Local Density Approximation for Pairing Correlations in Nuclei

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We introduce a natural and simple to implement renormalization scheme of the Hartree–Fock–Bogoliubov (HFB) equations for the case of zero range pairing interaction. This renormalization scheme proves to be equivalent to a simple energy cut–off with a position or density dependent running coupling constant. Subsequently, we present self–consistent HFB calculations with a full consideration of the continuum of long chains of spherical tin and lead nuclei (essentially from one drip line to another) using the SLy5 interaction. In the pairing channel we use a zero range interaction, treated by means of this new regularization scheme.

1 Introduction

Since the landmark paper of Bohr, Mottelson and Pines\textsuperscript{3} we have accumulated so much experimental and theoretical information about pairing in nuclei that one might be tempted to conclude that “hardly any rock was left unturned.” A closer analysis of the nuclear pairing properties will soon however reveal how little we really know. Let us briefly review some basic facts, which, even though are well known and do not raise any doubt, will help “drive our point home.” In closed shell/magic nuclei the last occupied single–particle (sp) state is separated by a gap from the closest unoccupied sp state, see Fig. (\textsuperscript{1}). In condensed matter physics closed shell nuclei would correspond to insulators, while open shell nuclei to conductors. The presence of the gap in magic nuclei is what makes them extremely stable. At the same time, the residual interaction can modify in a qualitative manner the structure of the sp spectrum around the fermi level in an open shell nucleus.

The textbook explanation of why and how pairing correlations lead to a restructuring of the sp spectrum is a simple rehash of the initial Cooper’s picture of a Cooper pair formation\textsuperscript{2} and it is illustrated in Fig. (\textsuperscript{2}). The last pair of nucleons, one with spin up, the other with spin down, can be easily “pushed around” by the allegedly weak residual interaction, since the spacing between unoccupied levels is small. The relatively weak residual interaction is effectively enhanced by the large number of accessible levels and the result is the marked separation of one of the levels from the rest, see the rightmost level scheme in Fig. (\textsuperscript{2}).

Once a gap appears at the fermi surface everybody declares victory, as in particular one can then explain why a superconductor has no resistance, or
Figure 1: Generic single-particle spectra of closed (insulators) and open shell (conductors) nuclei.

Figure 2: Cooper’s picture of how a Cooper pair is formed.
in other words, why there is no dissipation. A less often asked question, to which many have no answer when confronted with it, is: “How come that a superconductor conducts at all? Isn’t its spectrum similar to the spectrum of an insulator? A superconductor should be an insulator!”

Another picture of the Cooper pair formation is in the momentum representation, illustrated in Fig. 3. Pairs of nucleons with opposite momenta and spins residing on opposite sides of the fermi surface are “shuffled around” by a short range interaction all over the fermi surface. The effect of the interaction is larger the larger the fermi momentum is, as that corresponds to a larger fermi surface and therefore to more accessible states. At the same time, scattering particles from one side of the fermi surface to another requires on average a rather large transferred momentum, $|p_1 - p_2| = \mathcal{O}(p_F)$, where $p_F = \hbar k_F$ is the fermi momentum. Such a process is possible only if the residual interaction responsible for this scattering has a sufficiently small radius $\mathcal{O}(1/k_F)$. Consequently, the pairing interaction is relatively short ranged. It is firmly established so far that nuclei belong to the $s$–wave type of “superconductors” in the weak coupling limit, when the paring gap is much smaller than the fermi energy, $\Delta \ll \epsilon_F = \hbar^2 k_F^2 / 2m$. One can show that in such a case (in infinite matter) the rms radius of the Cooper pair significantly exceeds the interparticle separation, namely $\hbar^2 k_F / m \Delta \gg 1/k_F$.

It is easy to see then that under normal circumstances a Cooper pair
has barely any room in an everyday nucleus, as a Cooper pair “wants” to be larger than a nucleus. This is a remarkable fact, which for some hard to explain reasons is rarely mentioned in the nuclear literature and nobody really considered seriously the consequences of this outstanding feature. As the Cooper pair is a large and a loosely bound state of two nucleons, its wave function should be described by a single coupling constant of an essentially zero–range interaction. This is very much similar to the case of the deuteron, but much closer to the case of two neutrons (which have an almost bound state), where the scattering length is \( a = -18.5 \) fm. The theory in such a case should be simple, since there is a small parameter, the ratio = interaction radius/Cooper pair radius.

The fact that the Cooper pair is so much larger than the interaction radius should lead to a local pairing field. For many reasons it is much better to use a local description of the meanfield properties of many fermion systems. Not only the numerical treatment is much simpler, but also our intuition works much better when dealing with local equations. Moreover, there are firm theoretical arguments that a local treatment is possible and one can devise at least a local Hartree–Fock (HF), or better, a Kohn–Sham (KS) hamiltonian \( h(r) \).

We shall use the term LDA in the strict KS sense, as this is the prevailing tendency in the condensed matter physics and chemistry literature (which by sheer numbers dominate), and which slowly becomes an accepted term in this sense in nuclear physics as well.

The only attempts to introduce a density functional theory and subsequently a LDA for pairing known to us are Refs. 8. However, the LDA extension described in these references is in terms of the anomalous density matrix \( \nu(r_1, r_2) = \langle gs | \hat{\psi}^\dagger(r_1) \hat{\psi}(r_2) | gs \rangle \) and thus in terms of a nonlocal pairing field as well. If one can adopt the approximation of a zero range two–body interaction in the pairing channel as well, then the HFB (or Bogoliubov–de Gennes in condensed matter literature) equations become

\[
[h(r) - \mu]u_i(r) + \Delta(r)v_i(r) = E_i u_i(r), \quad (1)
\]

\[
\Delta^*(r)u_i(r) - [h^*(r) - \mu]v_i(r) = E_i v_i(r). \quad (2)
\]

Here \( u_i(r) \) and \( v_i(r) \) are the quasi–particle wave functions, \( \mu \) is the chemical potential, \( \Delta(r) = -\frac{\delta E_{gs}}{\delta \nu(r)} \) is the local pairing field, \( E_{gs} \) is the ground state energy of the system and \( \nu(r) \) is the anomalous density. In all the formulas presented here we shall not display the spin degrees of freedom, but we shall specify the spin degeneracy factor.
2 Divergence of the anomalous density for a local pairing field

If one takes at face value Eqs. (1,2) one can show that the diagonal part of the anomalous density matrix \( \nu(r, r) \) diverges. Only the mere fact that the pairing field is local is sufficient enough in order to arrive at this conclusion. When \(|r_1 - r_2| \to 0\) the anomalous density \( \nu(r_1, r_2) \) has the singular behavior

\[
\nu(r_1, r_2) = \sum_i v_i^*(r_1) u_i(r_2) \propto \frac{1}{|r_1 - r_2|},
\]

and as a result, a local selfconsistent pairing field \( \Delta(r) \) cannot be defined. One obviously needs a cut-off of some kind, as the divergence emerges when the sum extends over the entire HFB spectrum. In nuclei and especially in very dilute fermionic atomic systems, where \( k_F r_0 \ll 1 \) and \( r_0 \) is the radius of the interaction, there is effectively no well defined cut-off and one needs to regularize the theory. A finite range interaction will provide a natural cut-off at single-particle energies of the order of \( \varepsilon_c \sim \hbar^2 / m r_0^2 \). For such high sp energies the fast spatial oscillations of the quasi-particle wave functions \( u_i(r), v_i(r) \) will render the nonlocal pairing field \( \Delta(r_1, r_2) \) ineffective. Even though the presence of a finite range of the interaction in the pairing channel formally removes the ultraviolet divergence of the gap, it is very difficult to come to terms with the fact that a cut-off at an energy of the order of \( \hbar^2 / m r_0^2 \) could be the responsible for the definition of the gap both in the case of regular nuclei and very dilute nuclear matter as well. The characteristic depth of the nucleon–nucleon interaction potential, which is of the order of \( \hbar^2 / m r_0^2 \), being the largest energy in the system, can be effectively considered to be infinite in the case of dilute systems. This estimate for the potential energy comes from deuteron properties, where the expectation values for the kinetic and potential energies are almost equal in magnitude, leading to a small deuteron binding energy. A well defined theoretical scheme for the calculation of a local pairing field, should lead to a converged result when only single-particle states near the Fermi surface are taken into account.

In many treatments of the pairing correlations in infinite systems authors often underline the dependence of the pairing gap on momentum, that is \( \Delta(k) \), or in other words, the nonlocality of the pairing field. We gave already a number of arguments above why a nonlocal pairing, most likely, makes little sense. Let us consider this issue from a slightly different point of view. On one hand, typical calculations of the pairing field \( \Delta(k) \) in infinite systems (with no medium polarization effects taken into account so far) show that for large momenta the pairing field decreases, as one would naturally expect. On the other hand, as soon as the momentum of a quasiparticle state is sufficiently...
different from the fermi momentum, when $|k - k_F| \approx m\Delta(k_F)/\hbar^2 k_F \ll k_F$, the effect of the pairing correlations on the single–particle properties is small, if not negligible. For such momenta, to a very good accuracy $E(k) = \sqrt{(\varepsilon(k) - \mu)^2 + \Delta^2(k)} \approx \sqrt{(\varepsilon(k) - \mu)^2 + \Delta^2(k_F)} \approx \varepsilon(k) - \mu$ and thus the use of a $k$–independent pairing field is a fair approximation. This is just another way of stating that the size of the Cooper pair $\hbar^2 k_F/m\Delta$ is much larger than the average interparticle separation in the weak coupling limit. Typically this takes place when also the range of the pairing interaction is smaller than the size of the Cooper pair as well, and thus the pairing interaction could and should be described by a single coupling constant.

Most of the calculational schemes suggested so far for infinite systems reduce to replacing a zero range potential by a low energy expansion of the vacuum two–body scattering amplitude. The traditional approach in the calculations of finite nuclei consists however in introducing a simple energy cut–off, while the pairing field is computed by the means of a pseudo–zero–range interaction. In this approach the effective range of the interaction is obviously determined by the value of the energy cut–off and the two–body coupling constant in the pairing channel is chosen accordingly. Such a pure phenomenological approach lacks a solid theoretical underpinning and always leaves the reader with a feeling that “the dirt has been swept under the rug”. Another solution, often favored by other practitioners is to use a finite range two–body interaction from the outset, such as Gogny interaction. Besides the fact that the ensuing HFB equations are much more difficult to solve numerically, such an approach also lacks the elegance and transparency of a local treatment and this seemingly simple recipe is indeed as phenomenological in spirit as the treatment based on a pseudo–zero–range interaction, with an explicit energy cut–off. Moreover, in spite of the feeble arguments often put forward in favor of a finite range interaction in HFB calculations, the only real argument is the fact that the pairing field would otherwise diverge, and there is no clear cut mean–field observable which would be noticeable different in the case of a finite range interaction.

It is instructive to show how this divergence emerges and the simplest system to illustrate this, is an infinite homogeneous one. Since the divergence is due to high momenta, thus small distances $|r_1 - r_2|$, this type of divergence is universal and has the same character in both finite and infinite systems. Until recently methods to deal with this divergence were known only for infinite homogeneous systems, and only recently ideas were put forward on how to implement a renormalization scheme for the case of finite or inhomogeneous systems. Assuming for the sake of simplicity that the spectrum of the HF operator
is simply \( \varepsilon(k) = \hbar^2 k^2 / 2m \), one can represent the anomalous density matrix as follows:

\[
\nu(r_1, r_2) = \int \frac{d^3k}{(2\pi)^3} \frac{\exp[ik \cdot (r_1 - r_2)]\Delta}{2\sqrt{[\varepsilon(k) - \mu]^2 + \Delta^2}}
\]

\[
\equiv \int \frac{d^3k}{(2\pi)^3} \exp[ik \cdot (r_1 - r_2)] \left\{ \frac{\Delta}{2\sqrt{[\varepsilon(k) - \mu]^2 + \Delta^2}} - \frac{\Delta}{2[\varepsilon(k) - \mu - i\gamma]} \right\}
\]

\[
+ \frac{\Delta \exp(ik_F|r_1 - r_2|)}{4\pi \hbar^2 |r_1 - r_2|},
\]

where \( \mu = \hbar^2 k_F^2 / 2m \). The last integral expression is well defined for all values of the coordinates \( r_{1,2} \). However, it is now obvious that the limit \( r_1 \to r_2 \) cannot be taken, since the last term is manifestly divergent. This is the divergence we have to deal with and remove it from the theory in some meaningful manner in order to be able to introduce a local pairing field. The well known BCS divergence has a different nature, is infrared in character and appears while one approaches the fermi surface, where \( E(k) = \sqrt{[\varepsilon(k) - \mu]^2 + \Delta^2} \) almost vanishes (in the weak coupling limit) and that leads to an almost logarithmic divergence of the integral in Rel. (4).

### 3 Regularization procedure for the anomalous density in finite and inhomogeneous infinite systems

In a nutshell, the regularization of the theory amounts simply to “throwing away” the leading divergent part \( \Delta \rho / [4\pi \hbar^2 |r_1 - r_2|] \) from the rest in the limit \( |r_1 - r_2| \to 0 \). There are several ways to justify this apparently rather arbitrary procedure:

\( i \) one can use steps outlined typically in renormalizing the gap equation in infinite systems – by relating the divergent part with the scattering amplitude

\( ii \) or by using well–known approaches in Quantum Field Theory (QFT) – either dimensional regularization

\( iii \) or one can introduce explicit cut–offs and counterterms – \( iv \) or one can follow the pseudopotential approach known for a long time in quantum mechanics and used among others by Fermi in the 30’s. Irrespective of the approach chosen, one arrives at the same value for the gap. In particular, if one introduces an explicit cut–off one can show that the gap equation becomes

\[
\frac{1}{|y|} = \int_0^{k_c} dk \frac{k^2}{4\pi^2} \left[ \frac{1}{\sqrt{[\varepsilon(k) - \mu]^2 + \Delta^2}} - \frac{1}{[\varepsilon(k) - \mu - i\gamma]} \right] + \frac{ik_F m}{4\pi \hbar^2},
\]
where the coupling constant $g$ is defined as

$$g\delta(r_1 - r_2) = \frac{\delta^2 E_{gs}}{\delta \nu^*(r_1) \delta \nu(r_2)}.$$  \hspace{1cm} (7)

and $k_c$ is a momentum cut-off. We have assumed here the simplest dependence of the LDA energy density functional on the anomalous density $\nu(r)$, namely $E(\tau(r), \rho(r), |\nu(r)|^2)$, merely for the sake of the simplicity of the presentation, but more general forms can be used as well. In Eq. (6) $k_c$ can be taken to infinity without impunity. In Ref. 12 it is shown that the minimal value for the cut–off momentum is given by $E_c = O(\hbar^2 k_F^2 / 2m)$, where $E_c = \hbar^2 k_F^2 / 2m + U - \mu$ and $U$ is the meanfield potential. Previous approaches\cite{4,14,16,17,18,19,20,21} use $\varepsilon(k)$ only in the second term instead of $\varepsilon(k) - \mu$ under the integral\cite{29}. In that case the last imaginary term does no appear and only then one can relate the coupling constant $g$ with the scattering length $g = 4\pi \hbar^2 a / m$ as well.

A note of caution: it would be incorrect to interpret some of the above formulas in the same manner as similar looking formulas appearing in various treatments of the pairing correlations with a zero–range interaction $V(r_1 - r_2) = g\delta(r_1 - r_2)$ (which can be related with the zero–energy two–particle scattering amplitude $g = 4\pi \hbar^2 a / m$). As it is well known for quite some time, even in the low density region, where $k_F |a| \ll 1$, there are significant medium polarization corrections to the pairing gap\cite{26}. If one adopts a LDA treatment, then, one is not limited anymore by similar restrictions on the density. In the LDA energy density functional the polarization effects are already implicitly included in the definition of $E(\tau(r), \rho(r), |\nu(r)|^2)$ and the coupling constant $g$ has no simple and direct relation to the vacuum two–particle scattering amplitude $a$. In this sense the LDA is similar in spirit to the Landau fermi liquid theory.

The only attempt to implement a consistent regularization scheme for finite systems that we are aware of is that of Ref. 11. In agreement with the analysis of Ref. 9 the authors of Ref. 11 conclude that in the case of a zero range two–body interaction the anomalous density has a $1/|r_1 - r_2|$ singularity. The traditional regularization schemes for infinite homogeneous systems amounts to subtracting a term proportional to $1/k^2$ in the gap equation in momentum representation\cite{4}, which in coordinate representation corresponds naturally to the same type of divergence as well $1/|r_1 - r_2|$. Since the divergence in the anomalous density matrix $\nu(r_1, r_2)$ is due to large momenta and thus short distances, it is not surprising that the character of the divergence is not affected by the size of the system. Bruun et al. advocate the use of the following calculational procedure for the anomalous density. First of all one represents
the anomalous density as
\[ \nu(r_1, r_2) = \sum_{E_i > 0} \left[ v_i^*(r_1) u_i(r_2) + \frac{\psi_i^*(r_1) \Delta(r) \psi_i(r_2)}{2(\mu - \varepsilon_i)} \right] - \frac{\Delta(r) G_0(r_1, r_2, \mu)}{2} \] (8)

[\hbar(r) - \varepsilon_i] \psi_i(r) = 0, \quad [\mu - \hbar(r_1)] G_0(r_1, r_2, \mu) = \delta(r_1 - r_2), \] (9)

where \( r = (r_1 + r_2)/2 \). This particular representation for \( \nu(r_1, r_2) \) was introduced earlier in Ref. 9. One can easily justify this subtraction scheme in infinite homogeneous matter, since
\[ v_i^*(r_1) u_i(r_2) = \Delta \psi_i^*(r_1) \psi_i(r_2) / 2\sqrt{(\varepsilon_i - \mu)^2 + \Delta^2}. \]

In the limit \( r_1 \to r_2 \) the sum over single–particle states in Eq. (8) is converging now and one has only to extract the regulated part of the propagator \( G_0(r_1, r_2, \mu) \), using the pseudo–potential approach
\[ \nu_{reg}(r) := \sum_{E_i > 0} \left[ v_i^*(r) u_i(r) + \frac{\Delta(r) \psi_i^*(r) \psi_i(r)}{2(\mu - \varepsilon_i)} \right] \] (10)

\[ -\frac{\Delta(r)}{2} C_{0, reg}^{\nu}(r, \mu), \] (11)

\[ C_{0, reg}^{\nu}(r, \mu) = \lim_{r_1 \to r_2} G_0(r_1, r_2, \mu) + \frac{m}{2\pi \hbar^2 |r_1 - r_2|} \] (12)

obtaining for the local pairing field
\[ \Delta(r) = \frac{4\pi |a| \hbar^2}{m} \sum_{E_i > 0} \left[ v_i^*(r) u_i(r) + \frac{\Delta(r) \psi_i^*(r) \psi_i(r)}{2(\mu - \varepsilon_i)} \right] \] (13)

\[ -\frac{4\pi |a| \hbar^2}{m} \Delta(r) C_{0, reg}^{\nu}(r, \mu), \] (14)

where \( a \) is the two–particle scattering length (\( a < 0 \)). As one can see, the regularization procedure and the extraction of the regulated part from various diverging quantities is completely analogous to the familiar procedures in QFT, with the only difference that in this case everything is performed in coordinate space. One literally "throws away" the diverging terms and retains the nonvanishing finite contributions.

There are however problems with using this apparently meaningful regularization procedure. As it is formulated, the approach of Ref. 11 works for systems in a harmonic trap only and does not apply to atomic nuclei or other self–sustaining systems. Nobody would argue that pairing correlation depend on the sp properties in some, hopefully small, neighborhood of the fermi surface only. Consequently, after the divergence has been removed, what was left, namely the rhs of Eqs. (10, 13), should be defined entirely in terms of
sp properties at and around the fermi level. The problem is that around the fermi level one cannot establish a 1–1 correspondence between the HF and HFB properties. In order to arrive at these expressions the authors of Ref. 9 used explicitly this 1–1 correspondence in order to remove in a controlled manner the divergent part of the anomalous density matrix \( \nu(\mathbf{r}_1, \mathbf{r}_2) \). In Fig. (4) the nature of the HFB spectrum around the fermi surface is illustrated for two cases: the upper panel corresponds to a situation resembling nuclei along the \( \beta \)-stability valley (\( |\Delta| < |\mu| \)) while in the lower figure we show an HFB spectrum for nuclei very close to a nucleon drip line (\( |\Delta| \geq |\mu| \)). In the first case one can see that not all discrete HF levels have a discrete counterpart in the HFB spectrum, even in the interval \( 2\mu < \varepsilon_i < 0 \). In the second case, the HFB equations have no discrete spectrum whatsoever.

The fact that hole–like states in HFB have a continuous spectrum is known for quite some time. The explanation given in these references is somewhat formal and lacks a simple physical intuition and a pictorial representation. As a matter of fact this feature can be explained in rather simple terms, as the phenomenon has similarities with the so called Andreev reflection, known for quite some time in condensed matter physics. Let us imagine that a system is made half of a normal metal and the other half is a superconductor, see Fig. (5). In some respects nuclei with pairing correlations are like that, as they can be thought of drops of “superconductor nuclear matter” embedded in a perfect conductor, the vacuum. If a particle coming from the normal part, impinges of the interface, normally one can expect that with some probability this particle is reflected and with some other probability the particle is refracted. If however the other side is superconducting, then there is one more possibility, the particle can get to the other side, but on the way it picks–up another particle from the normal side and leaves behind a hole. If the initial impinging particle had the momentum \( p_1 \), it will pick another particle with momentum \( -p_1 \) and opposite spin and it will form a Cooper pair. Since Cooper pairs are (almost) bosons, the probability that such an event occurs is bigger, the larger the Cooper pair condensate is, as in lasers for example. By picking–up an additional particle from the normal side this process leads to a hole, which is reflected exactly in the opposite direction of the picked–up particle. What one achieves in this way is a coupling between particle and hole states. Since the hole states are coupled with continuum particle states, hole states acquire a continuum character as well.

Now, returning back to the regularization procedure suggested in Ref. 11 one can see that we have a serious problem. In order to arrive at Eqs. (10,11,13,14) one had to assume that for each HFB term there was a unique HF term. Such a correspondence could in principle be established far away
Figure 4: The empty and filled dots correspond to discrete states of Eqs. (1,2) for $\Delta \equiv 0$ (marked with HF and -HF respectively), and the continuing straight lines to the corresponding continuous spectra. The HFB spectra are marked with E and -E, and we use pentagrams for discrete states and continuous lines for the respective continuous parts of the spectra. Only for the discrete HF states marked with empty circles one can find corresponding discrete HFB states.
from the fermi surface, where pairing is ineffective. One can then represent
the anomalous density matrix as follows, by introducing an explicit cut–off

\[ \nu(r_1, r_2) = \sum_{E \leq E_c} v_E^*(r_1) u_E(r_2) \]  \hspace{1cm} (15)

\[ -\frac{1}{2}\Delta \left( \frac{r_1 + r_2}{2} \right) \sum_{\varepsilon - \mu < E_c} \psi_\varepsilon^*(r_1) \psi_\varepsilon(r_2) / (\varepsilon - \mu) \]  \hspace{1cm} (16)

\[ + \sum_{E > E_c} \left[ v_E^*(r_1) u_E(r_2) - \frac{1}{2}\Delta \left( \frac{r_1 + r_2}{2} \right) \psi_\varepsilon^*(r_1) \psi_\varepsilon(r_2) \right] / (\varepsilon - \mu) \]  \hspace{1cm} (17)

\[ + \frac{1}{2}\Delta \left( \frac{r_1 + r_2}{2} \right) \sum_{\varepsilon} \psi_\varepsilon^*(r_1) \psi_\varepsilon(r_2) / (\varepsilon - \mu), \]  \hspace{1cm} (18)

where for \( E > E_c \) there is a 1–1 correspondence \( E \leftrightarrow \varepsilon - \mu \), but not for
the the rest of the spectrum. However, one cannot combine (15) with (16)
into a single expression, be that either an integral or sum (depending on the
character of the spectrum) and eventually combine that with (17) to express
the entire quantity as a single sum/integral, independent of \( E_c \) as was done
in Ref. 11. Without introducing an explicit cut–off, beyond which such a 1–1
correspondence could be established, and treating in some other manner the
rest of the spectrum, it is completely unclear how one should proceed in order

Figure 5: Andreev reflection.
to calculate Eqs. (10,13), which depend on the HF and HFB sp properties around the fermi level only.

A related difficulty with the approach suggested in Ref. 11 and to a large extent an even more serious issue is however the calculation of Eqs. (11,14). This requires the extraction of the regularized part of the HF propagator for a potential of arbitrary shape. These two issues are intimately related, as the final answer is only the sum of Eqs. (10) and (11) or of Eqs. (13) and (14) respectively. One has obviously some freedom here on how to chose the particular form of the subtracted quantity, as the regulator is not uniquely defined. Any regulator with the general structure

$$\frac{m \Delta(r) F(r_1, r_2)}{2\pi \hbar^2 |r_1 - r_2|}, \quad \text{where} \quad F(r, r) \equiv 1,$$

and otherwise arbitrary function $F(r_1, r_2)$ would be adequate. The question is: “How should one choose this regulator?” The extraction of the regular part of the propagator is trivial in the case of free motion, and one more case, the spherical harmonic potential was worked out in Ref. 11. We have tried to devise numerical procedures to perform such an extraction for an arbitrary potential, but the numerical accuracy we could achieve was unsatisfactory. Until such a procedure is suggested, the only alternative one is left with is to devise a new regulator, which, maybe, could be handled accurately either numerically or analytically.

Fortunately a very simple solution indeed exists. One has to recognize again the physics, namely that the divergence is ultraviolet in character and thus has nothing to do with one particular geometrical shape or spatial extent of the meanfield potential. This also suggests that the problem can most likely be handled in a local manner. First of all we introduce an explicit energy cut–off $E_c$ in evaluating the anomalous density. In this way we “divorce” the HFB and HF sums in Eqs. (8,10,13) and evaluate them separately, irrespective of the existence of the 1–1 correspondence discussed above. The final result should be independent of $E_c$, if this is chosen appropriately, specifically, if $E_c$ is large enough, then the quantity given by Rel. (17) is negligible. Secondly, we remark that there is no compelling reason to use the exact HF sp wave functions, energies and propagator in Eqs. (8,10,11,12,13,14) and in order to construct the regulator we use a Thomas–Fermi approximation for the relevant quantities. Since the divergence has an ultraviolet character, the Thomas–Fermi approximation is particularly well suited. Thus we arrive at the following relations

$$G_0(r_1, r_2, \mu - U(r)) = -\frac{m \exp(i k_F(r)|r_1 - r_2|)}{2\pi \hbar^2 |r_1 - r_2|}$$
\[
\nu_{\text{reg}}(r) := \nu_c(r) + \int_0^{k_c(r)} \frac{k^2 dk}{4\pi^2} \frac{\Delta(r)}{\mu - \hbar^2 k^2 - U(r) + i\gamma} + \frac{i\Delta(r)k_F(r)m}{4\pi\hbar^2},
\]

where the cut–off energy \( E_c \) is chosen sufficiently far away from the fermi level to insure that the rhs of Eqs. (21,22) is independent of \( E_c \) and \( \gamma \to 0^+ \) at the end. If the fermi momentum becomes imaginary (outside nuclei for example) one can easily show that \( \nu_{\text{reg}}(r) \) is still real. It is useful to introduce an effective coupling constant. Then the regularized pairing field has the simple form

\[
\Delta(r) = -g\nu_{\text{reg}}(r) = -g_{\text{eff}}(r)\nu_c(r),
\]

\[
\frac{1}{g_{\text{eff}}(r)} = 1 - \frac{mk_c(r)}{2\pi^2\hbar^2} \left[ 1 - \frac{k_F(r)}{2k_c(r)} \ln \frac{k_c(r) + k_F(r)}{k_c(r) - k_F(r)} \right].
\]

The fact that the effective coupling constant depends on position can be interpreted either as a position dependent running coupling constant or as a density dependent running coupling constant. For a typical nuclear potential which monotonically increases with the radial coordinate \( (dU(r)/dr > 0) \) one can show that \( dg_{\text{eff}}(r)/dr > 0 \), thus the effective pairing interaction is stronger inside than outside nuclear matter (remember \( g < 0 \)). This is stark contrast with the behavior one would get using the popular energy cut–off of a \( g\delta(r_1 - r_2) \) interaction, namely the vacuum renormalization scheme. In this case the effective coupling constant is

\[
\frac{1}{g_{\text{vac}}(r)} = 1 - \frac{mk_c(r)}{2\pi^2\hbar^2},
\]

from which follows that \( dg_{\text{vac}}(r)/dr < 0 \), if \( dU(r)/dr > 0 \). If one uses this vacuum renormalization scheme for the case of an infinite homogeneous system
the gap equation is identical to the traditional regularization scheme and the gap equation can be written as

$$\frac{1}{|g|} = \int_0^{k_c} \frac{dk}{4\pi^2} \frac{k^2}{\sqrt{[\varepsilon(k) - \mu]^2 + \Delta^2}} - \frac{1}{\varepsilon(k)},$$

which should be compared to Eq. (30). One can take the limit $k_c \to \infty$, as the integral converges, rather slowly however.

In Ref. 12 it was shown that one can introduce an even faster converging regularization procedure. It is based on the simple observation that the problematic term in the expression for the anomalous density $\Delta/2E(k)$ behaves rather like $\Delta/2|\varepsilon(k) - \mu|$ instead of $\Delta/2(\varepsilon(k) - \mu)$. The main difference between these two subtraction procedures appears for hole–like states. Using the “traditional subtraction scheme” the integral over the hole states converges only for energies of the order of the fermi energy $\varepsilon_F = \hbar^2 k_F^2/2m$. Clearly, in most cases of interest, the so called weak coupling limit, when $\Delta \ll \varepsilon_F$, there is absolutely no physical reason to take into account single–particle states so far away from the fermi level in order to describe nuclear pairing properties. By
simply replacing in the regulator \( \varepsilon(k) - \mu \) with \( |\varepsilon(k) - \mu| \) one obtains an equally simple, but impressively much faster convergent regularization procedure, see Fig. (8). Now indeed one can claim that there is an explicit procedure, which defines the paring field and the anomalous density in terms of sp properties in the immediate vicinity of the fermi surface only.

A last point, when evaluating the total energy of the system one has to be careful and calculate the expression

\[
E_{gs} = \int d^3r \left[ \frac{\hbar^2}{2m} \tau_{c}(r) - \Delta(r) \nu_{c}(r) \right] + E_{pot},
\]  

(31)

where \( E_{pot} \) is the usual HF potential energy contribution, since the kinetic energy density \( \tau_{c}(r) = 2 \sum_{E \leq E_c} |\nabla v_E(r)|^2 \) diverges in a similar fashion as \( \nu_{c}(r) \) with \( E_c \), but \( E_{gs} \) does not.

4 HFB calculations of spherical tin and lead nuclei with SLy5 interaction and zero range pairing interaction

With a clear regularization scheme in place one can now aim for a selfconsistent description of nuclear properties within the HFB method. Perhaps the most appealing way to proceed is to use the Kohn–Sham LDA approximation. The philosophy of this approach is to first compute the properties of infinite homogeneous matter in an \textit{ab initio} framework\(^7\) in order to derive the energy density functional. Lacking that, one can resort to phenomenological approaches. Since we are interested in treating open shell nuclei, this functional should depend on the kinetic energy \( \tau(r) = 2 \sum_{i} |\nabla v_i(r)|^2 \) the normal \( \rho(r) = 2 \sum_{i} |v_i(r)|^2 \) and the anomalous \( \nu(r) = \sum_{i} v_i^*(r)u_i(r) \) densities. (The angular momentum density \( J(r) \) is naturally included as well in calculations, along with other necessary ingredients such as Coulomb interaction.) For the sake of simplicity of this initial exploratory survey of nuclear properties using this new regularization scheme, we shall choose a rather simple parametrization of the energy density functional as follows

\[
E_{LDA}(r) = E_0(r) + g|\nu(r)|^2,
\]  

(32)

where for energy density describing normal systems we have chosen \( E_0(r) \) given by the so called SLy5 interaction\(^3\). We could have also used the parametrization suggested by Fayans \(^7\), constructed directly from properties of infinite homogeneous symmetric nuclear matter and pure neutron matter\(^3\). A similar constraint was imposed for the SLy interaction. As for the dependence on the anomalous density no such information is available yet. There are quite a
number of calculations of pairing properties of homogeneous neutron and symmetric nuclear matter, see Refs. \cite{13,14,32} and further references therein. The usefulness of all these results is questionable however at this time. Some authors would try to convince the reader that the use of a bare NN–interaction in the pairing channel is appropriate\cite{13}. Others would not quite subscribe to this point of view, but in the absence of any meaningful theoretical input would proceed with pairing calculations using bare NN–interaction anyway\cite{14,32}. Even though there is a clear danger of double–counting, in some instances the Gogny interaction is used as well\cite{32}, claiming, however, that in this particular channel the Gogny interaction is perhaps closer to a bare NN–interaction rather then to a G–matrix, as was initially envisioned by its creators\cite{23,24}. The list of uncertainties however does not stop here. Assuming for the moment that indeed one can use the bare NN–interaction in the pairing channel, this is not going to help us too much. One might naively suspect that in very dilute matter polarization effects are negligible and thus one can indeed use the vacuum scattering amplitude to evaluate the pairing gap in the leading order in $k_F|a|$ expansion. That would correspond formally to the energy density functional we have chosen above, see Eq. (32). The medium polarization effects are however not negligible and, moreover, depending on the composition of the system they can either enhance significantly the pairing correlations in symmetric nuclear matter by a factor of $(4e)^{1/3} \approx 2.2$ or suppress them by the opposite factor $(4e)^{-1/3} \approx 0.45$ in the case of pure neutron matter. What happens at finite densities is so far a big unknown, as no comprehensive study of the isospin dependence of the pairing properties in infinite matter was performed, as far as we know.

In principle, if full microscopic calculations of the pairing properties of infinite homogeneous matter would be available and one would know for example the dependence of the pairing gap at the fermi level as a function of the chemical potential, then one could use Eq. (1) to extract the density dependence of the effective bare coupling constant $g$ on density. Ideally we would like to know both the isoscalar and the isovector nature of the pairing properties. In the absence of such input we have resorted to the only avenue left to us, assume the simplest form for the dependence of the energy density functional on the anomalous density and try to determine the single constant $g$ from available experimental information. The authors of Refs.\cite{32} suggested a somewhat similar approach, using as input however results from infinite matter calculations with bare NN–interaction. Besides the uncertainties mentioned above with such type of approaches, the zero–range interaction suggested by these authors is determined by three parameters, which have a rather unclear and doubtful theoretical underpinning. One of the reasons is of course the fact
Figure 7: The pairing field $\Delta(r)$ in spherical even–even tin and lead isotopes.
that until recently a meaningful regularization scheme for zero-range pairing interaction in finite systems was not available. We have shown here that such an effective zero-range interaction can be derived easily and it is fully characterized by a single effective position/density running coupling constant $g_{\text{eff}}$. A $g_{\text{eff}}$ extracted in this way will show an additional density dependence (besides the one originating from the regularization procedure), arising from the density dependence of the pairing gap as a function of the density in infinite nuclear matter.

Since we shall consider here nuclei with a magic proton number, pairing will appear only in the neutron system and thus we can limit ourselves to a single bare coupling constant $g$. The first part of the nuclear density functional $E_0$, apart from the Coulomb interaction, is isospin invariant, see discussion in Refs. 7, 33. The part describing the pairing correlation is not explicitly an isospin conserving functional of the anomalous density. An isospin conserving energy density functional should have the property (apart from the explicit Coulomb part)

$$E(\rho_n, \rho_p, \nu_n, \nu_p) \equiv E(\rho_p, \rho_n, \nu_p, \nu_n).$$

We have displayed here only the normal and anomalous density dependence. Perhaps the simplest parametrization of the pairing part of the energy density functional would be of the form

$$E_{\text{LDA}}(\rho_n, \rho_p, \nu_n, \nu_p) = E_0(\rho_n, \rho_p) + g_0|\nu_n + \nu_p|^2 + g_1|\nu_n - \nu_p|^2,$$

where $E_0(\rho_n, \rho_p)$ describes the normal nuclear properties and $g_0$ and $g_1$ would in principle depend on $\rho_n$ and $\rho_p$ as well. We want to stress here that the energy density functional should be isospin conserving, which is due to the strong isospin conserving character of the nuclear forces. However, in various particular ground states of various nuclear systems the isospin symmetry might and is as a rule broken. This is in complete analogy with magnetism. The Hamiltonian (effective or exact) describing a magnetic system is always rotational invariant, even though magnetization can spontaneously appear in particular systems. There is no a priori reason however to conclude that the energy density functional has such a simple dependence on the anomalous density and we might uncover phenomena which would require the introduction of at least quartic terms in the anomalous density. So far, it seems that nuclear pairing fields are relatively weak and quartic terms are not needed.

Limited by these uncertainties, concerning the description of pairing correlations, we performed a first exploratory calculation of tin and lead spherical nuclei, essentially from one drip line to the other. We have solved numerically
the ensuing HFB equations in coordinate representations and in order to treat correctly the continuum spectra of the HFB equations we have used the Green function technique of Fayans et al.\cite{Fayans} in order to evaluate the normal and anomalous densities, by integrating the corresponding normal and anomalous sp propagators in the complex energy plane. Typical results for the neutron selfconsistent pairing field in these nuclei are shown in Fig. (7). In Figs. (8) and (9) we show the neutron and proton density distribution for some selected nuclei and the corresponding expectation values for $r^2$. In the results shown in these figures for the tin isotopes we have used a bare coupling constant $g = -270$ MeV $\cdot$ fm$^3$ and $g = -300$ MeV $\cdot$ fm$^3$ for lead isotopes

For those nuclei for which the binding energies have been measured, we have compared the two–neutron separation energies calculated with a range of values for the bare coupling constant $g$ and compared with experimental data. By varying $g$ the densities are only slightly affected, while the pairing fields change roughly proportional to the value of $g$ used. The $S_{2n}$ energies however seem to be reproduced better for $g = -300$ MeV $\cdot$ fm$^3$. One has to take these apparently good results with a grain of salt, as a final fit of the energy density functional should involve both its normal part (especially its isovector dependence) along with its pairing properties. One can however conclude from here that it is very likely that one can achieve a very good description of masses, perhaps rms radii as well, with a single pairing coupling constant, maybe two, to account for the isospin dependence. More work is required to determine if any genuine density dependence (not that arising from regularization) is needed to describe nuclear properties. There is an ongoing debate on whether pairing has a volume or surface character in nuclei\cite{surface}, but no clear cut answer so far.

5 Conclusions

The main issue we have tried to address here is how to proceed in order to introduce a well defined LDA nuclear energy density functional, which includes a meaningful description of the pairing properties as well. Until now such a theoretical framework was missing. We have shown here that with very little effort such a framework can be formulated. The same procedure should be applied to relativistic meanfield calculations with pairing correlations\cite{relativistic} if one prefers an energy density functional derived in this manner. However, this is not the main achievement, as one might hastily conclude. With this new tool in hands we now understand that the nuclear pairing problem in a way it is much simpler then previously thought. There is absolutely no physical reason to perform calculations of the paring gap involving nuclear single–particle
Figure 8: The proton (dashes), neutron (dots) and total (full line) densities $\rho(r)$ in tin isotopes for $N = 52, 68, 84, 100, 116$ and in lead isotopes for $N = 100, 120, 140, 160, 180$. 
Figure 9: The proton and neutron expectation values for $r^2 - r_0^2$ in tin and lead isotopes, where for tin isotopes $r_0^2$ were the corresponding values for $^{132}\text{Sn}$, while for lead isotopes the values of $r^2$ corresponding to $^{208}\text{Pb}$.
Figure 10: The two-neutron separation energies $S_{2n}$ in tin and lead isotopes for several values of the bare coupling constant $g$ and the corresponding experimental values.
states with energies of the order of 1 GeV, as quite often one might find in literature. Pairing affects nuclear properties around a very small energy window around the fermi level, a few MeV’s or so, and any physically meaningful treatment of the pairing phenomena should involve only states in this energy region. We have shown that this is indeed the case. Along the way we have observed that the ensuing formalism is in some ways very “simple” and it requires the introduction of one or perhaps at most two effective coupling constants. Even if in the final analysis one will find the need for more parameters, it is very likely that those parameters will be needed in order to describe the genuine density dependence of the effective pairing interaction. This situation is to a large extent totally similar to the Landau theory of fermi liquids and its extension to nuclei by Migdal. As it was confirmed many times over in subsequent treatments of nuclei using Skyrme forces, Landau’s and Migdal’s ideas needed some relatively minor tweaking. In the end the description of nuclear properties within the Skyrme meanfield approximation is basically the Landau–Migdal theory made selfconsistent and based on a relatively small number of bare coupling constants. Where the theory needed completion was the pairing channel, which, in order to make the theory selfconsistent, required a regularization procedure.

With the success of the Hohenberg and Kohn density functional theory, and especially the LDA formulation of Kohn and Sham, we come to understand that the primary ingredient is the energy density functional. The road to construct it is basically clear. One has to calculate in an \emph{ab initio} approach the properties of infinite homogeneous matter in order to extract the energy density functional. To this one has to add the calculation of both normal and superconducting systems, in order to extract the dependence on the anomalous densities (proton and neutron) as well. There is one more step, the calculation of the gradient corrections. There is a lot of ambiguity here and even the condensed matter and chemistry communities, with their significantly larger human potential, were not able to arrive at a reasonable answer. Moreover, in condensed matter systems and chemistry the interaction is well known. One can however consider a pure phenomenological approach, such as that suggested by Fayans \cite{fayans}. There is also the question of whether one needs to consider gradient corrections in the pairing channel. Here the situation is not clear yet. On one hand, one might argue that since the pairing occurs in a very narrow energy strip around the fermi level, the nucleon momenta are always essentially equal in length to the fermi momentum $p_F$ and thus there should be no need to consider any momentum dependent terms in the effective pairing interaction. (One should not confuse density with momentum dependence.) On the other hand, the short range pairing interaction scatters
the nucleons in the Cooper pair at very large angles and the typical momentum transfer is of the order of the fermi momentum. This seems to indicate that a (specific) momentum dependence of the pairing interaction perhaps is needed and maybe even required. However, until one can point to an observable, which is clearly affected by the momentum dependence of the pairing interaction (we are not aware of any so far), one can perhaps use the principle of minimum information or maximum entropy and proceed with a simple pairing correction to the energy density functional suggested here. The exceptional value of such an energy density functional is its universality, that fact that it can and it should be used to describe both nuclei, irrespective of their Z/N ratio, along with infinite homogeneous and inhomogeneous systems.

There are still a couple of problems, which are not solved yet, and which might have a relatively simple and obvious solution. One has to derive rules for evaluating other observables involving the anomalous density, e.g. α–decay reduced widths. It is not a priori clear whether one should simply use \( \nu_c(r) \) or \( \nu_{reg}(r) \), or maybe even something else. One should as well extend the regularization procedure to the linear response theory, which, superficially, seems rather straightforward.

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