Superfluid LDA (SLDA): Describing pairing phenomena in nuclei, neutron stars and dilute fermi gases in traps

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Transparencies will be available shortly at <a href="http://www.phys.washington.edu/~bulgac">http://www.phys.washington.edu/~bulgac</a>



# Physics absences hamper research

#### by Dylan Lee Lehrke 10/21/2003

Yongle Yu, a physics graduate student, was optimistic when he went to Sweden last March to be interviewed for a postdoctoral position at the world-renowned Lund University. Yu got the position and had to return to UW only to take his final exams. But 10 months later, half a year after he was supposed to have graduated, Yu is in his home country of China waiting for a visa.



One of my favorite times in the academic year occurs in early spring when I give my class of extremely bright graduate students, who have mastered quantum mechanics but are otherwise unsuspecting and innocent, a takehome exam in which they are asked to deduce superfluidity from first principles, There is no doubt a special place in hell being reserved for me at this very moment for this mean trick, for the task is impossible. Superfluidity, like the fractional quantum Hall effect, is an emergent phenomenon - a low-energy collective effect of huge numbers of particles that cannot be deduced from the microscopic equations of motion in a rigorous way and that disappears completely when the system is taken apart<sup>A)</sup>. There are prototypes for superfluids, of course, and students who memorize them have taken the first step down the long road to understanding the phenomenon, but these are all approximate and in the end not deductive at all, but fits to experiment. The students feel betrayed and hurt by this experience because they have been trained to think in reductionist terms and thus to believe that everything not amenable to such thinking is unimportant. But nature is much more heartless than I am, and those students who stay in physics long enough to seriously confront the experimental record eventually come to understand that the reductionist idea is wrong a great deal of the time, and perhaps always.

Robert B. Laughlin, Nobel Lecture, December 8, 1998

## Superconductivity and superfluidity in Fermi systems

- ✓ Dilute atomic Fermi gases
- Liquid <sup>3</sup>He
- Metals, composite materials
- ✓ Nuclei, neutron stars
- QCD color superconductivity

$$\begin{split} T_c &> 10^{-12} \text{ eV} \\ T_c &> 10^{-7} \text{ eV} \\ T_c &> 10^{-3} - 10^{-2} \text{ eV} \\ T_c &> 10^5 - 10^6 \text{ eV} \\ T_c &> 10^7 - 10^8 \text{ eV} \end{split}$$

units (1 eV > 10<sup>4</sup> K)

Memorable years in the history of superfluidity and superconductivity of Fermi systems

- 1913 Kamerlingh Onnes
- 1972 Bardeen, Cooper and Schrieffer
- 1973 Esaki, Giaever and Josephson
- 1987 Bednorz and Muller
- 1996 Lee, Osheroff and Richardson
- 2003 Abrikosov, Ginzburg and Leggett







Alexei A. Abrikosov

Vitaly L. Ginzburg Anthony J. Leggett



#### How pairing emerges?

## Cooper's argument (1956)







## Contents

- Introduction (the part that you have just seen)
- > Description of the Superfluid LDA (SLDA).
- Application of SLDA to spherical nuclei in a fully self-consistent approach.
- Description of the vortex state in low density neutron matter (neutron stars).
- Application of SLDA in the strong coupling limit to the vortex state in a dilute atomic Fermi gas.
- ➢ Summary

#### References

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Phys. Rev. C **65**, 051305(R) (2002) nucl-th/0109083 (Lectures) nucl-th/0302007 (Appendix to PRL) nucl-th/0310066 in preparation Density Functional Theory (DFT) Hohenberg and <u>Kohn</u>, 1964

$$E_{gs} = \int d^3 r \varepsilon [\rho(\vec{r})]$$

Local Density Approximation (LDA) Kohn and Sham, 1965

$$E_{gs} = \int d^3 r \mathcal{E}[\rho(\vec{r}), \tau(\vec{r})]$$

$$\rho(\vec{r}) = \sum_{i=1}^{N} |\mathbf{v}_i(\vec{r})|^2$$
$$\tau(\vec{r}) = \sum_{i=1}^{N} |\vec{\nabla}\mathbf{v}_i(\vec{r})|^2$$

#### particle density

The energy density is typically determined in *ab initio* calculations of infinite homogeneous matter.

The main reason for the A in LDA is due to the inaccuracies of the gradient corrections.

#### Normal Fermi systems only!

Assume that there are two different manybody wave functions, corresponding to the same number particle density!

$$\Psi_{A}(\vec{r}_{1},...,\vec{r}_{N}) \neq \Psi_{B}(\vec{r}_{1},...,\vec{r}_{N}) \quad \text{Evaluation of the formation of the dense}$$

$$H = \sum_{i} T_{i} + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + ...$$

$$E_{A} = \left\langle \Psi_{A} \mid H + \sum_{i} V_{i} \mid \Psi_{A} \right\rangle = \left\langle \Psi_{A} \mid H \mid \Psi_{A} \right\rangle + \text{Tr}(V\rho)$$

$$E_{B} = \left\langle \Psi_{B} \mid H + \sum_{i} U_{i} \mid \Psi_{B} \right\rangle = \left\langle \Psi_{B} \mid H \mid \Psi_{B} \right\rangle + \text{Tr}(U\rho)$$

 $E_{A} < \left\langle \Psi_{B} \mid H \mid \Psi_{B} \right\rangle + \operatorname{Tr}(V\rho)$   $\frac{E_{B} < \left\langle \Psi_{A} \mid H \mid \Psi_{A} \right\rangle + \operatorname{Tr}(U\rho)}{E_{A} + E_{B} < E_{A} + E_{B}}$ 

 $\Psi_{A}(\vec{r}_{1},...,\vec{r}_{N}) \Rightarrow \rho(\vec{r})$ 

 $\Psi_{R}(\vec{r}_{1},...,\vec{r}_{N}) \Rightarrow \rho(\vec{r})$ 

Nonsense!

## LDA (Kohn-Sham) for superfluid fermi systems (Bogoliubov-de Gennes equations)

$$E_{gs} = \int d^{3}r \varepsilon(\rho(\vec{r}), \tau(\vec{r}), \nu(\vec{r}))$$
  

$$\rho(\vec{r}) = 2\sum_{k} |v_{k}(\vec{r})|^{2}, \quad \tau(\vec{r}) = 2\sum_{k} |\vec{\nabla}v_{k}(\vec{r})|^{2}$$
  

$$\nu(\vec{r}) = \sum_{k} u_{k}(\vec{r})v_{k}^{*}(\vec{r})$$
  

$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^{*}(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} u_{k}(\vec{r}) \\ v_{k}(\vec{r}) \end{pmatrix} = E_{k} \begin{pmatrix} u_{k}(\vec{r}) \\ v_{k}(\vec{r}) \end{pmatrix}$$

Mean-field and pairing field are both local fields! (for sake of simplicity spin degrees of freedom are not shown)

There is a little problem! The pairing field D diverges.

#### Why would one consider a local pairing field?

Because it makes sense physically!
The treatment is so much simpler!
Our intuition is so much better also.



$$r_0 \cong \frac{\hbar}{p_F} = k_F^{-1}$$

radius of interaction inter-particle separation

$$\Delta = \omega_D Exp\left(-\frac{1}{|V|N}\right) << \varepsilon_F$$

$$\boldsymbol{\xi} \approx \frac{1}{k_F} \frac{\boldsymbol{\varepsilon}_F}{\Delta} >> r_0$$

coherence length size of the Cooper pair

#### Nature of the problem

$$\nu(\vec{r}_{1},\vec{r}_{2}) = \sum_{E_{k}>0} v_{k}^{*}(\vec{r}_{1})u_{k}(\vec{r}_{2}) \propto \frac{1}{|\vec{r}_{1}-\vec{r}_{2}|} \quad \text{at small separation}$$
$$\Delta(\vec{r}_{1},\vec{r}_{2}) = \frac{1}{2}V(\vec{r}_{1},\vec{r}_{2})\nu(\vec{r}_{1},\vec{r}_{2})$$

ns

It is easier to show how this singularity appears in infinite homogeneous matter (BCS model)

$$v_{k}(\vec{r}_{1}) = v_{k} \exp(i\vec{k}\cdot\vec{r}_{1}), \quad u_{k}(\vec{r}_{2}) = u_{k} \exp(i\vec{k}\cdot\vec{r}_{2})$$
$$v_{k}^{2} = \frac{1}{2} \left( 1 - \frac{\varepsilon_{k} - \mu}{\sqrt{(\varepsilon_{k} - \mu)^{2} + \Delta^{2}}} \right), \quad u_{k}^{2} + v_{k}^{2} = 1, \quad \varepsilon_{k} = \frac{\hbar^{2}\vec{k}^{2}}{2m} + U, \quad \Delta = \frac{\hbar^{2}\delta}{2m}$$

$$\nu(r) = \frac{\Delta m}{2\pi^2 \hbar^2} \int_0^\infty dk \, \frac{\sin(kr)}{kr} \frac{k^2}{\sqrt{(k^2 - k_F^2)^2 + \delta^2}}, \qquad r = |\vec{r_1} - \vec{r_2}|$$

#### **Pseudo-potential approach**

(appropriate for very slow particles, very transparent but somewhat difficult to improve)

Lenz (1927), Fermi (1931), Blatt and Weiskopf (1952) Lee, Huang and Yang (1957)

$$-\frac{\hbar^{2}\Delta_{\vec{r}}}{m}\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}), \quad V(\vec{r}) \approx 0 \text{ if } r > R$$

$$\psi(\vec{r}) = \exp(i\vec{k}\cdot\vec{r}) + \frac{f}{r}\exp(ikr) \approx 1 + \frac{f}{r} + \dots \approx 1 - \frac{a}{r} + O(kr)$$

$$f^{-1} = -\frac{1}{a} + \frac{1}{2}r_{0}k^{2} - ik, \qquad g = \frac{4\pi \hbar^{2}a}{m(1 + ika)} + \dots$$

$$\text{if } kr_{0} << 1 \quad \text{then} \quad V(\vec{r})\psi(\vec{r}) \Rightarrow g\delta(\vec{r})\frac{\partial}{\partial r}[r\psi(\vec{r})]$$

$$\text{Example} : \psi(\vec{r}) = \frac{A}{r} + B + \dots \Rightarrow \delta(\vec{r})\frac{\partial}{\partial r}[r\psi(\vec{r})] = \delta(\vec{r})B$$

The SLDA (renormalized) equations

$$E_{gs} = \int d^{3}r \left\{ \varepsilon_{N} \left[ \rho(\vec{r}), \tau(\vec{r}) \right] + \varepsilon_{S} \left[ \rho(\vec{r}), \nu(\vec{r}) \right] \right\}$$
$$\varepsilon_{S} \left[ \rho(\vec{r}), \nu(\vec{r}) \right] \stackrel{def}{=} -\Delta(\vec{r}) \nu_{c}(\vec{r}) = g_{eff}(\vec{r}) |\nu_{c}(\vec{r})|^{2}$$

 $\begin{cases} [h(\vec{r}) - \mu] u_{i}(\vec{r}) + \Delta(\vec{r}) v_{i}(\vec{r}) = E_{i} u_{i}(\vec{r}) \\ \Delta^{*}(\vec{r}) u_{i}(\vec{r}) - [h(\vec{r}) - \mu] v_{i}(\vec{r}) = E_{i} v_{i}(\vec{r}) \end{cases} \begin{cases} h(\vec{r}) = -\vec{\nabla} \frac{\hbar^{2}}{2m(\vec{r})} \vec{\nabla} + U(\vec{r}) \\ \Delta(\vec{r}) = -g_{eff}(\vec{r}) v_{c}(\vec{r}) \end{cases}$ 

$$\frac{1}{g_{eff}(\vec{r})} = \frac{1}{g[\rho(\vec{r})]} - \frac{m(\vec{r})k_c(\vec{r})}{2\pi^2\hbar^2} \left\{ 1 - \frac{k_F(\vec{r})}{2k_c(\vec{r})} \ln \frac{k_c(\vec{r}) + k_F(\vec{r})}{k_c(\vec{r}) - k_F(\vec{r})} \right\}$$

$$\rho_{c}(\vec{r}) = 2\sum_{E_{i}\geq0}^{E_{c}} |\mathbf{v}_{i}(\vec{r})|^{2}, \quad v_{c}(\vec{r}) = \sum_{E_{i}\geq0}^{E_{c}} \mathbf{v}_{i}^{*}(\vec{r})\mathbf{u}_{i}(\vec{r})$$
$$E_{c} + \mu = \frac{\hbar^{2}k_{c}^{2}(\vec{r})}{2m(\vec{r})} + U(\vec{r}), \quad \mu = \frac{\hbar^{2}k_{F}^{2}(\vec{r})}{2m(\vec{r})} + U(\vec{r})$$

Position and momentum dependent running coupling constant Observables are (obviously) independent of cut-off energy (when chosen properly).





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November 10, 2003

Energy Secretary Spencer Abraham Announces Department of Energy 20-Year Science Facility Plan Sets Priorities for 28 New, Major Science Research Facilities





Facilities for the Future of Science: A Twenty-Year Outlook



**Reaccelerated Beams** 

A (significantly) abridged list of major questions still left unanswered in nuclear physics concerning pairing correlations:

- ✓ Do nuclear pairing correlations have a volume or/and surface character?
- The density dependence of the pairing gap (partially related to the previous topic), the role of higher partial waves (p-wave etc.) especially in neutron matter.
- The role of the isospin symmetry in nuclear pairing.
- Pairing in T = 0 channel?
- Does the presence or absence of neutron superfluidity have any influence on the presence and/or character of proton superfluidity and vice versa. New question raised recently: are neutron stars type I or II superconductors?

# Pairing correlations show prominently in the staggering of the binding energies.

Systems with odd particle number are less bound than systems with even particle number.



#### **One-neutron separation energies**



Volume pairing  $g(\vec{r}) = g$ 

Volume + Surface pairing

$$g(\vec{r}) = V_0 \left( 1 - \frac{\rho(\vec{r})}{\rho_c} \right)$$

Normal EDF:

SLy4 - Chabanat et al.
 Nucl. Phys. A627, 710 (1997)
 Nucl. Phys. A635, 231 (1998)
 Nucl. Phys. A643, 441(E)(1998)

➢ FaNDF<sup>0</sup> – Fayans JETP Lett. 68, 169 (1998)

#### Two-neutron separation energies



#### **One-nucleon separation energies**



How can one determine the density dependence of the coupling constant g? I know two methods.

✓ In homogeneous low density matter one can compute the pairing gap as a function of the density. NB this is not a BCS/HFB result!

$$\Delta = \left(\frac{2}{e}\right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right)$$

 One compute also the energy of the normal and superfluid phases as a function of density, as was recently done by Carlson et al, Phys. Rev. Lett. 91, 050401 (2003) for a Fermi system interacting with an infinite scattering length (Bertsch's MBX 1999 challenge)

In both cases one can extract from these results the superfluid contribution to the LDA energy density functional in a straight forward manner.

#### Anderson and Itoh, Nature, 1975

"Pulsar glitches and restlessness as a hard superfluidity phenomenon" *The crust of neutron stars is the only other place in the entire Universe where one can find solid matter, except planets.* Superfluidity phenomenon" A NEUTRON STAR: SURFACE and INTERIOR

A neutron star will cover the map at the bottom
The mass is about 1.5 solar masses
Density 10<sup>14</sup> g/cm<sup>3</sup>





#### **Author: Dany Page**

#### Landau criterion for superflow stability (flow without dissipation)

Consider a superfluid flowing in a pipe with velocity v<sub>s:</sub>

$$E_0 + \frac{Nmv_s^2}{2} < E_0 + \varepsilon_{\vec{p}} + \vec{v}_s \cdot \vec{p} + \frac{Nmv_s^2}{2} \Longrightarrow v_s < \frac{\varepsilon_{\vec{p}}}{p}$$

no internal excitations

One single quasi-particle excitation with momentum p

In the case of a Fermi superfluid this condition becomes



## Vortex in neutron matter

$$\begin{pmatrix} u_{\alpha \ln}(\vec{r}) \\ v_{\alpha \ln}(\vec{r}) \end{pmatrix} = \begin{pmatrix} u_{\alpha}(r) \exp[i(n+1/2)\phi - ikz] \\ v_{\alpha}(r) \exp[i(n-1/2)\phi - ikz] \end{pmatrix}, \quad n - \text{half-integer}$$

 $\Delta(\vec{r}) = \Delta(r) \exp(i\phi), \qquad \vec{r} = (r, \phi, z) \text{ [cyllindrical coordinates]}$ Oz - vortex symmetry axis

Ideal vortex, Onsager's quantization (one  $\hbar$  per Cooper pair)

$$\vec{\mathrm{V}}_{\mathrm{v}}(\vec{r}) = \frac{\hbar}{2mr^2}(y, -x, 0) \iff \frac{1}{2\pi} \oint_C \vec{\mathrm{V}}_{\mathrm{v}}(\vec{r}) \cdot d\vec{r} = \frac{\hbar}{2m}$$

## "Screening effects" are significant!





s-wave pairing gap in infinite neutron matter with realistic NN-interactions

# from Lombardo and Schulze astro-ph/0012209

These are major effects beyond the naïve HFB when it comes to describing pairing correlations.





# Dramatic structural changes of the vortex state naturally lead to significant changes in the energy balance of a neutron star

•  $\frac{\mathbf{v}_{\mathrm{S}}}{\mathbf{v}_{\mathrm{F}}} \leq \frac{\Delta}{2\varepsilon_{\mathrm{F}}}\Big|_{\mathrm{max}} \approx 0.12$ , extremely fast vortical motion,  $\frac{\lambda_{\mathrm{F}}}{\xi} \propto \frac{\Delta}{\varepsilon_{\mathrm{F}}}$ • In low density region  $\varepsilon(\rho_{out})\rho_{out} > \varepsilon(\rho_{in})\rho_{in}$ which thus leads to a large anti - pinning energy  $E_{pin}^{V} > 0$ :

 $E_{pin}^{V} = \left[ \varepsilon(\rho_{out}) \rho_{out} - \varepsilon(\rho_{in}) \rho_{in} \right] V$ 

• The energy per unit length is going to be changed dramatically when compared to previous estimates, by

$$\frac{\Delta E_{\text{vortex}}}{L} \approx \left[ \varepsilon(\rho_{out}) \rho_{out} - \varepsilon(\rho_{in}) \rho_{in} \right] \pi R^2$$

• Specific heat, transport properties are expected to significantly affected as well.

Some similar conclusions have been reached recently also by Donati and Pizzochero, Phys. Rev. Lett. <u>90</u>, 211101 (2003).

# Vortices in dilute atomic Fermi systems in traps

#### ✓ 1995 BEC was observed.

- ✓ 2000 vortices in BEC were created, thus BEC confirmed un-ambiguously.
- In 1999 DeMarco and Jin created a degenerate atomic Fermi gas.
- ✓ 2002 O'Hara, Hammer, Gehm, Granada and Thomas observed expansion of a Fermi cloud compatible with the existence of a superfluid fermionic phase.

Observation of stable/quantized vortices in Fermi systems would provide the ultimate and most spectacular proof for the existence of a Fermionic superfluid phase. Why would one study vortices in neutral Fermi superfluids?

They are perhaps just about the only phenomenon in which one can have a true stable superflow!

# How can one put in evidence a vortex in a Fermi superfluid?

Hard to see, since density changes are not expected, unlike the case of a Bose superfluid.

What we learned from the structure of a vortex in low density neutron matter can help however.

If the gap is not small one can expect a noticeable density depletion along the vortex core, and the bigger the gap the bigger the depletion.

One can change the magnitude of the gap by altering the scattering length between two atoms with magnetic fields by means of a Feshbach resonance.

# Feshbach resonance

$$H = \frac{\vec{p}^2}{2\mu_r} + \sum_{i=1}^2 (V_i^{hf} + V_i^Z) + V_0(\vec{r})P_0 + V_1(\vec{r})P_1 + V^d$$
$$V^{hf} = \frac{a_{hf}}{r^2} \vec{S}^e \cdot \vec{S}^n, \ V^Z = (\gamma_e S_z^e - \gamma_n S_z^n)B$$

#### Tiesinga, Verhaar, Stoof Phys. Rev. A47, 4114 (1993)

h



Regal and Jin Phys. Rev. Lett. **90**, 230404 (2003)



Consider Bertsch's MBX challenge (1999): "Find the ground state of infinite homogeneous neutron matter interacting with an infinite scattering length."  $r_0 \rightarrow 0 \ll \lambda_F \ll |a| \rightarrow \infty$ 

PRC 68, 025802 (2003), with Green Function Monte Carlo (GFMC)

$$\frac{E_N}{N} = \alpha_N \frac{3}{5} \varepsilon_{F,} \quad \alpha_N = 0.54$$

normal state

Carlson, Chang, Pandharipande and Schmidt, PRL 91, 050401 (2003), with GFMC

$$\frac{E_S}{N} = \alpha_S \frac{3}{5} \varepsilon_{F,} \quad \alpha_S = 0.44$$

superfluid state

This state is half the way from  $BCS \rightarrow BEC$  crossover, the pairing correlations are in the strong coupling limit and HFB invalid again.

#### BCS $\rightarrow$ BEC crossover

Leggett (1980), Nozieres and Schmitt-Rink (1985), Randeria *et al.* (1993),... If a<0 at T=0 a Fermi system is a BCS superfluid

$$\Delta \approx \left(\frac{2}{e}\right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right) << \varepsilon_F, \quad \text{iff} \quad k_F \mid a \mid << 1 \text{ and } \xi = \frac{1}{k_F} \frac{\varepsilon_F}{\Delta} >> \frac{1}{k_F}$$

If  $|a|=\infty$  and  $nr_0^{-3}\dot{a}$  1 a Fermi system is strongly coupled and its properties are universal. Carlson *et al.* PRL <u>91</u>, 050401 (2003)

$$\frac{E_{\text{normal}}}{N} \approx 0.54 \frac{3}{5} \varepsilon_F, \qquad \frac{E_{\text{superfluid}}}{N} \approx 0.44 \frac{3}{5} \varepsilon_F \quad \text{and } \xi = O(\lambda_F), \ \Delta = O(\varepsilon_F)$$

If a>0 ( $a>>r_0$ ) and  $na^3á$  1 the system is a dilute BEC of tightly bound dimers

$$\varepsilon_2 = -\frac{\hbar^2}{ma^2}$$
 and  $n_b a^3 << 1$ , where  $n_b = \frac{n_f}{2}$  and  $a_{bb} = 0.61a > 0$ 

# Now one can construct an LDA functional to describe this new state of Fermionic matter

$$\begin{aligned} \mathcal{E}(\boldsymbol{r})n(\boldsymbol{r}) &= \frac{\hbar^2}{m} \left[ \frac{m}{2m^*} \tau(\boldsymbol{r}) + \beta n(\boldsymbol{r})^{5/3} + \gamma \frac{|\nu(\boldsymbol{r})|^2}{n(\boldsymbol{r})^{1/3}} \right], \\ n(\boldsymbol{r}) &= \sum_{\alpha} |v_{\alpha}(\boldsymbol{r})|^2, \quad \tau(\boldsymbol{r}) = \sum_{\alpha} |\boldsymbol{\nabla} v_{\alpha}(\boldsymbol{r})|^2, \\ \nu(\boldsymbol{r}) &= \sum_{\alpha} v_{\alpha}^*(\boldsymbol{r}) u_{\alpha}(\boldsymbol{r}). \end{aligned}$$

This form is not unique, as one can have either:
 b=0 (set I) or b≠0 and m\*=m (set II).
 Gradient terms not determined yet (expected minor role).

Solid lines - parameter set I, \_\_\_\_\_ Dashed lines for parameter set II Dots – velocity profile for ideal vortex

The depletion along the vortex core is reminiscent of the corresponding density depletion in the case of a vortex in a Bose superfluid, when the density vanishes exactly along the axis for 100% BEC.



#### Extremely fast quantum vortical motion!





#### **Conclusions:**

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. . .

 An LDA-DFT formalism for describing pairing correlations in Fermi systems has been developed. This represents the first genuinely local extention of the Kohn-Sham LDA from normal to superfluid systems - <u>SLDA</u>



