscopic regularization schemes do not motivate the use of such a small active window. Of course, one has to assess whether this impacts physical observable. The right panel of Fig. 3 shows that the intrinsic increase of CPU time needed to tackle the finite-range force is compensated by its faster convergence as a function of the basis size. This is a very critical result since the size of the single-particle basis is (among the size of the box and of the mesh) what makes calculations on the 3D mesh expensive. With a mesh of 0.8 fm, 3D codes of the type of $\text{EV8}$ [37] can handle 800 wave functions for systematic calculations performed on supercomputers. For a large enough box [16], this allows one to go up to $E_{\text{max}} \approx 10/15$ MeV in medium mass nuclei. Depending on the convergence required, this may rule out some of the pairing schemes discussed presently. In any case, ULB, FR and ZFR are the most preferable ones in that respect.

One can nicely relate the convergence properties previously discussed to occupation of single-particle states in the continuum. As can be seen from Fig. 2, occupation numbers decrease much faster for the finite range force FR than for any DDDI, except for ULB. As a result, physical observable converge faster for FR than for ZFR, DFTM and RDFTM as a function of the basis size. Independently on the pairing scheme used, one can roughly relate the precision required on $E_{\text{tot}}$ to the occupation of single-particle states to be included in the calculation. For a precision of the order of 10 keV, one can see from Fig. 2 that states with $v_m^2 > 10^{-4}$ have been taken into account.

$^4$ What is a converged value depends on the observable and the situation. For instance, separation or excitation energies converge faster than absolute binding energies as a function of the basis/box/mesh sizes or the type of derivative used. On the other hand, quantities which are not minimized such as pairing gaps or radii are, at least, as sensitive as binding energies and maybe more in drip-line nuclei. What is a reasonable converged value also depends on other sources of numerical inaccuracy. For instance, 3D codes on the mesh can usually handle a mesh size of 0.8 fm compared to 0.1/0.25 fm in spherical codes. This can lead to inaccuracy of the order of 500 keV in heavy nuclei, even with the best formula for derivatives [36].
In fact, occupation probabilities reflect directly the properties of the underlying regularization scheme. Indeed, using a finite range force or a microscopically regularized DDDI, \( v^2_m \) follows closely the law one can derive for such forces in the limit \( \varepsilon_m \approx \hbar^2 k_m^2 / 2m \gg \lambda \). Such a limit is relevant in finite nuclei because plane-wave continuum states do not feel the finite nuclear potential at these energies. The laws obtained in this limit for the bare force used here [31] (thick dashed line in Fig. 2) and for the corresponding zero-range approximation (thin dashed line in Fig. 2) read respectively as \(^5\):

\[
v^2_m \approx \frac{\Delta^2}{4 \varepsilon^2_m} e^{-4 \alpha^2 / \pi (\varepsilon_m - \lambda)} \quad \text{and} \quad v^2_m \approx \frac{\Delta^2}{4 \varepsilon^2_m}.
\]

(3)

On the other hand, occupation numbers associated to DFTM and ULB do not follow the expected pattern of true zero-range forces and strongly reflect the properties of the underlying phenomenological regularization schemes (see the very abrupt decrease close to zero energy for ULB). Again, the relevant question is whether or not this influences the description of (pairing) properties of nuclei.

To obtain a first insight, let us focus on DFTM and RDFTM which only differ through the regularization recipe used. One can see from Fig. 1 that the converged binding energy provided by the two methods differs by about 300 keV in \(^{120}\)Sn, which is on the edge of being significant as far as microscopic mass tables are concerned. However, this is quite a constant shift over a large set of spherical nuclei (see for example the right panel of Fig. 1 for \(^{170}\)Sn) and can certainly be easily reabsorbed. As a matter of fact, DFTM and RDFTM provide identical \( S_{2N} \) for all spherical nuclei [16]. Regarding pairing properties, Fig. 3 shows that average neutron gaps \( \langle \Delta^v(N) \rangle \) obtained in tin isotopes with the two methods are not only equal where the forces are fitted but extrapolate in a very similar way up to the drip-lines. As a conclusion, the regularization recipe does not seem to matter too much. In order to tackle the same question regarding a ULB-type regularization, a parameterization with the same density form-factor as DFTM or RDFTM should be studied [16].

In any case, one has to be careful before concluding on the unimportance of employing a microscopic regularization scheme. Indeed, the conclusion could be different if using a more realistic density dependence as the one displayed by ZFR, that is, which reflects the large scattering length of the \( NN \) interaction at low density. Indeed, a DFT-type force was shown to lead to unrealistic densities and to an unrealistic reduction of the two-neutron separation energy across the magic number \( N = 82 \) when used together with such a strongly attractive form factor at low density. On the other hand, no such unrealistic behavior is seen with ZFR [16] for which the microscopic regularization method and the strongly attractive form factor at low density have been derived consistently [31].

\(^5\) Single-particle states which accumulates close to zero on Fig. 2 correspond to canonical states with very small occupation which are not well converged numerically. Also, \( v^2_m \) patterns reflect the fact that the calculation is performed for \( E_{\text{max}} = +130 \) MeV.
FIGURE 3. Left panel: $<\Delta^n(N)>_K$ along the Sn isotopic chain. Full dots are experimental five-point odd-even mass differences [39]. Right Panel: CPU time necessary to reach convergence in $^{120}$Sn as a function of $E_{\text{max}}$.

There are two elements to the role played by the density dependence: its spatial character and its isovector nature. Gaps calculated with ZFR and DFTM are very similar, both in absolute value and in terms of their isotopic trend $^6$. This is due to the behavior of ZFR between volume and surface which confirmed the phenomenological findings of Refs. [3, 4, 24, 25]. Surface-peaked DDDI on the other hand provide too strong pairing, especially in neutron rich nuclei. This is clear when comparing DFTM and DFTS which differ only through the spatial character of $f(\vec{r})$. The increasing difference between DFTM and DFTS as we move towards the drip-line reflects in fact mainly the isospin character associated with their dependence on $\rho_0$. Forces depending on $\rho_0$ only give too strong pairing correlations in neutron rich matter as explained in Ref. [33]. The latter effect being proportional to how much the density form-factor varies over the volume of the nucleus, it is much more pronounced for DFTS than for DFTM. The rather weak dependence of DFTM on $\rho_0$ explains why the pairing gaps predicted by DFTM and ZFR towards the drip-line remains similar and are not spoiled by their different isospin nature.

4. CONCLUSIONS

In the present paper, we briefly compare the main pairing schemes currently used in HFB calculations of nuclei (except for the Gogny force). We employ spherical 1D HFB calculations of tin isotopes to assess the impact of the regularization recipes and of the density dependence used in connection with zero-range forces. Beyond usual phenomenological DDDI, the recently proposed microscopic pairing force equivalent to the bare $NN$ force is discussed [31]. It was shown that only the latter finite-range force and phenomenological DDDI using small active pairing windows around the Fermi energy can currently be tackled in calculations on a 3D mesh.

The results presented here constitute a preview of a more extensive and systematic study of existing phenomenological and microscopic pairing schemes [16]. In addition to analyzing the formal and technical differences between those schemes, the forthcoming study will focus on the impact these differences may or may not have on physical properties of nuclear ground-states.

$^6$ The slight asymmetric behavior between magic numbers of the gaps obtained with FR and ZFR is due to the "asymmetric option" of the recast used and to the approximation associated to it when going from infinite matter to finite nuclei. This can be understood by employing the exact bare force directly or by performing the recast of the gap equation directly in the finite nucleus [38].

$^7$ Such a statement deals with pairing correlations generated by the bare $NN$ force. On the other hand, the isospin character of beyond mean-field effects is far from being understood.
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