The static and dynamic extension of DFT to superfluid fermionic systems:

SLDA, ASLDA and TDSLDA

Aurel Bulgac University of Washington

Collaborators: Yongle YU (now at Wuhan Institute of Physics and Mathematics) Michael M. FORBES (now at LANL) Sukjin YOON (UW) Kenneth J. ROCHE (ORNL) Yuan Lung LUO (UW) Piotr MAGIERSKI (Warsaw and UW) Ionel STETCU (UW)

Funding: DOE grants No. DE-FG02-97ER41014 (UW NT Group) DE-FC02-07ER41457 (SciDAC-UNEDF)

Outline:

- Extension of DFT to superfluid systems SLDA
- Extension of SLDA to asymmetric systems ASLDA
- Extension of SLDA to time dependent phenomena TDSLDA
- SLDA for nuclei (and vortices in neutron stars)
- SLDA for unitary gas (and vortices in a unitary gas), derivation of EDF from *ab initio* calculations and its validation
- Derivation of ASLDA and its verification
- New states of matter, new mechanisms of pairing
- Dynamics of superfluid fermionic systems and new type of collective modes
- Why TDSLDA is better than QRPA?

Very brief/skewed summary of DFT

Kohn-Sham theorem

$$\begin{split} H &= \sum_{i}^{N} T(i) + \sum_{i < j}^{N} U(ij) + \sum_{i < j < k}^{N} U(ijk) + \ldots + \sum_{i}^{N} V_{ext}(i) \\ H \Psi_{0}(1, 2, \ldots N) &= E_{0} \Psi_{0}(1, 2, \ldots N) \\ n(\vec{r}) &= \left\langle \Psi_{0} \right| \sum_{i}^{N} \delta(\vec{r} - \vec{r}_{i}) \left| \Psi_{0} \right\rangle \\ \Psi_{0}(1, 2, \ldots N) \iff V_{ext}(\vec{r}) \iff n(\vec{r}) \\ E_{0} &= \min_{n(\vec{r})} \int d^{3}r \left\{ \frac{\hbar^{2}}{2m} \tau(\vec{r}) + \varepsilon [n(\vec{r})] + V_{ext}(\vec{r})n(\vec{r}) \right\} \\ n(\vec{r}) &= \sum_{i}^{N} \left| \varphi_{i}(\vec{r}) \right|^{2}, \qquad \tau(\vec{r}) = \sum_{i}^{N} \left| \vec{\nabla} \varphi_{i}(\vec{r}) \right|^{2} \end{split}$$

Universal functional of particle density alone Independent of external potential

Injective map (one-to-one) How to construct and validate an *ab initio* EDF?

Given a many body Hamiltonian determine the properties of the infinite homogeneous system as a function of density

Extract the energy density functional (EDF)

Add gradient corrections, if needed or known how (?)

Determine in an *ab initio* calculation the properties of a select number of wisely selected finite systems

Apply the energy density functional to inhomogeneous systems and compare with the *ab initio* calculation, and if lucky declare Victory!

Extended Kohn-Sham equations

Position dependent mass

$$E_{gs} = \int d^3r \left\{ \frac{\hbar^2}{2m^*[n(\vec{r})]} \tau(\vec{r}) + \varepsilon[n(\vec{r})]n(\vec{r}) \right\}$$
$$n(\vec{r}) = \sum_{i=1}^N |\psi_i(\vec{r})|^2 \qquad \tau(\vec{r}) = \sum_{i=1}^N |\vec{\nabla}\psi_i(\vec{r})|^2$$
$$-\vec{\nabla} \frac{\hbar^2}{2m^*[n(\vec{r})]} \vec{\nabla}\psi_i(\vec{r}) + U(\vec{r})\psi_i(\vec{r}) = \varepsilon_i \psi_i(\vec{r})$$

Normal Fermi systems only!

However, not everyone is normal!

Superconductivity and superfluidity in Fermi systems

- ✓ Dilute atomic Fermi gases $T_c \approx 10^{-12} 10^{-9} \text{ eV}$
- \checkmark Liquid ³He $T_c \approx 10^{-7} \, eV$
- ✓ Metals, composite materials
- ✓ Nuclei, neutron stars
- QCD color superconductivity

 $\begin{array}{ll} T_c \approx & 10^{\text{-7}} \mbox{ eV} \\ T_c \approx & 10^{\text{-3}} - 10^{\text{-2}} \mbox{ eV} \\ T_c \approx & 10^5 - 10^6 \mbox{ eV} \end{array}$

$$T_c \approx 10^7 - 10^8 \, eV$$

units (1 eV \approx 10⁴ K)

SLDA - Extension of Kohn-Sham approach to

superfluid Fermi systems

$$\begin{split} E_{gs} &= \int d^3 r \, \varepsilon(n(\vec{r}), \tau(\vec{r}), \nu(\vec{r})) \\ n(\vec{r}) &= 2 \sum_{k} |\mathbf{v}_{k}(\vec{r})|^{2}, \quad \tau(\vec{r}) = 2 \sum_{k} |\vec{\nabla} \mathbf{v}_{k}(\vec{r})|^{2} \\ \nu(\vec{r}) &= \sum_{k} \mathbf{u}_{k}(\vec{r}) \mathbf{v}_{k}^{*}(\vec{r}) \\ \begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^{*}(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathbf{u}_{k}(\vec{r}) \\ \mathbf{v}_{k}(\vec{r}) \end{pmatrix} = E_{k} \begin{pmatrix} \mathbf{u}_{k}(\vec{r}) \\ \mathbf{v}_{k}(\vec{r}) \end{pmatrix} \end{split}$$

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 densities v and τ diverges!

$$\begin{aligned} \begin{array}{l} \begin{array}{l} \begin{array}{l} \text{The SLDA (renormalized) equations} \end{array} \\ E_{gs} &= \int d^{3}r \left\{ \begin{array}{l} \varepsilon_{N} \left[n\left(\vec{r} \right), \tau\left(\vec{r} \right) \right] + \varepsilon_{S} \left[n\left(\vec{r} \right), v\left(\vec{r} \right) \right] \end{array} \right\} \\ & \varepsilon_{S} \left[n\left(\vec{r} \right), v\left(\vec{r} \right) \right] \end{array} \overset{def}{=} -\Delta \left(\vec{r} \right) v_{c} \left(\vec{r} \right) = g_{\text{eff}} \left(\vec{r} \right) \left| v_{c} \left(\vec{r} \right) \right|^{2} \\ & \left\{ \begin{array}{l} \left[h(\vec{r}) - \mu \right] u_{i}(\vec{r}) + \Delta(\vec{r}) v_{i}(\vec{r}) = E_{i} u_{i}(\vec{r}) \\ \Delta^{*}(\vec{r}) u_{i}(\vec{r}) - \left[h(\vec{r}) - \mu \right] v_{i}(\vec{r}) = E_{i} v_{i}(\vec{r}) \end{array} \right. \\ & \left\{ \begin{array}{l} h(\vec{r}) = -\vec{\nabla} \frac{\hbar^{2}}{2m(\vec{r})} \ \vec{\nabla} + U(\vec{r}) \\ \Delta(\vec{r}) = -g_{\text{eff}} \left(\vec{r} \right) v_{c} \left(\vec{r} \right) \end{array} \right. \\ & \left. \frac{1}{g_{eff}(\vec{r})} = \frac{1}{g[n(\vec{r})]} - \frac{m(\vec{r})k_{c}(\vec{r})}{2\pi^{2}\hbar^{2}} \left\{ 1 - \frac{k_{F}(\vec{r})}{2k_{c}(\vec{r})} \ln \frac{k_{c}(\vec{r}) + k_{F}(\vec{r})}{k_{c}(\vec{r}) - k_{F}(\vec{r})} \right\} \\ & \left. n_{c}(\vec{r}) = 2 \sum_{k_{i} \geq 0}^{E_{c}} \left| v_{i}(\vec{r}) \right|^{2}, \quad v_{c}(\vec{r}) = \sum_{k_{i} \geq 0}^{E_{c}} v_{i}^{*}(\vec{r}) u_{i}(\vec{r}) \\ & E_{c} + \mu = \frac{\hbar^{2}k_{c}^{2}(\vec{r})}{2m(\vec{r})} + U(\vec{r}), \quad \mu = \frac{\hbar^{2}k_{F}^{2}(\vec{r})}{2m(\vec{r})} + U(\vec{r}) \end{aligned} \end{aligned}$$

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

Superfluid Local Density Approximation (SLDA) for a unitary Fermi gas

The renormalized SLDA energy density functional

Only this combination is cutoff independent

$$\varepsilon(\vec{r}) = \left[\alpha \frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right] + \beta \frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5}$$

$$\begin{split} n(\vec{r}) &= 2\sum_{k} \left| \mathbf{v}_{\mathbf{k}}(\vec{r}) \right|^{2}, \quad \tau_{c}(\vec{r}) = 2\sum_{E < E_{c}} \left| \vec{\nabla} \mathbf{v}_{\mathbf{k}}(\vec{r}) \right|^{2}, \quad \nu_{c}(\vec{r}) = \sum_{E < E_{c}} \mathbf{u}_{\mathbf{k}}(\vec{r}) \mathbf{v}_{\mathbf{k}}^{*}(\vec{r}) \\ \frac{1}{g_{eff}(\vec{r})} &= \frac{n^{1/3}(\vec{r})}{\gamma} - \frac{k_{c}(\vec{r})}{2\pi^{2}\alpha} \left[1 - \frac{k_{0}(\vec{r})}{2k_{c}(\vec{r})} \ln \frac{k_{c}(\vec{r}) + k_{0}(\vec{r})}{k_{c}(\vec{r}) - k_{0}(\vec{r})} \right] \\ E_{c} + \mu = \alpha \frac{k_{c}^{2}(\vec{r})}{2} + U(\vec{r}), \qquad \mu = \alpha \frac{k_{0}^{2}(\vec{r})}{2} + U(\vec{r}) \end{split}$$

$$\begin{split} U(\vec{r}) &= \beta \frac{(3\pi^2)^{2/3} n^{2/3}(\vec{r})}{2} - \frac{\left|\Delta(\vec{r})\right|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r})\\ \Delta(\vec{r}) &= -g_{eff}(\vec{r}) v_c(\vec{r}) \end{split}$$

No free parameters, EDF is fully determined by *ab initio* calculations

Bulgac, Phys. Rev. A <u>76</u>, 040502(R) (2007)

Parameters defining SLDA functional for a unitary gas:

$$\begin{cases} \xi_s = \frac{5E}{3N\varepsilon_F} = 0.42(2) \\ \eta = \frac{\Delta}{\varepsilon_F} = 0.504(24) \Rightarrow \begin{cases} \alpha = 1.14 \\ \beta = -0.553 \\ \frac{1}{\gamma} = -0.0906 \end{cases}$$

Quasiparticle spectrum in homogeneous matter



solid/dotted blue line red circles dashed blue line

Bonus!

- SLDA, homogeneous GFMC due to Carlson et al

- GFMC due to Carlson and Reddy
- SLDA, homogeneous MC due to Juillet

black dashed-dotted line - meanfield at unitarity

Extra Bonus!

The normal state has been also determined in GFMC

$$\xi_{\scriptscriptstyle N} = \frac{5E}{3N\varepsilon_{\scriptscriptstyle F}} = 0.55(2)$$

SLDA functional predicts

$$\xi_N = \alpha + \beta = 0.59$$

Fermions at unitarity in a harmonic trap



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007) FN-DMC - von Stecher, Greene and Blume, PRL <u>99</u>, 233201 (2007) PRA <u>76</u>, 053613 (2007) TABLE I: Table I. The energies E(N) calculated within the GFMC [14], FN-DMC [15] and SLDA. When two numbers are present the first was calculated as the expectation value of the Hamiltonian/functional, while the second is the value obtained using the virial theorem, namely $E(N) = m\omega^2 \int d^3r n(\mathbf{r})r^2$ [23].

N	E_{GFMC}	Efn-dmc	E_{SLDA}
1	1.5		1.37
2	2.01/1.95	2.002	2.33/2.34
3	4.28/4.19		4.62/4.62
4	5.10	5.069	5.52/5.56
5	7.60		7.98/8.02
6	8.70	8.67	9.07/9.14
7	11.3		11.83/11.91
8	12.6/11.9	12.57	12.94/13.06
9	15.6		16.06/16.20
10	17.2	16.79	17.15/17.33
11	19.9		20.36/20.56
12	21.5	21.26	21.63/21.88
13	25.2		24.96/25.23
14	26.6/26.0	25.90	26.32/26.65
15	30.0		29.78/30.14
16	31.9	30.92	31.21/31.62
17	35.4		34.81/35.26
18	37.4	36.00	36.27/36.78
19	41.1		40.02/40.58
20	43.2/40.8	41.35	41.51/42.12
21	46.9		45.42/46.10
22	49.3		46.92/47.64

NB Particle projection neither required nor needed in SLDA!!!

SLDA - Extension of Kohn-Sham approach to superfluid Fermi systems

$$E_{gs} = \int d^3r \left\{ \mathcal{E}(n(\vec{r}), \tau(\vec{r}), \nu(\vec{r})) + \leftarrow \begin{array}{l} \text{universal functional} \\ \text{(independent of external potential)} \\ V_{ext}(\vec{r})n(\vec{r}) + \Delta_{ext}(\vec{r})\nu(\vec{r}) + \Delta_{ext}^*(\vec{r})\nu^*(\vec{r}) \right\}$$

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

$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathbf{u}_k(\vec{r}) \\ \mathbf{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathbf{u}_k(\vec{r}) \\ \mathbf{v}_k(\vec{r}) \end{pmatrix}$$



GFMC - Chang and Bertsch, Phys. Rev. A <u>76</u>, 021603(R) (2007) FN-DMC - von Stecher, Greene and Blume, PRL <u>99</u>, 233201 (2007) PRA <u>76</u>, 053613 (2007) Agreement between GFMC/FN-DMC and SLDA extremely good, a few percent (at most) accuracy

Why not better? A better agreement would have really signaled big troubles!

• Energy density functional is not unique, in spite of the strong restrictions imposed by unitarity

- Self-interaction correction neglected smallest systems affected the most
- Absence of polarization effects spherical symmetry imposed, odd systems mostly affected
- Spin number densities not included extension from SLDA to SLSD(A) needed *ab initio* results for asymmetric system needed
- Gradient corrections not included, ... but very likely small!!!

Challenges towards implementation of SLDA in nuclei

JETP LETTERS

Service

₹ E 10 AUGUST 1998

Towards a universal nuclear density functional

S. A. Fayans

Kurchatov Institute Russian Science Center, 123182 Moscow, Russia

The total energy density of a nuclear system is represented as

$$\varepsilon = \varepsilon_{kin} + \varepsilon_v + \varepsilon_s + \varepsilon_{Coul} + \varepsilon_{sl} + \varepsilon_{anom}$$
,

where e_{kin} is the kinetic energy term which, since we are constructing a Kohn–Sham type functional, is taken with the free operator $t=p^2/2m$, i.e., with the effective mass $m^*=m$; all the other terms are discussed below. The surface t

The volume term in (1) is chosen to be in the form

$$\varepsilon_{v} = \frac{2}{3} \epsilon_{F}^{0} \rho_{0} \left[a_{+}^{v} \frac{1 - h_{1+}^{v} x_{+}^{\sigma}}{1 + h_{2+}^{v} x_{+}^{\sigma}} x_{+}^{2} + a_{-}^{v} \frac{1 - h_{1-}^{v} x_{+}}{1 + h_{2-}^{v} x_{+}} x_{-}^{2} \right]$$

Here and in the following $x_{\pm} = (\rho_n \pm \rho_p)/2\rho_0$, $\rho_{n(p)}$ is the neutron ($2\rho_0$ is the equilibrium density of symmetric nuclear matter with



The surface part in Eq. (1) is meant to describe the finite-range and nonlocal inmedium effects which may presumably be incorporated phenomenologically within the EDF framework in a localized form by introducing a dependence on density gradients. It is taken as follows:

$$\varepsilon_s = \frac{2}{3} \epsilon_F^0 \rho_0 \frac{a_+^s r_0^2 (\nabla x_+)^2}{1 + h_+^s x_+^\sigma + h_{\nabla}^s r_0^2 (\nabla x_+)^2},$$
(3)



with $h_{i}^{s} = h_{2}^{o}$, a_{i}^{s} and h_{π}^{s} the two free parameters. Such a form is obtained by adding







Gandolfi et al. arXiv:0805.2513



Gezerlis and Carlson, PRC 77, 032801 (2008)



Bulgac et al. arXiv:0801.1504, arXiv:0803.3238

Let us summarize some of the ingredients of the SLDA in nuclei

Energy Density (ED) describing the normal system

ED contribution due to superfluid correlations

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

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

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

<u>Isospin symmetry</u> (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.

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

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

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

Let us stare at the anomalous part of the ED for a moment, ... or two.

SU(2) invariant

$$\mathcal{E}_{S}[v_{p},v_{n}] = g_{0} |v_{p}+v_{n}|^{2} + g_{1} |v_{p}-v_{n}|^{2}$$
$$= g[|v_{p}|^{2} + |v_{n}|^{2}] + g'[v_{p}^{*}v_{n} + v_{n}^{*}v_{p}]$$
$$g = g_{0} + g_{1} \qquad g' = g_{0} - g_{1}$$

NB I am dealing here with s-wave pairing only (S=0 and T=1)!

The last term could not arise from a two-body bare interaction.

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

$$\varepsilon_{S}[v_{p}, v_{n}] = g(\rho_{p}, \rho_{n})[|v_{p}|^{2} + |v_{n}|^{2}]$$

$$+ f(\rho_{p}, \rho_{n})[|v_{p}|^{2} - |v_{n}|^{2}] \frac{\rho_{p} - \rho_{n}}{\rho_{p} + \rho_{n}}$$
where $g(\rho_{p}, \rho_{n}) = g(\rho_{n}, \rho_{p})$
and $f(\rho_{p}, \rho_{n}) = f(\rho_{n}, \rho_{p})$

C

The same coupling constant for both even and odd neutron/proton numbers!!!



<u>A single universal parameter for pairing in nuclei!</u> Yu and Bulgac , Phys. Rev. Lett. <u>90</u>, 222501 (2003) Bulgac and Yu, Phys. Rev. Lett. <u>88</u>, 042504 (2002) Until now we kept the numbers of spin-up and spin-down equal.

What happens when there are not enough partners for everyone to pair with?

(In particular this is what one expects to happen in color superconductivity, due to the heavier strange quark)

What theory tells us?

Green – Fermi sphere of spin-up fermions Yellow – Fermi sphere of spin-down fermions

If
$$|\mu_{\uparrow} - \mu_{\downarrow}| < \frac{\Delta}{\sqrt{2}}$$
 the same solution as for $\mu_{\uparrow} = \mu_{\downarrow}$



LOFF/FFLO solution (1964) Pairing gap becomes a spatially varying function Translational invariance broken



Muether and Sedrakian (2002) Translational invariant solution Rotational invariance broken

What we think is happening in spin imbalanced systems?

Induced P-wave superfluidity

Two new superfluid phases where before they were not expected



What happens at unitarity?



Predicted quantum first phase order transition, subsequently observed in MIT experiment , Shin *et al*. Nature, <u>451</u>, 689 (2008)

Red points with error bars – subsequent DMC calculations for normal state due to Lobo et al, PRL <u>97</u>, 200403 (2006)

$$E(n_a, n_b) = \frac{3}{5} \frac{(6\pi^2)^{2/3} \hbar^2}{2m} \left[n_a g\left(\frac{n_b}{n_a}\right) \right]^{5/3}, \quad n_a \ge n_b$$

Bulgac and Forbes, PRA 75, 031605(R) (2007)

A refined EOS for spin unbalanced systems



Red line: Larkin-Ovchinnikov phase

Black line:normal part of the energy densityBlue points:DMC calculations for normal state, Lobo et al, PRL <u>97</u>, 200403 (2006)Gray crosses:experimental EOS due to Shin, Phys. Rev. A <u>77</u>, 041603(R) (2008)

$$E(n_a, n_b) = \frac{3}{5} \frac{(6\pi^2)^{2/3} \hbar^2}{2m} \left[n_a g\left(\frac{n_b}{n_a}\right) \right]^{5/3}$$

Bulgac and Forbes, Phys. Rev. Lett. <u>101</u>, 215301 (2008)

How this new refined EOS for spin imbalanced systems was obtained?

Through the use of the (A)SLDA , which is an extension of the Kohn-Sham LDA to superfluid systems

A Unitary Fermi Supersolid: the Larkin-Ovchinnikov phase



Phys. Rev. Lett. <u>101</u>, 215301 (2008)

$$P[\mu_a,\mu_b] = \frac{2}{30\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \left[\mu_a h\left(\frac{\mu_b}{\mu_a}\right)\right]^{5/2}$$

Time Dependent Phenomena and Formalism

The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only singleparticle properties are considered.

A.K. Rajagopal and J. Callaway, Phys. Rev. B <u>7</u>, 1912 (1973)
V. Peuckert, J. Phys. C <u>11</u>, 4945 (1978)
E. Runge and E.K.U. Gross, Phys. Rev. Lett. <u>52</u>, 997 (1984)

http://www.tddft.org

$$[h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathbf{u}_{i}(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)] \mathbf{v}_{i}(\vec{r},t) = i\hbar \frac{\partial \mathbf{u}_{i}(\vec{r},t)}{\partial t}$$
$$[\Delta^{*}(\vec{r},t) + \Delta^{*}_{ext}(\vec{r},t)] \mathbf{u}_{i}(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathbf{v}_{i}(\vec{r},t) = i\hbar \frac{\partial \mathbf{v}_{i}(\vec{r},t)}{\partial t}$$

Full 3D implementation of TD-SLDA is a petaflop problem and is almost complete.

Bulgac and Roche, J. Phys. Conf. Series <u>125</u>, 012064 (2008)

Lots of contributions due to Yu, Yoon, Luo, Magierski, and Stetcu

New issues arising in formulating and implementing a TD-DFT:

In ground states currents vanish, but they are present in excited states.

The dependence of the EDF on some currents can be established from general principles, e.g. Galilean invariance:

$$\tau(\vec{r}) \Rightarrow \tau(\vec{r}) - \frac{\vec{j}^2(\vec{r})}{n(\vec{r})}$$

Not all currents and densities can be introduced into the formalism in a such a manner however.

Energy of a (unitary) Fermi system as a function of the pairing gap



Response of a unitary Fermi system to changing the scattering length with time

Tool: TD DFT extension to superfluid systems (TD-SLDA)



• All these modes have a very low frequency below the pairing gap and a very large amplitude and excitation energy as well

 None of these modes can be described either within Quantum Hydrodynamics or Landau-Ginzburg like approaches

Bulgac and Yoon, Phys. Rev. Lett. 102, 085302 (2009)

3D unitary Fermi gas confined to a 1D ho potential well (pancake)

New qualitative excitation mode of a superfluid Fermi system (non-spherical Fermi momentum distribution)



Black solid line – Time dependence of the cloud radius Black dashed line – Time dependence of the quadrupole moment of momentum distribution

Bulgac and Yoon, Phys. Rev. Lett. 102, 085302 (2009)

Vortex generation (show movie)

Time-Dependent Superfluid Local Density Approximation

This is a general many-body problem with direct applications, which will provide the time dependent response of superfluid fermionic systems to a large variety of external probes for both cases of small and large amplitude collective motion.

- Nuclear physics: fission, heavy-ion collision, nuclear reactions, response electromagnetic fields, beta-decay, ...
- Neutron star crust, dynamics of vortices, vortex pinning mechanism
- Cold atom physics, optical lattices, ...
- Condensed matter physics

Next frontier: Stochastic TDSLDA

Generic adiabatic large amplitude potential energy SURFACES



In LACM adiabaticity is not a guaranteed
Level crossings are a great source of :

entropy production (dissipation) dynamical symmetry breaking non-abelian gauge fields

Known disease of QRPA, the particle number of excited states is ill defined see Terasaki, Engel and Bertsch, Phys. Rev. C <u>77</u>, 044311 (2008)



FIG. 1. Particle-hole character of the lowest 2^+ solutions. The histogram displays the quantity ΔN defined in Eq. (1) for 155 nuclei in the SLy4 data set (one of which we drop—see text). The values -2, 0, +2 correspond to excitations of hole-hole, particle-hole, and particle-particle character, respectively.

However in TDSLDA the particle number is not violated and all states have a well defined average particle number.

Plato's cave

