Superfluid LDA (SLDA): Local Density Approximation for Systems with Superfluid Correlations

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We present a concise account of our development of the first genuine Local Density Approximation (LDA) to the Energy Density Functional (EDF) for fermionic systems with superfluid correlations, with a particular emphasis to nuclear systems.

1. General remarks

The theorem of Hohenberg and Kohn\textsuperscript{1} concerning the existence of a universal Energy Density Functional (EDF), and its subsequent implementation as a Local Density Approximation (LDA), lead to a new qualitative approach to the study of electron systems, from atoms, to molecules, to condensed matter systems and macromolecules in particular and other fermionic systems in general. Even though neither Hohenberg and Kohn nor Kohn and Sham gave us recipes on how to construct the EDF, various approximation schemes with increasing level of sophistication have been created. Moreover, the EDF ideology has been extended to finite temperatures and finite excitation energies as well. However, essentially all of the implementations of the LDA and EDF have been limited so far to normal Fermi systems, namely, systems with no pairing correlations. There were two attempts to extend the LDA to superconducting systems\textsuperscript{2}, however, the pairing field in this approach was still a nonlocal object. One can present the argument that because electron superconductivity is phonon mediated, and since phonons have a spectrum limited by the Debye frequency, such a genuinely nonlocal character of the electron pairing field is natural. In our opinion this kind of argumentation is somewhat tenuous. The normal part of the EDF arises from Coulomb interaction, which in itself has an infinite range. Nevertheless, a coherent LDA approach to normal systems is possible. In recent works\textsuperscript{3,4,5,6,7,8,9,10} we have been able to develop a genuinely local extention of the LDA to systems with superfluid correlations and apply it to a number of nuclear and atomic systems. Besides the fact that a genuine local approach to pairing correlations within an LDA à la Kohn and Sham is certainly possible, such a framework is physically meaningful. In nuclear physics for example, the so called coherence length, or in other words the size of the Cooper pair,
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is significantly larger than the radius of the NN-interaction. The binding energy of the Cooper pair, roughly equal to the pairing gap, is significantly smaller than the Fermi energy. Thus a zero range approximation to the pairing interaction is definitely a meaningful thing to pursue, once one learns how to deal with the inherent short range/ultraviolet divergence characteristic to any local pairing field. Not the last among various arguments that one can bring forward, is the fact that our intuition is so much better in the case of local potentials, when compared to the case of nonlocal potentials. This argument alone, together with the intrinsic simplicity of a local treatment will alone warrant the quest for a suitable, from a pure pragmatic point of view, local scheme, even if such a scheme would not be possible in principle.

2. Formulation of the Superfluid LDA (SLDA)

We suggest a new acronym for the extension of the LDA to superfluid systems, namely SLDA, standing for Superfluid LDA. The starting point of the entire formalism is naturally the assumption that a local EDF for superfluid systems exists, namely 3.4.5.6.7.8.9.10

\[ \mathcal{E}(\mathbf{r}) = \mathcal{E}_N[\rho(\mathbf{r}), \tau(\mathbf{r})] + \mathcal{E}_S[\rho(\mathbf{r}), \nu(\mathbf{r})], \]  

\[ \rho(\mathbf{r}) = \sum_i 2|v_i(\mathbf{r})|^2, \]  

\[ \tau(\mathbf{r}) = \sum_i 2|\nabla v_i(\mathbf{r})|^2, \]  

\[ \nu(\mathbf{r}) = \sum_i v_i(\mathbf{r})^* u_i(\mathbf{r}), \]  

where \( \mathcal{E}_N[\rho(\mathbf{r}), \tau(\mathbf{r})] \) is the normal contribution and \( \mathcal{E}_S[\rho(\mathbf{r}), \nu(\mathbf{r})] \) is the superfluid counterpart. \( \rho(\mathbf{r}) \) and \( \tau(\mathbf{r}) \) are the normal density and kinetic energy densities and \( \nu(\mathbf{r}) \) is the anomalous (superfluid) density, all expressed through the quasiparticle wave functions \( u_i(\mathbf{r}), v_i(\mathbf{r}) \). We have not shown explicitly the spin degrees of freedom (so far we have limited ourselves to systems with \( s \)-wave pairing only). The EDF can and does depend on a number of other local densities, which for the sake of the simplicity of the presentation we choose not to display as well. We assume that the normal part of the EDF is known and we shall not discuss its origin and form.

In most physical systems the magnitude of the anomalous density is relatively small, which reflects the fact that in most cases the pairing is in the weak coupling regime. One can then safely assume that, in nuclei for example, the superfluid EDF is only quadratic in the anomalous density and in that case SLDA equations acquire the following structure (shown here only for one kind of fermions):

\[ E_{gs} = \int d^3r \{\mathcal{E}_N[\rho(\mathbf{r}), \tau(\mathbf{r})] + \mathcal{E}_S[\rho(\mathbf{r}), \nu(\mathbf{r})]\}, \]  

\[ \mathcal{E}_S[\rho(\mathbf{r}), \nu(\mathbf{r})] := -\Delta(\mathbf{r})\nu_c(\mathbf{r}) = g_{\text{eff}}(\mathbf{r})|\nu_c(\mathbf{r})|^2, \]
\[
\begin{align*}
\{ [h(\mathbf{r}) - \mu]u_i(\mathbf{r}) + \Delta(\mathbf{r})v_i(\mathbf{r}) &= E_i u_i(\mathbf{r}), \\
\Delta^*(\mathbf{r})u_i(\mathbf{r}) - [h(\mathbf{r}) - \mu]v_i(\mathbf{r}) &= E_i v_i(\mathbf{r}),
\}
\tag{7}
\end{align*}
\]

\[
\begin{align*}
h(\mathbf{r}) &= -\nabla \cdot \frac{\hbar^2}{2m(\mathbf{r})} \nabla + U(\mathbf{r}), \\
\Delta(\mathbf{r}) &= -g_{\text{eff}}(\mathbf{r})\nu_c(\mathbf{r}), \\
\frac{1}{g_{\text{eff}}(\mathbf{r})} &= \frac{1}{g(\rho(\mathbf{r}))} - \frac{m(\mathbf{r})k_c(\mathbf{r})}{2\pi^2\hbar^2} \left\{ 1 - \frac{k_F(\mathbf{r})}{2k_c(\mathbf{r})} \ln \frac{k_c(\mathbf{r})}{k_c(\mathbf{r})} - \frac{k_F(\mathbf{r})}{k_c(\mathbf{r})} \right\}
\tag{10}
\end{align*}
\]

\[
\begin{align*}
\rho_c(\mathbf{r}) &= \sum_{E_i \geq 0} 2|v_i(\mathbf{r})|^2, \\
\nu_c(\mathbf{r}) &= \sum_{E_i \geq 0} v_i^*(\mathbf{r})u_i(\mathbf{r}), \\
E_c + \mu &= \frac{\hbar^2k^2_c(\mathbf{r})}{2m(\mathbf{r})} + U(\mathbf{r}), \\
\mu &= \frac{\hbar^2k^2_F(\mathbf{r})}{2m(\mathbf{r})} + U(\mathbf{r}).
\tag{14}
\end{align*}
\]

(NB In Ref. 5 in the equation for the renormalized coupling constant there is a typo and the effective mass should be used as shown above.) The SLDA equations for the quasiparticle wave functions have exactly the same structure as the HFB/Bogoliubov-de Gennes equations, for the trivial reason that the corresponding EDF depends on one-body densities alone. Unlike the HFB approximation, however, SLDA does in principle lead to the exact ground state energy and densities, up to gradient corrections. The gradient corrections are additional terms in EDF determined by \(\nabla\rho(\mathbf{r})\) and \(\nabla\nu(\mathbf{r})\), which otherwise vanish identically in infinite homogeneous matter. While the dependence of the EDF on densities can be inferred from \textit{ab initio} calculations of infinite homogeneous matter, the gradient corrections require additional input. The uncertainties still existing in their determination are the source of the largest errors in various EDF approaches and the main \textit{raison d’être} for the letter “\(\Lambda\)” in the acronym LDA. As the vast experience accumulated over the years (mainly in the study of a large number of electron systems) amply shows, gradient corrections are never dominant and are indeed always (relatively small) corrections.

Above \(E_c\) is a cutoff energy, which should be chosen \(\approx 1.5\) times the value of the Fermi energy or larger. In such a case any dependence of the results/observables on the value of the cutoff energy \(E_c\) disappears. The only new element in the formalism, when compared to a formalism with an explicit energy cutoff, is the position and energy cutoff running coupling constant \(g_{\text{eff}}(\mathbf{r})\). The main difference with the similar running coupling constants in Quantum Field Theory (QFT) for example, is the fact that \(g_{\text{eff}}(\mathbf{r})\) depends on position as well, because we are dealing with inhomogeneous systems, unlike the QFT case of particles interacting in vacuum, which is by default homogeneous. The apparent quantum mechanical inconsistency that one can have
at the same time a dependence of the running coupling constant on both position and energy (more exactly on momentum) cutoff is easily resolved if one remembers that as a matter of fact there is a clear separation of scales, similar to the separation of scales in the Landau Fermi liquids theory for example.

3. Application of SLDA to atomic nuclei

Our knowledge of the normal part of the nuclear EDF is more or less satisfactory\(^\text{11}\). In our calculations of nuclear properties we have used the so called SLy4 interaction\(^\text{12}\) in order to generate \(E_N[\rho(r), \tau(r)]\) and also Fayans’ FuNDF\(^\text{0} 13\), both of which where in somewhat different ways fitted to the canonical infinite matter results\(^\text{14}\).

As far as \(E_S[\rho(r), \nu(r)]\) goes, the theoretical knowledge is in a very unsatisfactory overall state. Infinite matter calculations made within the HFB/BCS framework lead to maximum pairing gaps of the order of 3 MeV for \(k_F \approx 1 \text{ fm}^{-1}\) and essentially vanishing pairing gaps at nuclear saturation densities. Various ”correlation effects” taken \textit{a posteriori} into account are essentially never in agreement with each other, except for the fact that the maximum value of the gap is \textit{reduced} to about 1 MeV, a value which a number of people think is a reasonable one\(^\text{15,16,17}\). In qualitative agreement with these results is a somewhat less known result in the nuclear community, established more than four decades ago. In very dilute systems the BCS value for the pairing gap is incorrect and the actual value, which can be estimated quite accurately, is smaller by a factor of about 2.2\(^\text{18,19}\). The situation becomes even more confusing in a way when one takes into account the fact that nuclei have a surface. It was shown that surface modes lead to a significant \textit{enhancement} of the pairing gap\(^\text{20}\), thus just to the opposite effect.

Nuclear phenomenology does not fare much better in this respect and one can find claims that the nuclear pairing energy has either a volume, or a surface or a surface + volume character\(^\text{21,22,23,24,25}\). Thus the density dependence suggested by nuclear matter calculations (weak pairing inside and somewhat stronger outside) does not seem to be either confirmed or disproved in phenomenological studies of finite nuclei. Moreover, so far we really have no clue on whether pairing interaction is momentum dependent and/or energy dependent and/or isospin dependent. Just about the only thing we can state with some certainty is the fact that pairing correlations are indeed present in nuclei and on some kind of average the pairing gap is about 1 MeV or so. And since most of the phenomenological studies of the pairing effects are made with quite a number of restrictions, widely varying from one study to another, the more detailed information about pairing effects is often contradictory and thus cannot be trusted.

In our fully self-consistent treatment of nuclei, with an exact treatment of the continuum spectrum as well, we have resorted to the most simple and meaningful approach, and we have decided to use a single bare coupling constant for both neutrons and protons. We have studied the case of \(T = 1\) pairing only so far. Unlike many/most of the existing treatments available in the literature, our ap-
The approach is fully consistent with the isospin symmetry of the nuclear forces. Within this framework we have been able to achieve an agreement with experiment for the single-nucleon and two-nucleon separation energies which compares extremely favorably with any of the previous calculations, see Refs. 5, 9.

We have tried to determine whether the pairing coupling constant has any noticeable density dependence and were unable to find any. We attribute this to the fact that a nuclear Cooper pair is unable to resolve such fine details, since it effectively averages the pairing interaction over the entire nuclear volume. In a recent fully self-consistent analysis of all known nuclear masses Goriely et al. 26 have arrived independently at the same conclusion. This particular aspect deserves a little more discussion. Often it is argued that the pairing strength among nucleons should be weaker/vanishing inside and reach its maximum at the nuclear surface and beyond. Such a behavior follows from a naive implementation of a "local density approximation" (not to be confused with LDA for EDF) to the pairing gaps as a function of density in infinite homogeneous nuclear matter 27. A better alternative to the naive local density approximation is either the Thomas-Fermi approximation. A discussion of the merits and demerits of the Thomas-Fermi approximation, which indeed would provide only an approximate solution to the SLDA equations, was performed by Grasso and Urban 28 in the HFB limit. In Ref. 28 one can find as well a comparison between the renormalization scheme proposed by 3 us and its precursor 29. In the weak coupling limit, the value of the HFB/BCS pairing gap is quite accurately given by the Emery’s formula 30. When one introduces the low-density corrective pre-exponential factor 18,19, the corrected HFB/BCS Emery’s formula for the pairing gap becomes (if \( n^* = n \))

\[
\Delta = \left( \frac{2}{\hbar} \right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp \left( -\frac{\pi}{2 \tan \delta(k_F)} \right) \\
\approx \left( \frac{2}{\hbar} \right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp \left( -\frac{\pi}{2mk_F V(k_F, k_F)} \right).
\]

In the naive local density approximation, when the value of the pairing gap at a given point inside a nucleus is given by the value of the pairing gap in infinite homogeneous matter at the corresponding local density, a strong density dependence can arise if the \( ^1S_0 \) effective pairing interaction in momentum representation \( V(k_F, k_F) \) has a strong momentum dependence. A strong momentum dependence arises if the range of the effective NN pairing interaction is relative large, namely of the order of \( 1/k_F \) or larger. In the usual HFB approximation a density dependence of this type does also lead to a large nonlocality of the pairing field. Notice, however, that in SLDA the pairing field is local and has no momentum dependence. In SLDA the momentum dependence of the pairing field can arise only if one were to introduce a dependence of the EDF on a new anomalous density, similar to the normal kinetic energy density \( \tau(r) \), namely

\[
\nu_\tau(r) = \sum_i \bar{\nabla} u_i(r)^* \cdot \nabla u_i(r).
\]
This simple argument, based on naive local density approximation, that a noticeable density dependence should be present in nuclei, is not without its merits and it is indeed surprising that our and Goriely et al.,\textsuperscript{26} analyses could not find any convincing trace of such a behavior. Even if one is willing to accept our argument that a spatially large and weakly bound Cooper pair cannot really resolve such small details and it effectively averages the strength of the pairing coupling constant over the entire nuclear volume, it is not clear why such an average is independent of the atomic number. Clearly the ratio surface/volume is not constant over the periodic table.

It is worth noticing as well, that so far, in the somewhat limited study we have performed, we never found a reason to introduce an isospin dependent coupling, even though we have definitely covered the nuclear region where such a dependence was advocated rather strongly by others. Moreover, to stress it again, both proton and neutron pairing correlations have been described with the same coupling constant, as indeed one would expect (up to relatively small Coulomb and CSB forces corrections).

4. Isospin structure of the superfluid contribution to the nuclear EDF

Even though we have not been able to identify any isospin dependence of the pairing EDF, such a dependence could exist and it was suggested in various ways before. Very often however, various authors have violated the isospin symmetry of the pairing EDF, either invoking phenomenological arguments, or simply in order to be able to obtain a better description of various nuclear properties, in particular masses\textsuperscript{26,31,32}. We suspect that one can reconcile to some extent (not fully though) the lack of isospin symmetry in Refs.\textsuperscript{26,31,32} for example, in a rather simple manner, by simply noticing that so far experimentalists have been able to create more neutron rich nuclei than proton rich nuclei. It can be shown that

\[
\left\langle \frac{N - Z}{A} \right\rangle = 0.1473, \tag{17}
\]

where the average is computed over all measured nuclear masses with \( A \geq 8 \) used in Ref.\textsuperscript{31}. One can then easily show that the following superfluid EDF

\[
\mathcal{E}_S(\rho_n, \rho_p, |\nu_n|^2, |\nu_p|^2) = g(\rho_n, \rho_p) \left[ |\nu_n|^2 + |\nu_p|^2 \right] + f(\rho_n, \rho_p) \left[ |\nu_n|^2 - |\nu_p|^2 \right] \frac{\rho_n - \rho_p}{\rho_n + \rho_p}, \tag{18}
\]

\[
g(\rho_n, \rho_p) = g(\rho_p, \rho_n) < 0, \quad f(\rho_n, \rho_p) = f(\rho_p, \rho_n) > 0, \tag{19}
\]

\[
\frac{f(\rho_n, \rho_p)}{g(\rho_n, \rho_p)} \approx -0.39 \tag{20}
\]

will reproduce the fact than on average the proton pairing is stronger than the neutron pairing, in agreement with the otherwise isospin violating treatment of pairing correlations in Refs.\textsuperscript{31,32,26}. The above nuclear superfluid EDF has two
parts. The first part, proportional to \((|\nu_n|^2 + |\nu_p|^2)\), is indeed isospin symmetric. However, the second part, which is proportional to \((|\nu_n|^2 - |\nu_p|^2)(\rho_n - \rho_p)\), is only charge symmetric.\(^a\) It is highly debatable, however, whether one can really accept a charge symmetric only (as opposed to an isospin symmetric one) contribution to the nuclear superfluid EDF, merely for the sake of improving the agreement of the calculated masses for example with the experimental values.

So far we could not find a suitable candidate for a nuclear superfluid EDF, which could in principle directly couple the proton and neutron superfluids and which is not more than quadratic in the anomalous densities. There have been suggestions for superfluid nuclear EDF in literature,\(^33\) quartic in character. Recently this question has been raised again,\(^34\) in order to determine whether protons in neutron stars form a type I or type II superconductor, following the observations of a long period precession in isolated pulsars,\(^35\) which apparently do not support the standard picture of protons being a type II superconductor. We find the superfluid EDF suggested in Ref.\(^34\), however, very hard to reconcile with our knowledge of the pairing correlations at the corresponding densities\(^15\).

5. Concluding Remarks

A relatively simple in structure and very easy to implement LDA to EDF of fermion systems with superfluid correlations has been developed, which in itself apparently represents the first genuinely local extension of the Kohn-Sham ideology to such systems.

This Superfluid LDA (SLDA) has been applied by us so far to study single-nucleon and two-nucleon separation energies of a relatively large number of nuclei (more than 200) with a surprisingly high accuracy. We have used the simplest possible ansatz for the superfluid energy density, compatible with all basic nuclear symmetries, and have used standard forms for the normal energy density part of the nuclear EDF. Namely, we have used a superfluid EDF characterized by a single, density independent and universal bare coupling constant. And even though we did not try to obtain the best overall description of these basic energy nuclear properties, which are affected most significantly by the pairing correlations, our results proved to be of a better quality than any of the previous results we are aware of. Of course, there is no guarantee that by extending the analysis to more nuclei the accuracy of this simple approach will survive unscathed. But there is plenty of room for "improvements," if such would be needed.

There is no question in our minds that a more sophisticated form of the superfluid EDF is going to be needed in order to improve even further the quality of the agreement between theory and experiment. In particular, it is very likely that an explicit isospin dependence of the pairing couplings will eventually emerge.

There are a number of questions our results left so far unanswered, for vari-

\(^a\)AB is grateful to J. Dobaczewski for helping him in clarifying this issue.
ous reasons. In particular, it is still unclear whether a contribution to the nuclear superfluid EDF exists, which couples directly the proton and neutron superfluids.

The microscopic calculations available in literature, concerning the dependence of the pairing gaps on density leave so far a lot to desire, as no consensus seem to have emerged to what is the true value of the pairing gap for example in neutron matter $^{15,16,17}$. Moreover, one can expect that the values and the density dependence of the pairing gaps could be entirely different in symmetric nuclear matter, if one were to naively extrapolate the arguments of Heiselberg et al.,$^{19}$ to finite densities, and we should expect an enhancement of the pairing correlations when compared to simple BCS/HFB calculations, thus an effect opposite to that established so far in pure neutron matter. The dependence of the pairing gap on the isospin composition of the matter is still unknown microscopically. Things are however somewhat worse, as an additional density dependence should appear in finite nuclei. Since nuclei have clear and well defined surface collective modes and as it appears that their contribution to the pairing gaps are about 50% or so $^{20}$, this leads us to believe that gradient density corrections to the superfluid EDF could be rather large.

Some of these aspects of the nuclear superfluid EDF become particularly acute in neutron stars, as at higher than nuclear saturation densities the pairing in $p$- and $f$-waves becomes important. For example, it is a matter of current debate whether at such densities protons are a superconductor of type I or of type II $^{34,35}$, and the answer to this question can change a lot of the neutron stars physics.

The SLDA formalism developed by us has been applied to other systems as well, the vortex state in low density superfluid neutron matter $^6$, the vortex in a superfluid dilute atomic Fermi gas $^7$, overall properties of superfluid correlations in such systems $^{10}$, 2-dimensional quantum dots $^{36}$, in many cases leading to new qualitative findings. The range of phenomena to which SLDA has been applied so far, with pairing gaps spanning almost twenty orders of magnitude, is a measure of its flexibility and relevance.

It is worth mentioning that there are at least two cases in which the SLDA approach can be implemented already in a fully controlled manner. Namely, in the low density regime both the normal EDF and the pairing gap are known to a high degree of accuracy $^{18,19}$. Unlike the HF approach, which would be valid in the leading order in this case, the HFB/BCS fails in this limit, however, SLDA works. The HF approximation is accurate for electrons in high density regime as well. As a matter of fact we are not aware of any physical system in any regime where the unadulterated HFB/BCS approximation will have a satisfactory accuracy. Another extremely interesting and universal regime is that of a dilute system, but with an infinite scattering length $^{37}$, a regime which is nowadays routinely achieved in dilute atomic gases. Quite accurate calculations of such homogeneous systems became available recently $^{38,39}$ and subsequently the SLDA approach was implemented for inhomogeneous systems, specifically to describe the vortex state, see Ref. $^7$.

It is fair to conclude that our knowledge of the pairing properties of both finite nuclei and infinite neutron and nuclear matter are in a very unsatisfactory state.
The heavily phenomenological trend, which dominated the study of pairing nuclear properties over the last forty years left us with no answers to most of the questions discussed here. It is our hope that the existence of a theoretically consistent SLDA framework should be of significant help in settling some of these aspects.

A fundamental aspect of the nuclear pairing problem concerns the calculations of nuclear masses. The emphasis in nuclear physics so far was to generate, following one strategy or another, see Refs. 26, 31, 32, 40, the best possible nuclear mass formula. Our attitude should change, from trying to describe these masses with the best possible accuracy, to trying to understand why, when using a meaningful formalism, which incorporates our best established physical input, we still fail at some level or another. We should realize that by now we have at our disposal close to 2,500 measured masses and we should treat this as an object in its entirety, from which we may learn new physics perhaps, by using a framework consistent with what we have learned so far about nuclear interactions.

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