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Local density approximation for systems with pairing correlations

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This paper presents a formulation of a local density approximation for fermion systems with pairing correlations based on a rapidly converging renormalization scheme for the pairing field.

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The proof that for any fermion system there exists a unique energy density functional of the density matter distribution $\rho(\boldsymbol{r})$ alone, namely $E_{gs}=\min\int d^3r\mathcal{E}_{\rm DFT}(\rho(\boldsymbol{r}))$, is disarmingly simple [1]. However, except for some trivial cases, the exact form of this functional is still a mystery and no constructive algorithms for its determination have been suggested so far. Significant progress has been achieved however within the Kohn-Sham local density approximation (LDA) of the density functional theory (DFT). For a normal fermion system (with no pairing correlations) Kohn and Sham have shown that the ground state energy of any fermion system is a functional of its kinetic energy and matter density distributions, namely, $E_{gs}=\min\int d^3r\mathcal{E}_{\rm LDA}(\tau(\boldsymbol{r}),\rho(\boldsymbol{r}))$. The current philosophy is that one should determine this functional from homogeneous infinite matter calculations and then use it to describe properties of either infinite inhomogeneous or finite systems [1]. By the same token, one would expect that the formulation of a LDA for fermion systems with pairing correlations should be straightforward and that a corresponding universal LDA energy density functional $\mathcal{E}_{\rm LDA}(\tau,\rho,\nu)$ of the kinetic energy $\tau(\boldsymbol{r})=2\Sigma_i|\boldsymbol{\nabla}v_i(\boldsymbol{r})|^2$, normal $\rho(\boldsymbol{r})=2\Sigma_i|v_i(\boldsymbol{r})|^2$ and anomalous $\nu(\boldsymbol{r})=\Sigma_i v_i^*(\boldsymbol{r})u_i(\boldsymbol{r})$ densities exists. (I shall be concerned here explicitly with the case of s pairing in the so-called weak coupling limit. Generalizations seem possible however.) The LDA extension described in Refs. [2] is in terms of the anomalous density matrix $\nu(\boldsymbol{r}_1,\boldsymbol{r}_2)=\langle gs|\hat{\psi}_\uparrow(\boldsymbol{r}_1)\hat{\psi}_\downarrow(\boldsymbol{r}_2)|gs\rangle$. Upon variation of the quasiparticle wave functions $v_i(\boldsymbol{r}),u_i(\boldsymbol{r})$ under standard restrictions one obtains the Kohn-Sham equations, with a structure identical to the Hartree-Fock-Bogoliubov (HFB) or Bogoliubov–de Genes equations:

$$[h(\boldsymbol{r})-\mu]u_E(\boldsymbol{r})+\Delta(\boldsymbol{r})v_E(\boldsymbol{r})=Eu_E(\boldsymbol{r}), \tag{1}$$

$$\Delta^*(\boldsymbol{r})u_E(\boldsymbol{r})-[h^*(\boldsymbol{r})-\mu]v_E(\boldsymbol{r})=Ev_E(\boldsymbol{r}), \tag{2}$$

where $h(\boldsymbol{r})$ is the single-particle Hamiltonian, $\Delta(\boldsymbol{r})=-\delta E_{gs}/\delta\nu^*(\boldsymbol{r})$ and μ is the chemical potential. Each quasiparticle state could be characterized by additional quantum numbers besides the quasiparticle energy E, which I shall not explicitly display however. In all the formulas presented here I shall likewise not display the spin degrees of freedom. One can show that the mere locality of the pairing field $\Delta(\boldsymbol{r})$ leads to a divergent diagonal part of the anomalous density $\nu(\boldsymbol{r},\boldsymbol{r})$ [3–5]. When $|\boldsymbol{r}_1-\boldsymbol{r}_2|\to 0$ the anomalous density matrix has the singular behavior $\nu(\boldsymbol{r}_1,\boldsymbol{r}_2)=\Sigma_{E\geqslant 0}v_E^*(\boldsymbol{r}_2)u_E(\boldsymbol{r}_1)\propto 1/|\boldsymbol{r}_1-\boldsymbol{r}_2|$. As a result, the local self-consistent pairing field $\Delta(\boldsymbol{r})$ cannot be defined. (When summing over the spectrum, the sum becomes an integral if the spectrum is continuous and vice versa for an integral. I shall be casual in using either a summation or integration notation, hoping that the context makes this distinction obvious.) The existence of this particular divergence was the main obstacle in introducing an extension of the LDA approach to systems with pairing correlations. Fortunately, this divergence is one more example of the infinities that infest quantum field theory (QFT) and for which the techniques to regularize them in a controlled fashion exist and can be extended and applied to inhomogeneous systems as well now.

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 $|\boldsymbol{r}_1-\boldsymbol{r}_2|$, 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 [6–12] and only recently ideas were put forward on how to implement a renormalization scheme for the case of finite or inhomogeneous systems [4,5]. Assuming for the sake of simplicity that the spectrum of the HF operator is simply $\varepsilon(\boldsymbol{k})=\hbar^2k^2/2m$, one can represent the anomalous density matrix as follows [3–5]:

$$\nu(\boldsymbol{r}_1,\boldsymbol{r}_2)=\int\frac{d^3k}{(2\pi)^3}\frac{\exp[i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)]\Delta}{2\sqrt{[\varepsilon(\boldsymbol{k})-\mu]^2+\Delta^2}} \tag{3}$$

$$\equiv\int\frac{d^3k}{(2\pi)^3}\exp[i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)]\left\{\frac{\Delta}{2\sqrt{[\varepsilon(\boldsymbol{k})-\mu]^2+\Delta^2}}-\frac{\Delta}{2[\varepsilon(\boldsymbol{k})-\mu-i\gamma]}\right\}+\frac{\Delta m\exp(ik_F|\boldsymbol{r}_1-\boldsymbol{r}_2|)}{4\pi\hbar^2|\boldsymbol{r}_1-\boldsymbol{r}_2|}, \tag{4}$$

where $\mu=\hbar^2k_F^2/2m$. The last integral expression is well defined for all values of the coordinates $\boldsymbol{r}_{1,2}$. Once one has recognized the existence of a divergence, the next step is to devise a way to regularize the theory. In a nutshell, what one has to do is to subtract the divergent part $\Delta m/(4\pi\hbar^2|\boldsymbol{r}_1-\boldsymbol{r}_2|)$ from the rest in the limit $|\boldsymbol{r}_1-\boldsymbol{r}_2|\to 0$. Formally one can justify this apparently rather arbitrary procedure, either by following the steps outlined typically in renormalizing the gap equation in infinite systems—by relating the divergent part with the scattering amplitude [6–10]—or by using well-known approaches in QFT—for example, dimensional regu-

larization [11,12], or another QFT approach of introducing appropriate counterterms with explicit cutoffs—or one can follow the philosophy of the pseudopotential approach [4,5,13]. In all cases one naturally arrives at the same final value for the gap. The renormalized gap equation can be written as

$$-\frac{1}{g}=\int\frac{d^3k}{(2\pi)^3}\left[\frac{1}{2\sqrt{[\varepsilon(\boldsymbol{k})-\mu]^2+\Delta^2}}-\frac{1}{2[\varepsilon(\boldsymbol{k})-\mu-i\gamma]}\right]+\frac{ik_Fm}{4\pi\hbar^2}, \tag{5}$$

where the coupling constant g is defined as

$$g\,\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)=\frac{\delta^2E_{gs}}{\delta\nu^*(\boldsymbol{r}_1)\,\delta\nu(\boldsymbol{r}_2)}. \tag{6}$$

Previous approaches [6–12] use $\varepsilon(\boldsymbol{k})$ only in the second term under the integral and in that case the last imaginary term does not appear. I have assumed here the simplest dependence of the LDA energy density functional on the anomalous density $\nu(\boldsymbol{r})$, namely, $\mathcal{E}(\tau(\boldsymbol{r}),\rho(\boldsymbol{r}),|\nu(\boldsymbol{r})|^2)$, merely for the sake of the simplicity of the presentation, but more general forms can be used 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 $V(\boldsymbol{r}_1-\boldsymbol{r}_2)=g\,\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$ (which can be related to the zero energy two-particle scattering amplitude $g=4\pi\hbar^2a/m$). As it has been well known for quite some time, even in the low density region, when $k_F|a|\ll1$, there are significant medium polarization corrections to the pairing gap [14]. The present LDA treatment is not limited by similar restrictions on the density. In the LDA energy density functional the polarization effects are already implicitly included in the definition of $\mathcal{E}(\tau(\boldsymbol{r}),\rho(\boldsymbol{r}),|\nu(\boldsymbol{r})|^2)$ 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.

Equation (5) can be used to extract from known properties of homogeneous infinite matter [such as $\varepsilon(\boldsymbol{k})$, Δ and density] the specific value of the coupling constant g to be used in constructing $\mathcal{E}(\tau(\boldsymbol{r}),\rho(\boldsymbol{r}),|\nu(\boldsymbol{r})|^2)$. Assuming that a full microscopic calculation of homogeneous matter at a given density $\rho=k_F^3/3\pi^2$ has been performed and that the value of the pairing gap at the Fermi level is known, one can, using Eq. (5), calculate directly $g(\rho)$ and thus obtain the simplest approximation to the LDA energy density functional $\mathcal{E}_{LDA}(\tau(\boldsymbol{r}),\,\rho(\boldsymbol{r}),\,|\nu(\boldsymbol{r})|^2)=\mathcal{E}_0(\tau(\boldsymbol{r}),\,\rho(\boldsymbol{r}))+g(\rho(\boldsymbol{r}))|\nu(\boldsymbol{r})|^2$, where $\mathcal{E}_0(\tau(\boldsymbol{r}),\rho(\boldsymbol{r}))$ is the Kohn-Sham energy density functional in the absence of pairing correlations. In many treatments of the pairing correlations in infinite systems authors often underline the dependence of the pairing gap on momentum, that is $\Delta(\boldsymbol{k})$. On one hand, typical calculations [15] of the pairing field $\Delta(\boldsymbol{k})$ 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 $|k-k_F|\approx m\Delta(k_F)/\hbar^2k_F\ll k_F$, the effect of the pairing correlations on the single-particle properties is small, if not negligible. To a very good accuracy

$$E(\boldsymbol{k})=\sqrt{[\varepsilon(\boldsymbol{k})-\mu]^2+\Delta^2(\boldsymbol{k})}\approx\sqrt{[\varepsilon(\boldsymbol{k})-\mu]^2+\Delta^2(\boldsymbol{k}_F)}\approx|\varepsilon(\boldsymbol{k})-\mu|$$

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 $\hbar^2k_F/m\Delta$ [9] is much larger then the average interparticle separation in the weak coupling limit. Typically this takes place when the range of the pairing interaction is smaller than the size of the Cooper pair as well, and thus the pairing interaction could be described by a single coupling constant.

Even though apparently the divergence has been successfully dealt with (in infinite homogeneous systems), a closer inspection of the entire approach reveals an inconsistency, which is somewhat hard to spot. The divergence is due to high momenta and for that reason one has subtracted the term $\Delta/2[\varepsilon(\boldsymbol{k})-\mu-i\gamma]$ in Eqs. (4) and (5). Far away from the Fermi surface, however, the problematic term $\Delta/2\sqrt{[\varepsilon(\boldsymbol{k})-\mu]^2+\Delta^2}$ behaves rather like $\Delta/2|\varepsilon(\boldsymbol{k})-\mu|$ instead. The main difference between these two subtraction procedures appears for holelike states. As the Fermi energy is finite, the integral over states below the Fermi level is also finite. This feature, which breaks the approximate symmetry between the particle and hole states, is rather unsatisfactory and it has no theoretical underpinning. On one hand, in calculating the integral over the single-particle spectrum above the fermi level one expects a relatively fast convergence, when the energy of the particle states is a ''few gaps Δ away.'' On the other hand, the integral over the hole states converges only for energies of the order of the Fermi energy $\epsilon_F=\hbar^2k_F^2/2m$. Clearly, in most cases of interest, the so called weak coupling limit, when $\Delta\ll\epsilon_F$, there is absolutely no physical reason to take into account single-particle states so far away from the Fermi level in order to describe global or mean-field properties of nuclei in particular.

I show here how a relatively simple regularization scheme can easily deal with this problem in a very clear and easily implementable manner, suitable for any system, finite or infinite, homogeneous or inhomogeneous. The regularized anomalous density is calculated from the following expression:

$$\nu_{reg}(\boldsymbol{r}):=\int_0^{E_c}dE\,g_{HFB}(E)\,v_E^*(\boldsymbol{r})\,u_E(\boldsymbol{r})-\int_{\mu-E_c}^{\mu+E_c}d\varepsilon\,g_{HF}(\varepsilon)\,\frac{\Delta(\boldsymbol{r})}{2}\,\frac{\psi_\varepsilon^*(\boldsymbol{r})\,\psi_\varepsilon(\boldsymbol{r})}{|\varepsilon-\mu|+i\gamma}+\frac{\Delta(\boldsymbol{r})}{2}\Gamma^{reg}(\boldsymbol{r},\mu), \tag{7}$$

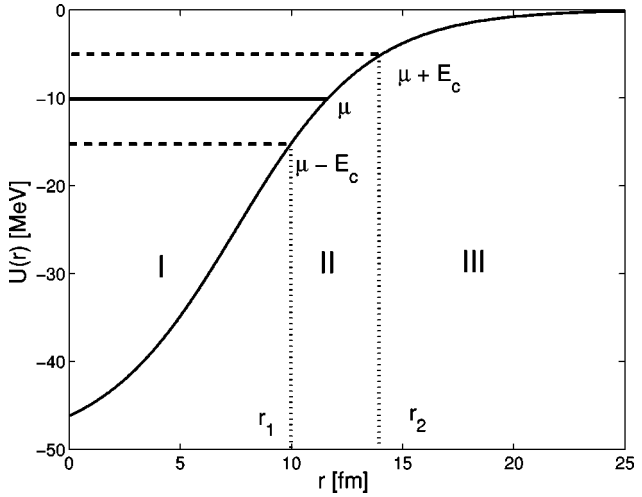

FIG. 1. In region I all three wave vectors $l_c(\boldsymbol{r}), k_F(\boldsymbol{r})$ and $k_c(\boldsymbol{r})$ are real and both subtraction terms are present. In region II $l_c(\boldsymbol{r})$ is imaginary and the corresponding subtraction term in Eq. (15) should be dropped. In region III all three wave vectors are imaginary and both subtraction terms in Eq. (15) should be dropped. Even though in region II $k_F(\boldsymbol{r})$ becomes imaginary for larger r, the corresponding subtraction term containing $k_F(\boldsymbol{r})$ is real everywhere and it should be retained.

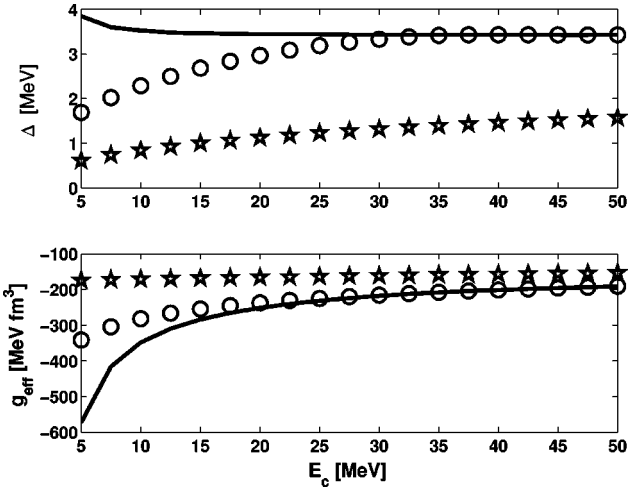

FIG. 2. The gap Δ and the effective coupling constant g_{eff} as a function of the cutoff energy E_c for three regularization schemes. The full lines correspond to calculations using Eqs. (15)–(17). Circles correspond to the regularization scheme presented in Ref. [5] (when only terms with k_c are present). The pentagrams correspond to the vacuum regularization scheme [16]. The calculation was performed for homogeneous neutron matter with $\rho = 0.08\ \mathrm{fm}^{-3}$ and $g = -250\ \mathrm{MeV\,fm}^3$.

where $g_{HFB}(E)$ and $g_{HF}(\varepsilon)$ are the HFB and HF density of states, respectively,

$$[h(\boldsymbol{r})-\varepsilon]\psi_\varepsilon(\boldsymbol{r})=0, \tag{8}$$

$$\Gamma(\boldsymbol{r}_1,\boldsymbol{r}_2,\mu)=\int d\varepsilon g_{HF}(\varepsilon)\frac{\psi^*_\varepsilon(\boldsymbol{r}_1)\psi_\varepsilon(\boldsymbol{r}_2)}{|\varepsilon-\mu|+i\gamma} \tag{9}$$

$$=\frac{m}{2\pi\hbar^2|\boldsymbol{r}_1-\boldsymbol{r}_2|}+\Gamma^{reg}(\boldsymbol{r},\mu)+O(|\boldsymbol{r}_1-\boldsymbol{r}_2|). \tag{10}$$

γ is as usual a small infinitesimal quantity and $\boldsymbol{r}=\boldsymbol{r}_{1,2}$ in the limit $|\boldsymbol{r}_1-\boldsymbol{r}_2|\to 0$. As in Ref. [5], I shall use a Thomas-Fermi approximation for the single-particle wave functions $\psi_\varepsilon(\boldsymbol{r})$ and energies in order to evaluate the regulator. After introducing the local wave vectors $l_c(\boldsymbol{r})\leqslant k_F(\boldsymbol{r})\leqslant k_c(\boldsymbol{r})$

$$h(\boldsymbol{r})=-\frac{\hbar^2\nabla^2}{2m}+U(\boldsymbol{r}), \tag{11}$$

$$\left[\frac{\hbar^2k_c^2(\boldsymbol{r})}{2m}+U(\boldsymbol{r})\right]=E_c+\mu, \tag{12}$$

$$\left[\frac{\hbar^2l_c^2(\boldsymbol{r})}{2m}+U(\boldsymbol{r})\right]=-E_c+\mu, \tag{13}$$

$$\frac{\hbar^2k_F^2(\boldsymbol{r})}{2m}+U(\boldsymbol{r})=\mu \tag{14}$$

and after some straightforward manipulations one can show that the renormalized anomalous density introduced above acquires the following form:

$$\nu_{reg}(\boldsymbol{r}):=\int_0^{E_c}dEg_{HFB}(E)v_E^*(\boldsymbol{r})u_E(\boldsymbol{r})-\frac{\Delta(\boldsymbol{r})mk_c(\boldsymbol{r})}{2\pi^2\hbar^2}\times\left\{1-\frac{k_F(\boldsymbol{r})}{2k_c(\boldsymbol{r})}\ln\frac{k_c(\boldsymbol{r})+k_F(\boldsymbol{r})}{k_c(\boldsymbol{r})-k_F(\boldsymbol{r})}\right\}-\frac{\Delta(\boldsymbol{r})ml_c(\boldsymbol{r})}{2\pi^2\hbar^2}\times\left\{1-\frac{k_F(\boldsymbol{r})}{2l_c(\boldsymbol{r})}\ln\frac{k_F(\boldsymbol{r})+l_c(\boldsymbol{r})}{k_F(\boldsymbol{r})-l_c(\boldsymbol{r})}\right\}. \tag{15}$$

The only formal difference between this expression and the corresponding expression introduced in Ref. [5] is in the terms containing the second cutoff momentum $l_c(\boldsymbol{r})$ (last line). If either one of the wave vectors $l_c(\boldsymbol{r})$ or $k_c(\boldsymbol{r})$ becomes imaginary, then the corresponding terms in the renormalized anomalous density $\nu_{reg}(\boldsymbol{r})$ should be dropped. However, if the wave vector $k_F(\boldsymbol{r})$ becomes imaginary, the renormalized anomalous density is real and the above definition should be used, see Fig. 1 for a generic situation.

It is convenient to introduce a notation for the cut-off anomalous density $\nu_c(\boldsymbol{r}):=\int_0^{E_c}dEg_{HFB}(E)v_E^*(\boldsymbol{r})u_E(\boldsymbol{r})$ and an effective position running coupling constant

$$\frac{1}{g_{eff}(\boldsymbol{r})}=\frac{1}{g}-\frac{mk_c(\boldsymbol{r})}{2\pi^2\hbar^2}\left\{1-\frac{k_F(\boldsymbol{r})}{2k_c(\boldsymbol{r})}\ln\frac{k_c(\boldsymbol{r})+k_F(\boldsymbol{r})}{k_c(\boldsymbol{r})-k_F(\boldsymbol{r})}\right\}-\frac{ml_c(\boldsymbol{r})}{2\pi^2\hbar^2}\left\{1-\frac{k_F(\boldsymbol{r})}{2l_c(\boldsymbol{r})}\ln\frac{k_F(\boldsymbol{r})+l_c(\boldsymbol{r})}{k_F(\boldsymbol{r})-l_c(\boldsymbol{r})}\right\}. \tag{16}$$

In the limit $k_F \to 0$ (in vacuum) the value of this effective running coupling constant agrees with that derived in Ref. [16]. Using these notations one obtains for the renormalized pairing field

$$\Delta(\boldsymbol{r}) = -g\,\nu_{reg}(\boldsymbol{r}) = -g_{eff}(\boldsymbol{r})\,\nu_c(\boldsymbol{r}). \tag{17}$$

Even though the cutoff momenta $k_c(\boldsymbol{r})$ and $l_c(\boldsymbol{r})$ and the cutoff quasiparticle energy E_c explicitly appear in the definition of both the effective coupling constant and of the cutoff anomalous density, the gap $\Delta(\boldsymbol{r})$ is indeed cutoff independent, once the cutoff energy E_c has been taken sufficiently far from the Fermi surface. This situation is similar to the situation described in Ref. [5], with the single difference that in the present case the convergence is achieved for significantly smaller values of E_c. As one can judge from Fig. 2, the present regularization scheme is indeed very fast converging, while the regularization scheme presented in Ref. [5] converges as expected at energies of the order of the Fermi energy $\epsilon_F = \hbar^2 k_F^2/2m$. At the same time, the traditional approach based on a δ function with cutoff energy E_c [16] (for which $g_{eff}(\boldsymbol{r}) = g/[1 - g m k_c(\boldsymbol{r})/2\pi^2\hbar^2]$) converges extremely slowly, and even at $E_c = 1000$ MeV is still about 20% off the converged value.

When computing the total energy of such a system one has to be careful and evaluate

$$E_{gs} = \int d^3r \left[\frac{\hbar^2}{2m}\tau_c(\boldsymbol{r}) - \Delta(\boldsymbol{r})\,\nu_c(\boldsymbol{r}) \right] + \int d^3r\, \mathcal{E}_0(0,\rho(\boldsymbol{r})), \tag{18}$$

where the kinetic energy density is evaluated as $\tau_c(\boldsymbol{r}) := 2\int_0^{E_c} dE\, g_{HFB}(E) |\boldsymbol{\nabla} v_E(\boldsymbol{r})|^2$. [I have assumed here the simplest dependence of $\mathcal{E}_0(\tau,\rho)$ on τ.] Only this combined expression, containing the trace of the kinetic energy with the trace of the pairing field and of the cutoff anomalous density, is converging as a function of the cutoff quasiparticle energy E_c [11]. The reason is that $\tau_c(\boldsymbol{r})$ diverges in a similar manner as $\nu_c(\boldsymbol{r})$ as a function of E_c.

The formalism described here paves the way to a LDA to pairing in the spirit of the Kohn-Sham theory [1]. One has simply to add to the usual LDA energy density functional a pairing term $g(\rho(\boldsymbol{r}))|\nu_c(\boldsymbol{r})|^2$ with a density dependent "bare coupling constant $g(\rho(\boldsymbol{r}))$," extracted from homogeneous infinite matter calculations. For the descriptions of many systems (e.g., nuclei, Fermionic atomic condensates, ^{3}He and neutron matter) a term linear in $|\nu_c(\boldsymbol{r})|^2$ will most likely suffice. However, as we already know from the Landau-Ginzburg theory, terms proportional to $|\nu_c(\boldsymbol{r})|^4$ might become relevant and in such a case the energy density functional should be generalized appropriately. Irrespective of the specific functional dependence of the energy density functional on the anomalous density $\nu_c(\boldsymbol{r})$, the emerging Kohn-Sham equations will be local and the ultraviolet divergence in the pairing field will have exactly the same character as the one studied here and consequently, can be dealt with using the same approach.

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