Ground State and Vortex State Properties of Strongly Coupled Fermi Superfluids

Aurel Bulgac

Colaborators: Yongle Yu (for the most part), P.F. Bedaque, A.C. Fonseca

Transparencies (both in ppt and pdf format) shall become shortly available at http://www.phys.washington.edu/~bulgac

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!

What shall I cover in this talk?

SLDA - Superfluid LDA

A brief introduction into the extension of the Kohn-Shall LDA to superfluid fermionic systems (A. Bulgac and Y. Yu, Phys. Rev. Lett. <u>88</u>, 042504 (2002) Y. Yu and A. Bulgac, Phys. Rev. Lett. <u>90</u>, 222501 (2003))

Vortices in the crust of neutron stars

Vortices in dilute superfluid Fermi gases and some related issues

 Density profiles of dilute normal and superfluid Fermi gases in traps Density Functional Theory (DFT) Hohenberg and Kohn, 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

Normal Fermi systems only!

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

$$\Psi_{A}(\vec{r}_{1},...,\vec{r}_{N}) \neq \Psi_{B}(\vec{r}_{1},...,\vec{r}_{N})$$

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

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

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

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

 $\Psi_A(\vec{r}_1,...,\vec{r}_N) \Rightarrow \rho(\vec{r})$

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

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

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

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

$$\nu(\vec{r}) = \sum_{k} \mathbf{u}_{k}(\vec{r})\mathbf{v}_{k}^{*}(\vec{r})$$

$$\begin{pmatrix} T + U(\vec{r}) - \lambda & \Delta(\vec{r}) \\ \Delta^{*}(\vec{r}) & -(T + U(\vec{r}) - \lambda) \end{pmatrix} \begin{pmatrix} \mathbf{u}_{k}(\vec{r}) \\ \mathbf{v}_{k}(\vec{r}) \end{pmatrix} = E_{k} \begin{pmatrix} \mathbf{u}_{k}(\vec{r}) \\ \mathbf{v}_{k}(\vec{r}) \end{pmatrix}$$

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

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

$$\xi \approx \frac{1}{k_F} \frac{\varepsilon_F}{\Delta} >> r_0$$

coherence length size of the Cooper pair

Nature of the problem

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

ations

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

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

$$v(r) = \frac{\Delta m}{2\pi^2 \hbar^2} \int_0^\infty dk \, \frac{\sin(kr)}{kr} \frac{k^2}{\sqrt{(k^2 - k_F^2)^2 + \delta^2}}$$

Solution of the problem in the case of the homogeneous matter (Lee, Huang and Yang and others)

Gap equation

$$V(\vec{r}_{1} - \vec{r}_{2}) = g\delta(\vec{r}_{1} - \vec{r}_{2})$$

$$1 = -\frac{g}{2} \int \frac{d^3k}{\left(2\pi\right)^3} \frac{1}{\sqrt{\left(\varepsilon_k - \lambda\right)^2 + \Delta^2}}$$

Lippmann-Schwinger equation (zero energy collision) T = V + VGT

$$-\frac{mg}{4\pi\hbar^2 a} + 1 = -\frac{g}{2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\varepsilon_k}$$

Now combine the two equations and the divergence is (magically) removed!

$$\frac{m}{4\pi\hbar^2 a} = -\frac{1}{2} \int \frac{d^3 k}{\left(2\pi\right)^3} \left\{ \frac{1}{\sqrt{\left(\varepsilon_k - \lambda\right)^2 + \Delta^2}} - \frac{1}{\varepsilon_k} \right\}$$

How people deal with this problem in finite (nuclei) systems?

- ✓ Introduce an explicit energy cut-off, which can vary from 5 MeV to 100 MeV (sometimes significantly higher) from the Fermi energy.
- Use a particle-particle interaction with a finite range, the most popular one being Gogny's interaction.
- Both approaches are in the final analysis equivalent in principle, as a potential with a finite range $\mathbf{r_0}$ provides a (smooth) cut-off at an energy $\mathbf{E_c} = \hbar^2/mr_0^2$
- The argument that nuclear forces have a finite range is superfluous, because nuclear pairing is manifest at small energies and distances of the order of the coherence length, which is much smaller than nuclear radii.
- > Moreover, LDA works pretty well for the regular mean-field.

A similar argument fails as well in case of electrons, where the radius of the interaction is infinite and LDA is fine.

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)

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

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

$$f^{-1} = -\frac{1}{a} + \frac{1}{2}r_{0}k^{2} - ik, \qquad g = \frac{4\pi \hbar^{2}a}{m(1+ika)} + \dots$$
if $kr_{0} << 1$ then $V(\vec{r})\psi(\vec{r}) \Rightarrow g\delta(\vec{r})\frac{\partial}{\partial r}[r\psi(\vec{r})]$
Example : $\psi(\vec{r}) = \frac{A}{r} + B + \dots \Rightarrow \delta(\vec{r})\frac{\partial}{\partial r}[r\psi(\vec{r})] = \delta(\vec{r})B$

How to deal with an inhomogeneous/finite system?

$$\begin{split} \nu_{reg}(\vec{r}) &= \sum_{i} \left[v_{i}^{*}(\vec{r})u_{i}(\vec{r}) + \frac{\Delta(\vec{r})\psi_{i}^{*}(\vec{r})\psi_{i}(\vec{r})}{2(\lambda - \varepsilon_{i})} \right] - \frac{\Delta(\vec{r})}{2}G_{reg}(\lambda, \vec{r}) \\ G_{reg}(\lambda, \vec{r}) &= \lim_{\vec{r}' \to \vec{r}} \left[G(\vec{r}, \vec{r}', \lambda) + \frac{m}{2\pi\hbar^{2}|\vec{r} - \vec{r}'|} \right] \\ \left[h(\vec{r}) - \varepsilon_{i} \right] \psi_{i}(\vec{r}) = 0 \\ \left[\lambda - h(\vec{r}) \right] G(\vec{r}, \vec{r}', \lambda) = \delta(\vec{r} - \vec{r}') \end{split}$$

There is complete freedom in choosing the Hamiltonian h and we are going to take advantage of this!

We shall use a "Thomas-Fermi" approximation for the propagator G.

$$\begin{aligned} G(\vec{r}, \vec{r}', \lambda) &= -\frac{m \exp(ik_F(\vec{r})|\vec{r} - \vec{r}'|)}{2\pi\hbar^2 |\vec{r} - \vec{r}'|} \\ &\approx -\frac{m}{2\pi\hbar^2 |\vec{r} - \vec{r}'|} - \frac{ik_F(\vec{r})m}{2\pi\hbar^2} + O(|\vec{r} - \vec{r}'|) \\ \frac{\hbar^2 k_F^2(\vec{r})}{2m} + U(\vec{r}) &= \lambda, \quad \frac{\hbar^2 k_c^2(\vec{r})}{2m} + U(\vec{r}) = \lambda + E_c \end{aligned}$$

$$v_{\text{reg}}(\vec{r}) \stackrel{def}{=} \left\{ \sum_{E_i \le E_c} v_i^*(\vec{r}) u_i(\vec{r}) + \frac{\Delta(\vec{r})}{4\pi^2} \int_0^{k_c(\vec{r})} \frac{1}{\lambda - \frac{\hbar^2 k^2}{2m} - U(\vec{r}) + i\gamma} k^2 dk \right\} + \frac{i\Delta(\vec{r})k_F(\vec{r})m}{4\pi\hbar^2}$$

Regularized anomalous density

Regular part of G

SLDA equations for superfluid Fermi systems:

Energy Density (ED) describing the normal phase

Additional contribution to ED due to superfluid correlations

$$\begin{split} E_{gs} &= \int d^{3}r [\mathcal{E}_{N}(\mathbf{r}) + \mathcal{E}_{S}(\mathbf{r})], \\ \mathcal{E}_{S}(\mathbf{r}) &:= -\Delta(\mathbf{r})\nu_{c}(\mathbf{r}) = g_{eff}(\mathbf{r})|\nu_{c}(\mathbf{r})|^{2}, \\ &\left\{ \begin{array}{l} [h(\mathbf{r}) - \mu]u_{i}(\mathbf{r}) + \Delta(\mathbf{r})v_{i}(\mathbf{r}) = E_{i}u_{i}(\mathbf{r}), \\ \Delta^{*}(\mathbf{r})u_{i}(\mathbf{r}) - [h(\mathbf{r}) - \mu]v_{i}(\mathbf{r}) = E_{i}v_{i}(\mathbf{r}), \end{array} \right. \\ h(\mathbf{r}) &= -\nabla \frac{\hbar^{2}}{2m(\mathbf{r})}\nabla + U(\mathbf{r}), \quad \Delta(\mathbf{r}) := -g_{eff}(\mathbf{r})\nu_{c}(\mathbf{r}), \\ &\left. \frac{1}{g_{eff}(\mathbf{r})} = \frac{1}{g(\mathbf{r})} - \frac{mk_{c}(\mathbf{r})}{2\pi^{2}\hbar^{2}} \left[1 - \frac{k_{F}(\mathbf{r})}{2k_{c}(\mathbf{r})} \ln \frac{k_{c}(\mathbf{r}) + k_{F}(\mathbf{r})}{k_{c}(\mathbf{r}) - k_{F}(\mathbf{r})} \right] \\ &\rho_{c}(\mathbf{r}) = \sum_{E_{i}\geq0}^{E_{c}} 2|v_{i}(\mathbf{r})|^{2}, \quad \nu_{c}(\mathbf{r}) = \sum_{E_{i}\geq0}^{E_{c}} v_{i}^{*}(\mathbf{r})u_{i}(\mathbf{r}), \\ &E_{c} + \mu = \frac{\hbar^{2}k_{c}^{2}(\mathbf{r})}{2m(\mathbf{r})} + U(\mathbf{r}), \quad \mu = \frac{\hbar^{2}k_{F}^{2}(\mathbf{r})}{2m(\mathbf{r})} + U(\mathbf{r}). \end{split}$$

Typo: replace m by m(r)

Y.Yu and A. Bulgac, PRL <u>90</u>, 222501 (2003)

Peculiarity of the finite systems: deep hole states are continuum states.

Andreev reflection



Integration contours used to construct the normal and anomalous densities from the Gorkov Green functions Belyaev *et al,* Sov. J. Nucl. Phys. <u>45</u>, 783 (1987).

$$\begin{pmatrix} E - (h - \lambda) & -\Delta \\ * & * \\ -\Delta & E + (h^* - \lambda) \end{pmatrix} \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



Even systems

Odd systems

Let me backtrack a bit and summarize some of the SLDA ingredients.

Energy Density (ED) describing the normal system

ED contribution due to superfluid correlations

$$E_{gs} = \int d^3r \left\{ \varepsilon_N^* [\rho_n(\vec{r}), \rho_p(\vec{r})] + \varepsilon_S^* [\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] \right\}$$

$$\left\{ \varepsilon_N^* [\rho_n(\vec{r}), \rho_p(\vec{r})] = \varepsilon_N^* [\rho_p(\vec{r}), \rho_n(\vec{r})]$$

$$\left\{ \varepsilon_S^* [\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] = \varepsilon_S^* [\rho_p(\vec{r}), \rho_n(\vec{r}), \nu_p(\vec{r}), \nu_n(\vec{r})] \right\}$$

Isospin symmetry

(Coulomb energy and other relatively small terms not shown here.)

Let us consider the simplest possible ED compatible with nuclear symmetries and with the fact that nuclear pairing corrrelations are relatively weak.

$$\mathcal{E}_{S}\left[\rho_{p},\rho_{n},\nu_{p},\nu_{n}\right] = g_{0}\left[\nu_{p}+\nu_{n}\right]^{2} + g_{1}\left[\nu_{p}-\nu_{n}\right]^{2}$$

$$\underbrace{\nu_{p}-\nu_{n}}_{\text{like }\rho_{p}+\rho_{n}} = \frac{1}{2}\left[\nu_{p}-\nu_{n}\right]^{2}$$

 g_0 and g_1 could depend as well on ρ_p and ρ_n

In the end one finds that a suitable superfluid nuclear EDF has the following structure:

Isospin symmetric $\mathcal{E}_{S}[v_{p},v_{n}] = g(\rho_{p},\rho_{n})[|v_{p}|^{2} + |v_{n}|^{2}]$ + $f(\rho_p, \rho_n)[|v_p|^2 - |v_n|^2] \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$ where $g(\rho_n, \rho_n) = g(\rho_n, \rho_n)$ and $f(\rho_p, \rho_n) = f(\rho_n, \rho_p)$

Charge symmetric

Let us now remember that there are more neutron rich nuclei and let me estimate the following quantity from all measured nuclear masses:

$$\frac{\overline{N-Z}}{A} = 0.1473$$

Conjecturing now that Goriely *et al*, Phys. Rev. C <u>66</u>, 024326 (2002) have as a matter of fact replaced in the "true" pairing EDF the isospin density dependence simply by its average over all masses, one can easily extract from their pairing parameters the following relation:

$$\varepsilon_{S} \left[v_{p}, v_{n} \right] = g \left[|v_{p}|^{2} + |v_{n}|^{2} \right]$$

$$+ f \left[|v_{p}|^{2} - |v_{n}|^{2} \right] \frac{\rho_{p} - \rho_{n}}{\rho_{p} + \rho_{n}}$$
where $f \approx -0.39 \ g > 0$ and $g < 0$
repulsion

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 or 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. <u>91</u>, 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.

What shall I cover in this talk?

SLDA - Superfluid LDA

A brief introduction into the extension of the Kohn-Shall LDA to superfluid fermion systems

 Vortices in the crust of neutron stars (Y. Yu and A. Bulgac, Phys. Rev. Lett. <u>90</u>, 161101 (2003))

Vortices in dilute superfluid Fermi gases and some related issues

 Density profiles of dilute normal and superfluid Fermi gases in traps



Borrowed from http://www.lsw.uni-heidelberg.de/~mcamenzi/NS Mass.html, author Dany Page

"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.

Let us check a simple example, homogeneous dilute Fermi gas with a weak attractive interaction, when pairing correlations occur in the ground state.

$$\Delta = \frac{8}{e^2} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right)$$

BCS result

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

An additional factor of $1/(4e)^{1/3} \approx 0.45$ is due to induced interactions Gorkov and Melik-Barkhudarov in 1961.

BCS/HFB in error even when the interaction is very weak, <u>unlike HF</u>!



FIG. 1. Diagrams for the induced interactions between two fermions in different internal states to second order in the effective interaction.

from Heiselberg et al Phys. Rev. Lett. <u>85</u>, 2418, (2000)



$$\Delta = \left(\frac{2}{e}\right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp\left[-\frac{\pi}{2\tan\delta(k_F)}\right]$$

RG- renormalization group calculation Schwenk, Friman, Brown, Nucl.Phys. <u>A713</u>, 191 (2003)R

Landau criterion for superflow stability (flow without dissipation)

Consider a superfluid flowing in a pipe with velocity v_{s:}

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

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

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

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

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

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

Y. Yu and A. Bulgac, PRL <u>90</u>, 161101 (2003)



Fayans's FaNDF⁰

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

An additional factor of **1/(4e)**^{1/3} is due to induced interactions Again, HFB not valid.



FIG. 1. Diagrams for the induced interactions between two fermions in different internal states to second order in the effective interaction.

from Heiselberg et al Phys. Rev. Lett. <u>85</u>, 2418, (2000)



Y. Yu and A. Bulgac, PRL 90, 161101 (2003)

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).

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(A. Bulgac and Y. Yu, Phys. Rev. Lett. <u>91</u>, 190404 (2003))

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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. A<u>47</u>, 4114 (1993)

 \hbar^2



Regal and Jin Phys. Rev. Lett. <u>90</u>, 230404 (2003)



Reagal, Ticknor, Bohm and Jin, Nature 424, 47 (2003)





Number of atoms after ramping B from 228.25 G to 216.15 (black dots) and for ramping B down (at 40 ns/G) and up at various rates (squares).

- a) Loss of atoms |9/2,-9/2> and |9/2,-5/2> as a function of final B. The initial value of B=227.81 G.
- b) Scattering length between hyperfine states |9/2,-9/2> and |9/2,-5/2> as a function of the magnetic field B.

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

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

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)

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

If a>0 ($a>>r_0$) and na^3a 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 $a_{bb} = 0.61a > 0$

What do we know about dilute normal Fermi systems? (For a recent review see Hammer and Furnstahl, Nucl. Phys. <u>A678</u>, 277 (2000))

$$\frac{E}{N} = \frac{k_{\rm F}^2}{2M} \left[\frac{3}{5} + (g-1) \left\{ \frac{2}{3\pi} (k_{\rm F}a_s) + \frac{4}{35\pi^2} (11-2\ln2)(k_{\rm F}a_s)^2 + \frac{1}{10\pi} (k_{\rm F}r_s)(k_{\rm F}a_s)^2 + (0.076 + 0.057(g-3))(k_{\rm F}a_s)^3 \right\} + (g+1)\frac{1}{5\pi} (k_{\rm F}a_p)^3 + (g-1)(g-2)\frac{16}{27\pi^3} (4\pi - 3\sqrt{3})(k_{\rm F}a_s)^4 \ln(k_{\rm F}a_s) + \cdots \right].$$
(1)

g – spin degeneracy, a_s – s-wave scattering length, a_p – p-wave scattering length, r_s – s-wave effective range



correlation energy

$$\frac{1}{2}\sum_{i}\left(\omega_{i}^{RPA}-\omega_{i}^{HF}\right)$$

effective range corrections appears at this order



- The first type of correction to be accounted for in both Bose and Fermi systems is the Lee & Yang, Huang, Luttinger (1957) correlation energy, which is still determined by the scattering length.
- ✓ Effective range corrections appear only much later.
- More importantly, the corrections to mean-field are <u>always</u> controlled by the parameter na³
- \checkmark When the parameter na³ becomes large, other methods are required.

"Fundamental" and "effective" Hamiltonians

$$egin{aligned} H_{ ext{fund}} &= -\sum_{s} \int d^{3}r \psi_{s}^{\dagger}(r) rac{\hbar^{2} oldsymbol{
abla}^{2}}{2m} \psi_{s}(r) \ &+ rac{1}{2} \sum_{s_{1},s_{2}} \int d^{3}r_{1} d^{3}r_{2} \psi_{s_{1}}^{\dagger}(r_{1}) \psi_{s_{2}}^{\dagger}(r_{2}) \psi_{s_{2}}(r_{2}) \psi_{s_{1}}(r_{1}) V_{s_{1}s_{2}}(|r_{1}-r_{2}|), \end{aligned}$$

If one is interested in phenomena with momenta $p = hk \le h/r_0$, where r_0 is the typical range of the interaction, the "fundamental" Hamiltonian is too complex.

$$\begin{split} H_{eff}(\boldsymbol{r}) &= -\psi^{\dagger}(\boldsymbol{r}) \frac{\hbar^{2} \boldsymbol{\nabla}_{a}^{2}}{2m} \psi_{a}(\boldsymbol{r}) + \frac{1}{2} \lambda_{aa} \psi_{a}^{\dagger}(\boldsymbol{r}) \psi_{a}(\boldsymbol{r}) \psi_{a}(\boldsymbol{r}) \psi_{a}(\boldsymbol{r}) \\ &- \psi^{\dagger}(\boldsymbol{r}) \frac{\hbar^{2} \boldsymbol{\nabla}_{m}^{2}}{4m} \psi_{m}(\boldsymbol{r}) + \varepsilon \psi_{m}^{\dagger}(\boldsymbol{r}) \psi_{m}(\boldsymbol{r}) + \frac{1}{2} \lambda_{mm} \psi_{m}^{\dagger}(\boldsymbol{r}) \psi_{m}(\boldsymbol{r}) \psi_{m}(\boldsymbol{r}) \\ &+ \lambda_{am} \psi_{m}^{\dagger}(\boldsymbol{r}) \psi_{a}^{\dagger}(\boldsymbol{r}) \psi_{a}(\boldsymbol{r}) \psi_{m}(\boldsymbol{r}) + \boldsymbol{\alpha} \psi_{m}^{\dagger}(\boldsymbol{r}) \psi_{a}(\boldsymbol{r}) \psi_{a}(\boldsymbol{r}) + \boldsymbol{\alpha} \psi_{a}^{\dagger}(\boldsymbol{r}) \psi_{a}(\boldsymbol{r}) , \end{split}$$

Working with contact couplings requires regularization and renormalization, which can be done in several different, but equivalent ways.

We will show that H_{eff} is over-determined.

Explicit introduction of "Feshbach molecules"

Example: open channel — two ⁸⁵Rb atoms in f = 2, m_f = -2 state each closed channel — two ⁸⁵Rb atoms in f = 3 each and total M_f = -4



Köhler, Gasenzer, Jullienne and Burnett, cond-mat/0305028.



closed channel {-2,-2} open channel 0.04 separable potential $\left(4\pi\right)^{1/2}r\phi_{\rm b}(r)$ 0.02 B_{evolve} =16.0 mT -0.02 0.015 $(4\pi)^{1/2} r_{b}^{(1)} r_{b}^{(2)} r_{b}^{(2)} r_{b}^{(2)}$ B_{min}=15.55 mT -0.005 10^{2} 10^{4} 10^{3} $r [a_{Bohr}]$

0.06 r

Feshbach resonance

NB The size of the "Feshbach molecule" (closed channel state) is largely B-independent and smaller than the interparticle separation.

Some simple estimates in case a > 0 and $a \gg r_0$

wf in open channel at
$$r > r_0$$
 wfs in region $r < r_0$
 $r\psi_1(r) = Ar_0 \left[1 + O\left(\frac{r_0}{a}\right) \right] \exp\left(-\frac{r}{a}\right)$ $r\psi_1(r) \approx r\psi_2(r) \approx r_0 A$
Probability to find two atoms :
 $P(r < r_0) = \int_0^{r_0} r^2 dr \left[\psi_1(r)^2 + \psi_2(r)^2\right] \approx \frac{2A^2 r_0^3}{3} \left(\text{or } \frac{A^2 r_0^3}{3} \text{ if oscillate} \right)$
 $P(r > r_0) = \int_{r_0}^{\infty} r^2 dr \psi_1(r)^2 \approx \frac{A^2 a r_0^2}{2}$
 $\frac{P(r > r_0)}{P(r < r_0)} \approx \frac{3a}{4r_0} >> 1 \left(\text{or } \frac{3a}{2r_0} \right)$

Most of the time the two atoms spend at large separations, $y_1(r)$ — open channel (dimer), $y_2(r)$ — closed channel (Feshbach molecule)

- So far we discussed only interaction between atoms and one needs to include molecules.
- If atoms and molecules coexist, it makes sense to introduce molecules as independent degrees of freedom.
- Previously various authors, starting with Timmermans *et al. (1998)* introduced explicitly the "Feshbach molecules" for several reasons:
- ☆ There was hope to overcome the restriction na³ á 1 close to a Feshbach resonance, when |a|≫r₀, and replace it hopefully with the milder condition nr₀³ á 1 and thus still be able to use the many-body tools developed for dilute systems.
- Develop a formalism for a mixture of atoms and molecules.

> It is relatively easy to convince oneself that corrections to the energy of a system of either Bose atoms and molecules, or Fermi atoms and Bose molecules (bound state of two Fermi atoms) are <u>always</u> controlled by the parameter na^3 and <u>never</u> by the parameter nr_0^3 .

(Essentially one has to repeat the old Lee, Young and Huang 1957 calculations and compute the correlation energy.)

In order to decide whether a given program is feasible one has to construct the ground state properties of the system under consideration within the framework of the formalism of choice and then consider higher order corrections. This aspect was largely ignored in previous works.

One can develop a theoretical framework to describe atoms and dimers (not Feshbach molecules) for the case a>0, a>>r₀ and na³Ü 1 and one can show that in this regime a mixture of atoms and dimers can be described by one coupling constant, the scattering length a.

The regime a > 0 and na³>>1 (strong coupling) can be studied as well, but using different methods (*ab initio*).

➤ The regime a<0 and |a|≫r₀, n|a|³Ü 1 is also universal and a new class of truly quantum liquids (not gases) appears, see AB Phys. Rev. Lett. 89, 050402 (2002) In order to develop our program we have at first to have a well defined procedure for constructing an effective Hamiltonian for interacting atoms and dimers starting from the "fundamental" Hamiltonian describing bare interacting atoms.

$$H_{a} = -\psi_{a}^{+} \frac{\hbar^{2} \nabla^{2}}{2m} \psi_{a} + \frac{1}{2} \lambda_{2} \psi_{a}^{+} \psi_{a}^{+} \psi_{a} \psi_{a} + \frac{1}{3} \lambda_{3} \psi_{a}^{+} \psi_{a}^{+} \psi_{a} \psi_{a} \psi_{a} \psi_{a}$$
$$H_{am} = \psi_{a}^{+} \left(-\frac{\hbar^{2} \nabla^{2}}{2m} \right) \psi_{a} + \psi_{m}^{+} \left(-\frac{\hbar^{2} \nabla^{2}}{4m} + \varepsilon_{2} \right) \psi_{m}$$
$$+ \frac{1}{2} \lambda_{aa} \psi_{a}^{+} \psi_{a}^{+} \psi_{a} \psi_{a} + \lambda_{am} \psi_{a}^{+} \psi_{m}^{+} \psi_{m} \psi_{a} + \frac{1}{2} \lambda_{mm} \psi_{m}^{+} \psi_{m}^{+} \psi_{m} \psi_{m} \psi_{m}$$

 H_a is a low energy reduction of the "fundamental" Hamiltonian, I_2 and I_3 are determined by the scattering length **a** and a three-body characteristic (denoted below by a_3 '). Interaction terms with derivatives are small as long as $kr_0 a$ 1.

H_{am} is determined by the matching" to be briefly described below.



Matching between the 2--, 3-- and 4--particle amplitudes computed with H_a and H_{am} . Only diagrams containing I_2 --vertices are shown.

The effective vertices thus defined (right side) can then be used to compute the ground state interaction energy in the leading order terms in an na³ expansion, which is given by the diagrams after the arrows.

✓ In medium the magnitude of the relevant momenta are determined by estimating The quantum fluctuations of the mean-field. One thus easily can show that $p = hk \approx h(na)^{1/2}/m$. As long as $kr_0 \mu ka \mu (na^3)^{1/2} \ddot{U} 1$ one can use contact couplings.

 \checkmark The accuracy of the mean-field approximation can be ascertained by estimating the magnitude of the quantum fluctuations to the energy density μ n (na³)^{3/2}ħ²/ma².

✓ We shall consider the regime when $a \gg r_0$ when the relevant momenta satisfy $p = \hbar k \approx \hbar/a \neq (na^3)^{1/2} \ddot{U} \hbar/a \ddot{U} \hbar/r_0$.

 \checkmark Note that both Hamiltonians H_a and H_{am} are appropriate for kaÜ 1 and kr₀Ü 1.

✓ However, while perturbation theory is not valid for H_a when $p \approx h/a$, all the non-perturbative physics at this scale (dimers of size $\approx a$ and the Efimov effect) Have been encapsulated in the couplings of the Hamiltonian H_{am} .

✓ The "matching" described here was performed in vaccum, at length scales of order O(a) and this matching is not modified by the many-body physics, which occurs at scales $O(a/(na^3)^{1/2}) \gg O(a)$.

Fermi atoms

$$\lambda_{aa} = \frac{4\pi\hbar^{2}a}{m}, \qquad \varepsilon_{2} = -\frac{\hbar^{2}}{ma^{2}}$$
$$\lambda_{am} = \frac{3\pi\hbar^{2}a_{am}}{m} = \frac{3.537\pi\hbar^{2}a}{m}, \qquad a_{am} = 1.179a$$
$$\lambda_{mm} = \frac{2\pi\hbar^{2}a_{mm}}{m} = \frac{1.22\pi\hbar^{2}a}{m}, \qquad a_{mm} = 0.61a$$

4 was first computed first by Skornyakov and Ter-Martirosian (1957) who studied neutron-deuteron scattering.

a_{mm} was computed by Petrov (2003) and Fonseca (2003).

Consider now a dilute mixture of fermionic atoms and (bosonic) dimers at temperatures smaller than the dimer binding energy (a>0 and $a>r_0$)

$$\frac{E}{V} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} n_f + \frac{\pi \hbar^2 a}{m} n_f^2 + \frac{3.537 \pi \hbar^2 a}{m} n_f n_b + \frac{0.62 \pi \hbar^2 a}{m} n_b^2 + \varepsilon_2 n_b + \text{corrections}$$
$$n_f = \frac{k_F^3}{3\pi^2}, \qquad \varepsilon_2 = -\frac{\hbar^2}{ma^2}$$

$$U_{fbf}(q,\omega) = U_{fb}^2 \frac{2n_b\varepsilon_q}{\hbar^2\omega^2 - \varepsilon_q(\varepsilon_q + 2n_bU_{bb})}$$

$$U_{bb} = \frac{4\pi\hbar^2 a_{bb}}{m_b}, \qquad \mathcal{E}_q = \frac{\hbar^2 q^2}{2m_b}$$

in coordinate representation at $\omega = 0$

$$U_{fbf}(r) = -\frac{U_{fb}^2}{U_{bb}} \frac{1}{4\pi\xi_b^2 r} \exp\left(-\frac{r}{\xi_b}\right)$$

$$\xi_b = \frac{\hbar}{2m_b s_s} = \frac{a_{bb}}{\sqrt{16\pi n_b a_{bb}^3}} >> a_{bb}, \qquad s_b^2 = \frac{n_b U_{bb}}{m_b}$$

One can show that pairing is typically weak!

Induced fermion-fermion interaction

Bardeen *et al.* (1967), Heiselberg *et al.* (2000), Bijlsma *et al.* (2000) Viverit (2000), Viverit and Giorgini (2000)

> coherence/healing length and speed of sound

The atom-dimer mixture can potentially be a system where relatively strong coupling pairing can occur.

$$\Delta = \left(\frac{2}{e}\right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp\left[\frac{2}{\pi k_F a} \left(1 - 10.25 \frac{\ln\left(1 + 4k_F^2 \xi_b^2\right)}{4k_F^2 \xi_b^2}\right)^{-1}\right]$$



 $a = n_b^{-1/3}/2.5$ (solid line) $a = n_b^{-1/3}/3$ (dashed line)

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. Consider Bertsch's MBX challenge (1999): "Find the ground state of infinite homogeneous neutron matter interacting with an infinite scattering length."

Carlson, Morales, Pandharipande and Ravenhall, Phys.Rev. C<u>68</u> (2003) 025802, with Green Function Monte Carlo (GFMC)

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

Carlson, Chang, Pandharipande and Schmidt, Phys. Rev. Lett. <u>91</u>, 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.

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.

Now one can construct an SLDA 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).

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.



Solid lines are results for parameter set I, dashed lines for parameter set II (dots – velocity profile for ideal vortex)



Extremely fast quantum vortical motion!



What shall I cover in this talk?

SLDA - Superfluid LDA

A brief introduction into the extension of the Kohn-Shall LDA to superfluid fermion systems

- Vortices in the crust of neutron stars
- Vortices in dilute superfluid Fermi gases and some related issues

 Density profiles of dilute normal and superfluid Fermi gases in traps

40K (Fermi) atoms in a spherical harmonic trap

Effect of interaction, with and without weak and strong pairing correlations with fixed chemical potential.



 $m = 0.14 \mu 10^{-10} eV$, $\hbar w = 0.568 \mu 10^{-12} eV$, a = -12.63nm (when finite)

40K (Fermi) atoms in a spherical harmonic trap

Effect of interaction, with and without weak and strong pairing correlations with fixed particle number, N = 5200.



 $\hbar w = 0.568 \mu 10^{-12} eV$, a = -12.63nm (when finite)