**INT Program:** **Fermions from Cold Atoms to Neutron Stars, Seattle, 5/12/2011**

# Coordinate-space HFB description of superfluid Fermi systems

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# Cold Fermi gas: rich implications

- W. Ketterle, M.W. Zwierlein, arXiv:0801.2500v1

Our ultimate goal is to control Nature and create and explore new forms of matter. But in the end, it is Nature who sets the rules, and in the case of ultracold fermions, she has been very kind to us.

- Reasons:
  - Interactions controllable through Feshbach resonances;
  - High critical temperature $T_c$;
  - Exciting observations: vortex, novel superfluid phases(phase separation; FFLO), anisotropic expansion, collective oscillations, and to be… (see talks given at INT)

# Interfaces to nuclear physics

- Cold atoms as a testing ground of neutron matter

superfluidity is a generic feature in strongly correlated Fermi systems

- *ab inito* benchmarking of neutron drops in a trap for DFT;

  S. Gandolfi et al, PRL 106, 012501(2011)

- effective 3-body force for DFT;

  A. Gezerlis et al., PRL 105, 212501(2010)

- benchmarking for *ab inito* DFT;

  J. Drut, arXiv: 1104.4357

- $^3P_2$ superfluidity for rapid cooling of neutron stars;

  D. Page et al. PRL 106, 081106(2011)

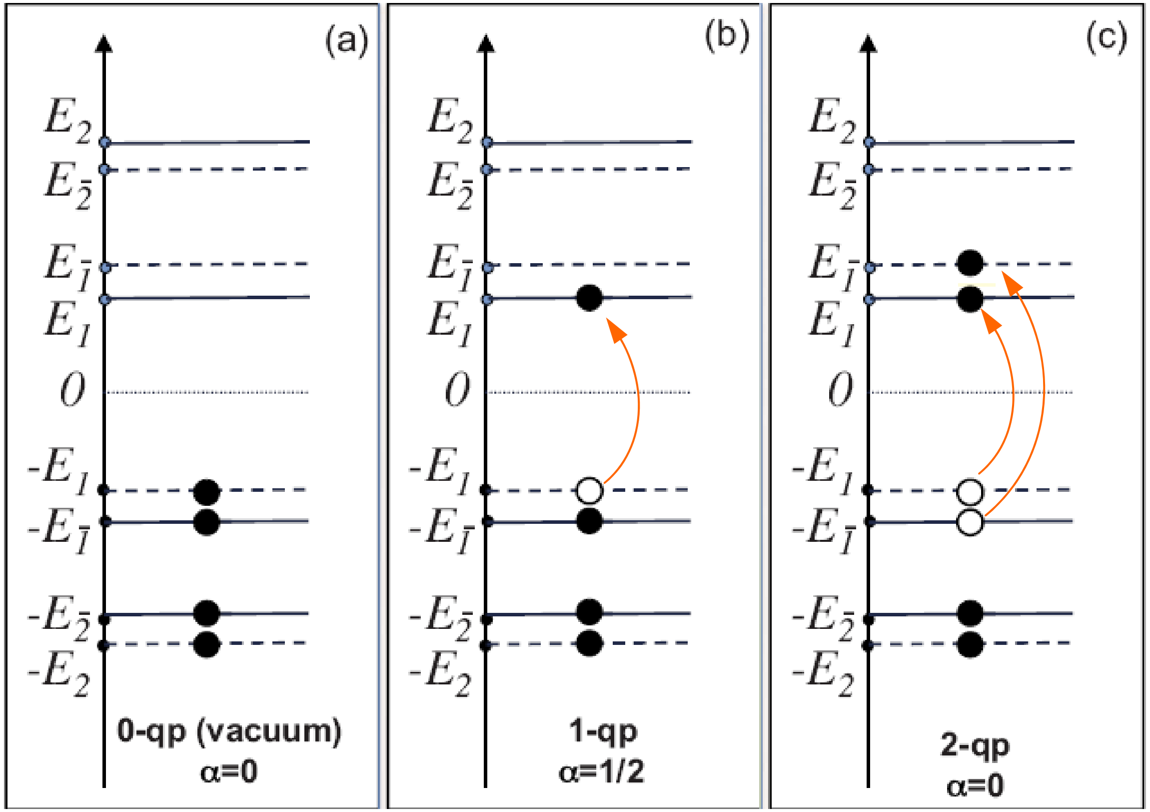
- Constrains on neutron matter EOS and nuclear properties

  D. Wen et al, PRL **103**, 211102 (2009)

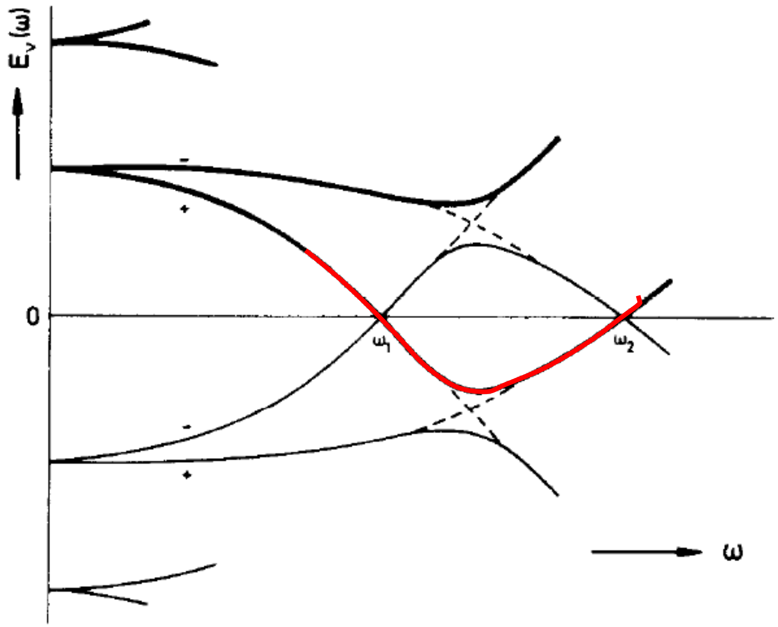
  K. Hebeler et al, PRL 105, 161102(2010)

  C. J. Horowitz et al, PRL **86**, 5647 (2001)

- Spin-polarization: quasiparticle excitation ("blocking" ) & imbalanced Fermi gas (two-Fermi level approach) G. Bertsch et al. PRA 79, 043602(2009)



- Gapless superfluidity: high-spin rotation nuclear states




B. Banerjee, Nucl. Phys. A 221, 564(1974)

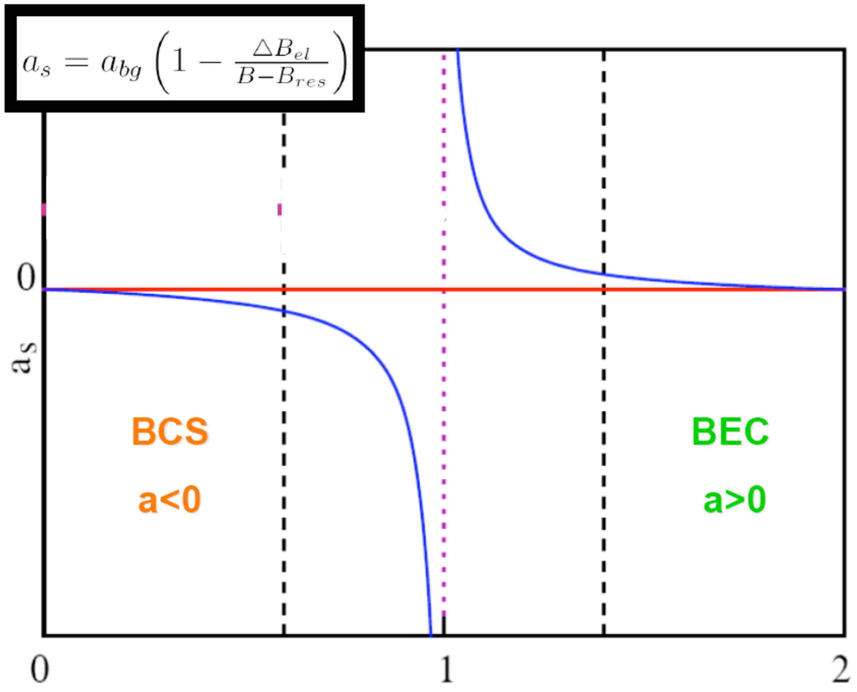
$$\begin{pmatrix} h-\omega J_x & \Delta \\ -\Delta^* & -(h-\omega J_x)^* \end{pmatrix} \begin{pmatrix} A_\mu \\ B_\mu \end{pmatrix} = E_\mu \begin{pmatrix} A_\mu \\ B_\mu \end{pmatrix}$$

# Unitarity Fermi gases

- Unitary limit: two body *s*-wave scattering length diverges: $a_s \to \pm\infty$

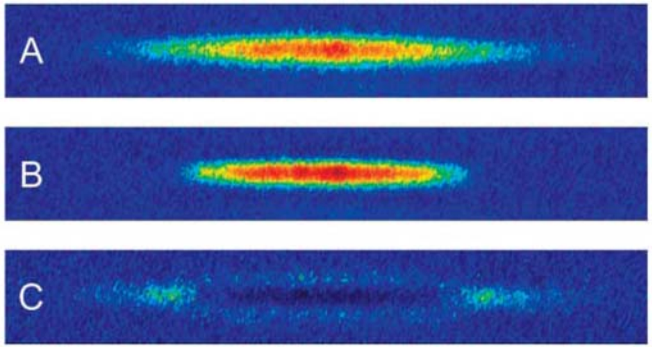
  System is strongly correlated and its properties do not dependent on the value of scattering length $a_s$, providing clear many-body physics picture
- Bertsch parameter ( $\xi$ ~0.4): $\epsilon_{\text{unitary}}(n) = \xi \epsilon_{\text{free}}(n)$
- Ideally suited for DFT description

  (A. Bulgac, PRA 76, 040502(2007), T. Papenbrock, PRA 72, 041603(2005))



# Imbalanced Fermi gases

- New phases: phase separation (*in situ*)




Spin-up density

Spin-down density

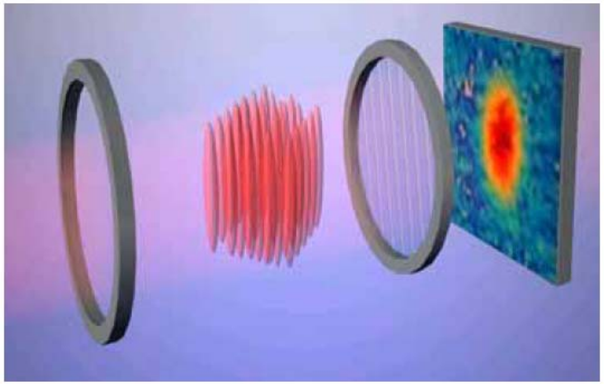
polarized density

Science 311(2006)503

- Experiments performed with highly elongated traps

$$U(r,z) = U_0(1-\exp(-\frac{1}{2}(w_r^2 r^2 + w_z^2 z^2)/U_0))$$

- A good chance for looking for FFLO (one-dimensional limit)



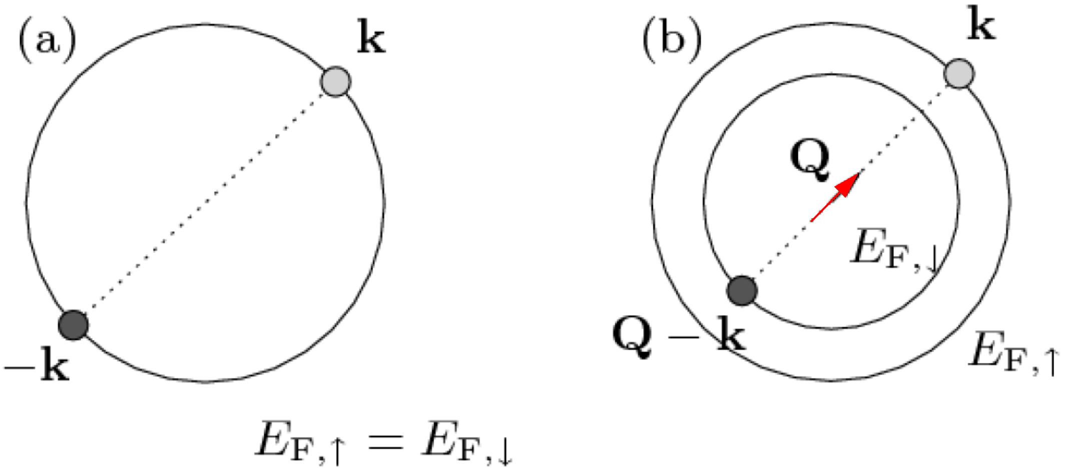
Liao, et al, Nature 467, 567-569 (2010)

# Expected exotic FFLO pairing

- In imbalanced Fermi systems, pairing with none-zero momentum can happen: Flude-Ferrell-Larkin-Ovchinnikov (**FFLO**)

  Oscillation pairing gap is expected; Modulated densities (crystallized).
- It exists in many theoretical calculations, but difficult to find.
- Some signatures in heavy fermions systems. Radovan, et al. Nature 425, 51, 2003.

$$\Delta(\vec{x}) = \Delta_0 \sum_n C_n e^{i\vec{q}_n \cdot \vec{x}}$$



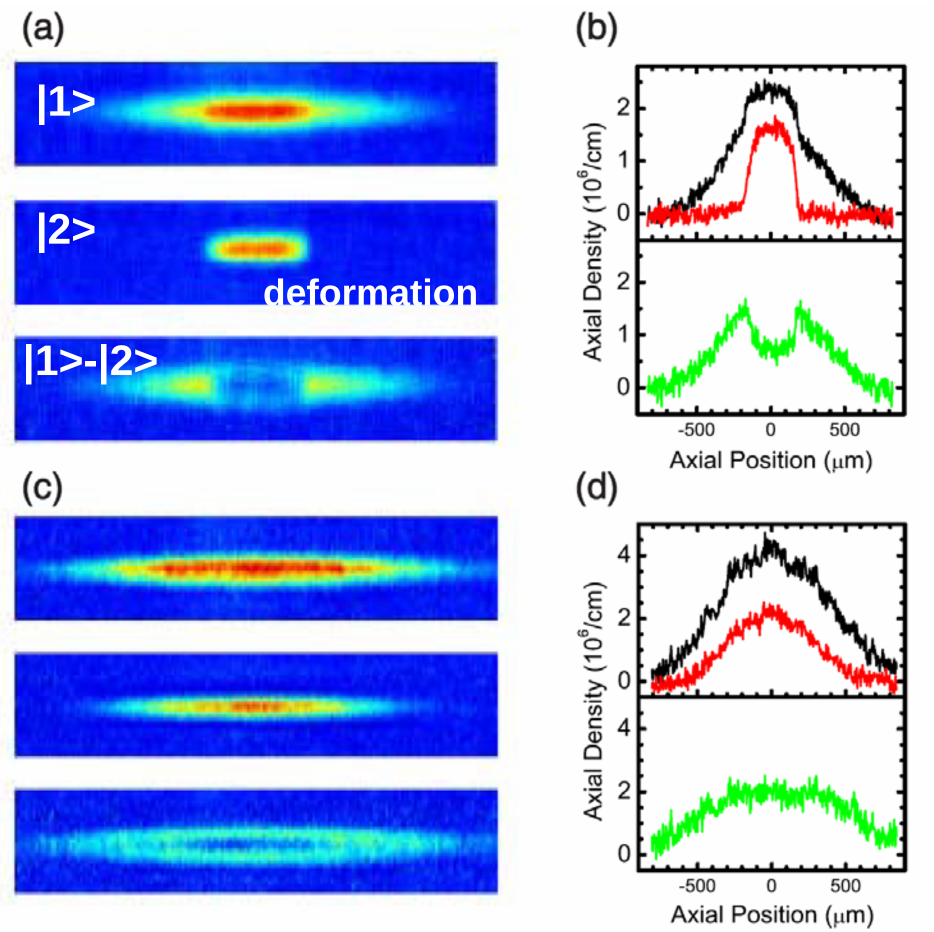
# Experiments (Rice)

- Phase Separation
- Superfluid Core is deformed from the trap shape (violation of LDA) and such deformation effects disappear at high temperatures

- Trap aspect ratio～**50**: highly elongate
- Particle numbers～$10^5$

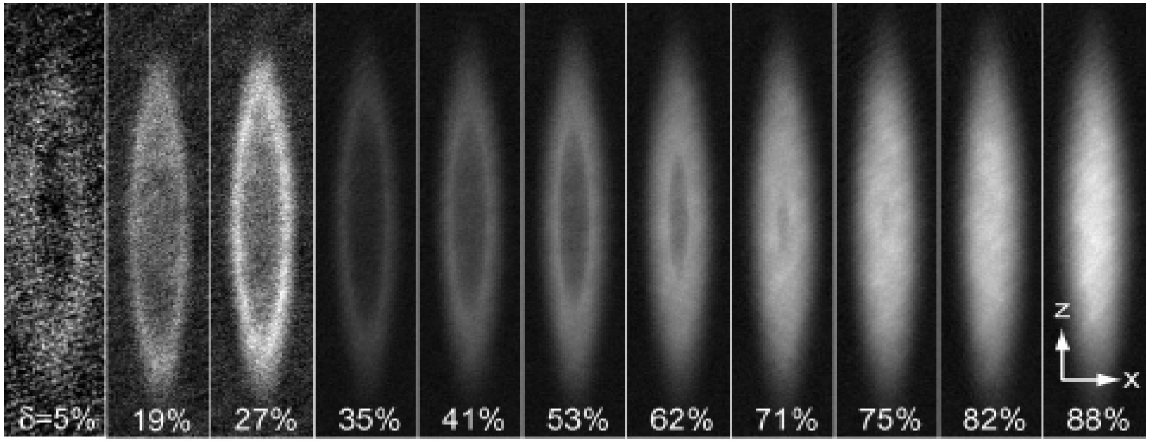
G.B.Partridge, et al, PRL97,190407,2006

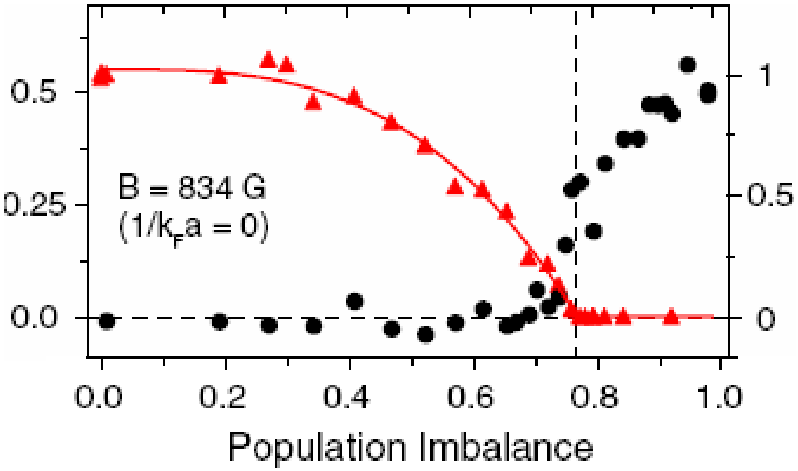
G.B.Partridge, et al, Science,311,503,2006



# Experiments (MIT)

- Phase separation
- However, no superfluid core deformation effects



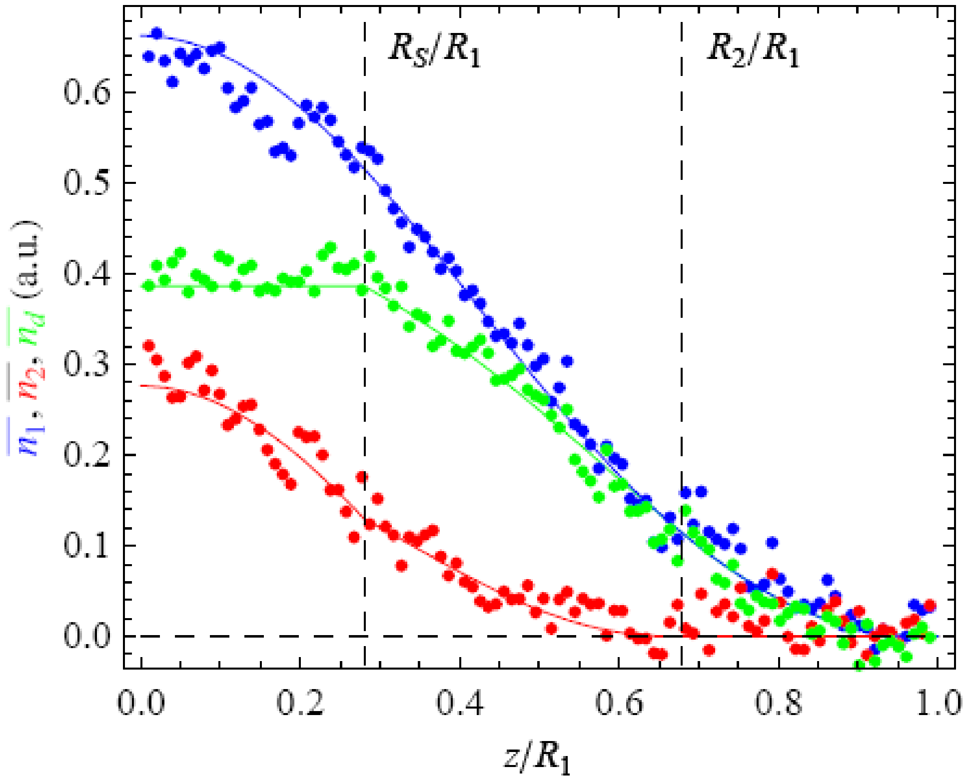

Y.Shin, et al, PRL 97,03401,2006

- Clogston-Chandrasekhar limit of superfluidity (of polarization), not exist in Rice experiment
- Trap aspect ratio=5, particles=$10^6$

# Experiments-ENS

- $10^5$ particles, aspect ratio=23 (agree with MIT)

No core deformation




S. Nascimbène, et al, PRL103, 18 (2009) 170402

**Question?**

1. different experimental conditions
2. or theory is not precise

- Finite-size effects

M.Ku, PRL 102, 255301, 2009

- Surface tension effects

T.N. De Silva, et al, PRL 97, 070402(2006)

- Non-equilibrium state?

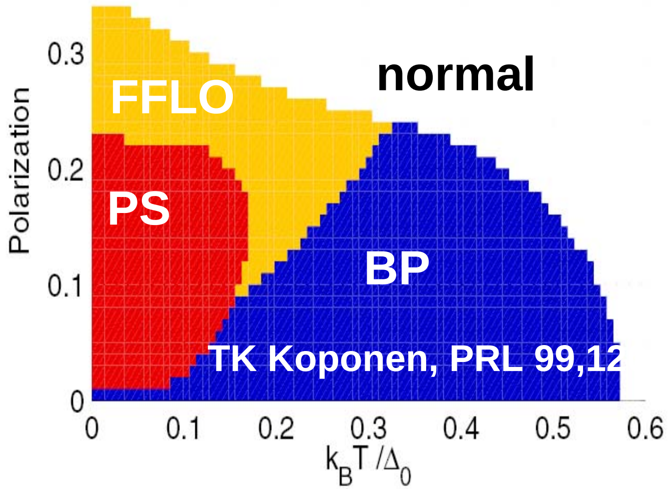
Parish, et al. PRA 063305(2009)

# Theories

- Quantum Monte Carlo for benchmarks: QMC is very precise but limited to small systems
- Bogoliubov de-Genes equation: Mean Field approximation

$$H(\mathbf{r}) = \sum_\sigma \Psi_\sigma^\dagger(\mathbf{r})[H_0(\mathbf{r}) - \mu_\sigma]\Psi_\sigma(\mathbf{r}) - g\Psi_\uparrow^\dagger(\mathbf{r})\Psi_\downarrow^\dagger(\mathbf{r})\Psi_\downarrow(\mathbf{r})\Psi_\uparrow(\mathbf{r})$$

$$\begin{pmatrix} H_0(\mathbf{r}) - \mu & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) + \mu \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = E_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$




Plenty of calculations, no Hartree potential, and not quantitatively accurate

A contest of computation: Tokyo U:3×$10^4$ particles; Rice U: $10^5$ particles

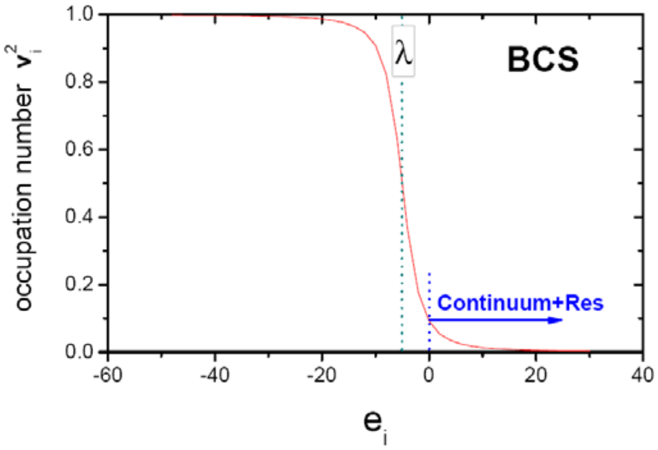
M. Tezuka, arXiv: 0811.1605, 2010

L.O. Baksmaty, Phys. Rev. A **83**, 023604 (2011)

- DFT at the unitary limit. Study a large number of particles. Superfluid Local Density Approximation (SLDA) is very precise.

# Quasiparticle spectrum in nuclei

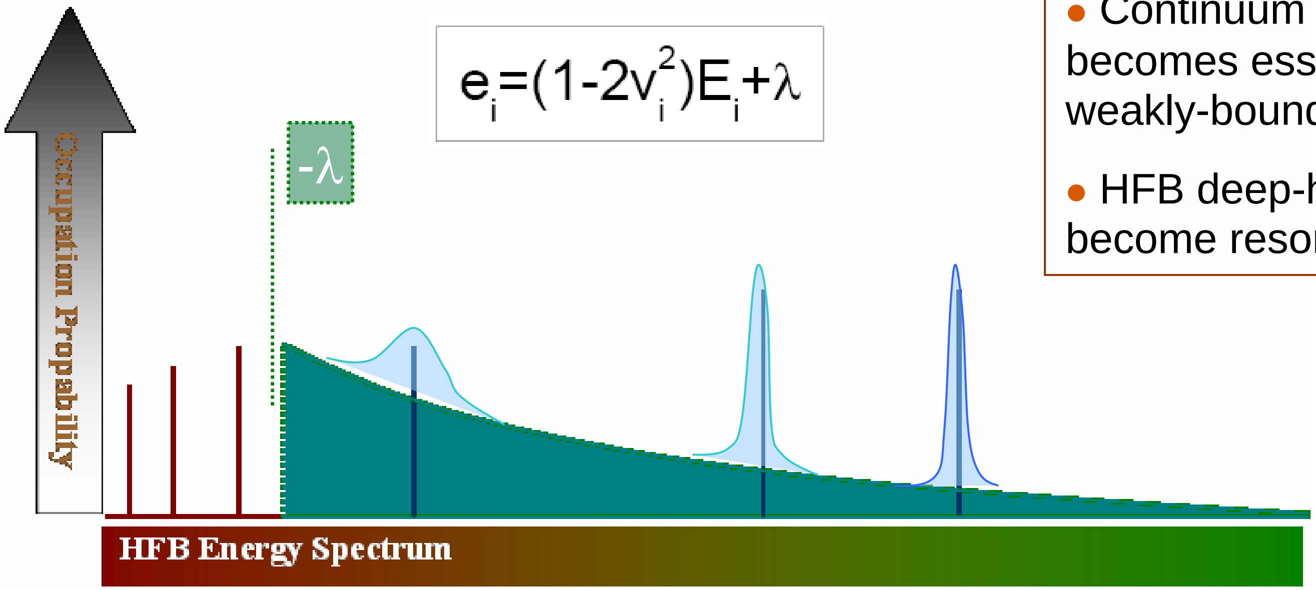
- BCS




Occupation numbers

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\tilde{\varepsilon}_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}\right)$$

- Hartree-Fock-Bogoliubov (HFB)




$$e_i = (1-2v_i^2)E_i + \lambda$$

- Continuum coupling becomes essential for weakly-bound nuclei.
- HFB deep-hole states become resonances

# Coordinate-space HFB calculations

- It is the advantage of coordinate-space Hartree-Fock-Bogoliubov (HFB) to treat elongated potential; developed to describe nuclear fission process

  HFB-AX code: using B-spline techniques; Axially symmetry; Very precise for deformed and weakly bound nuclei.

  2000 atoms employed. dimensionless 2D-box: R=25×0.3, Z=(125～300)×0.3 (very dense spectrum)

  the trap aspect ratio is set to be η=10, 20, 30, 40. ASLDA is very time consuming

  *Pei et al, PRC 78, 064306, 2007*

- 3D HFB-MADNESS is under development (multi-resolution adaptive wavelet basis): SLDA and ASLDA has been benchmarked. can treat 100-particles in elongated trap

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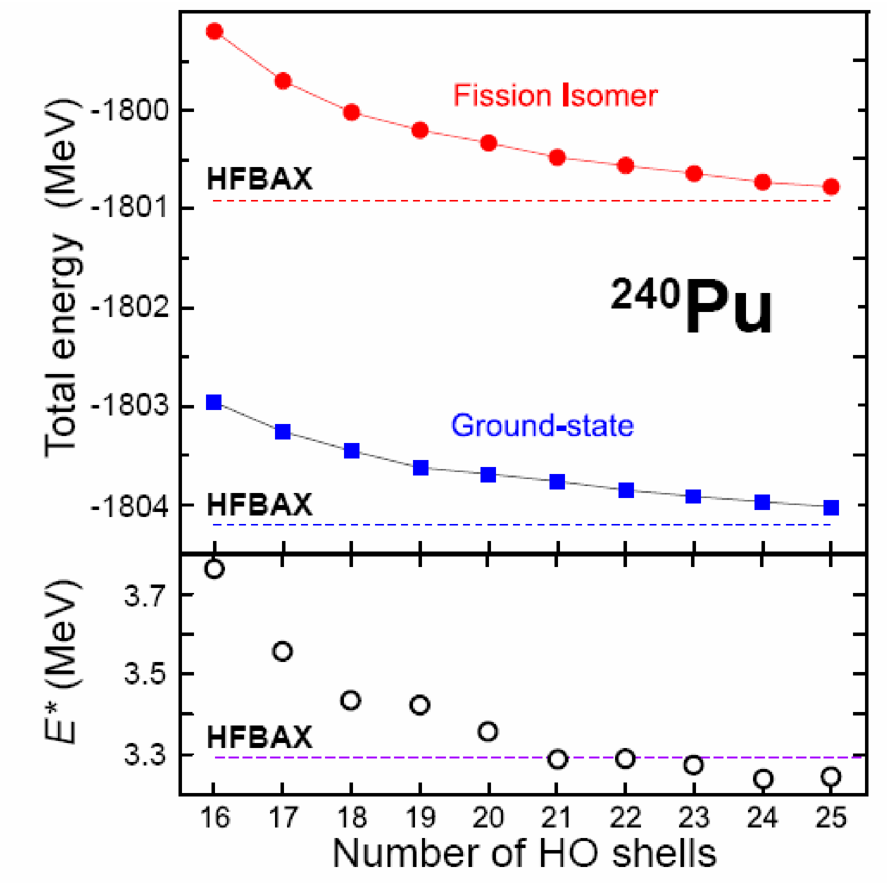
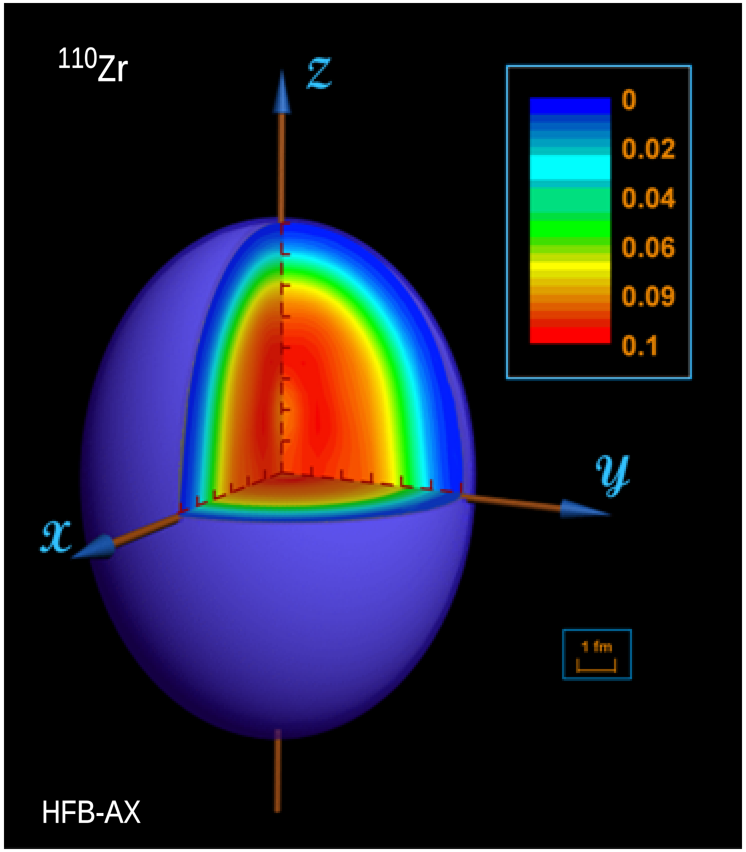
# Coordinate-space solutions

- Benchmarking (see how precise it is)




N. Nikolov et al. Phys. Rev. C 83, 034305 (2011)

- 2D nuclear density distributions

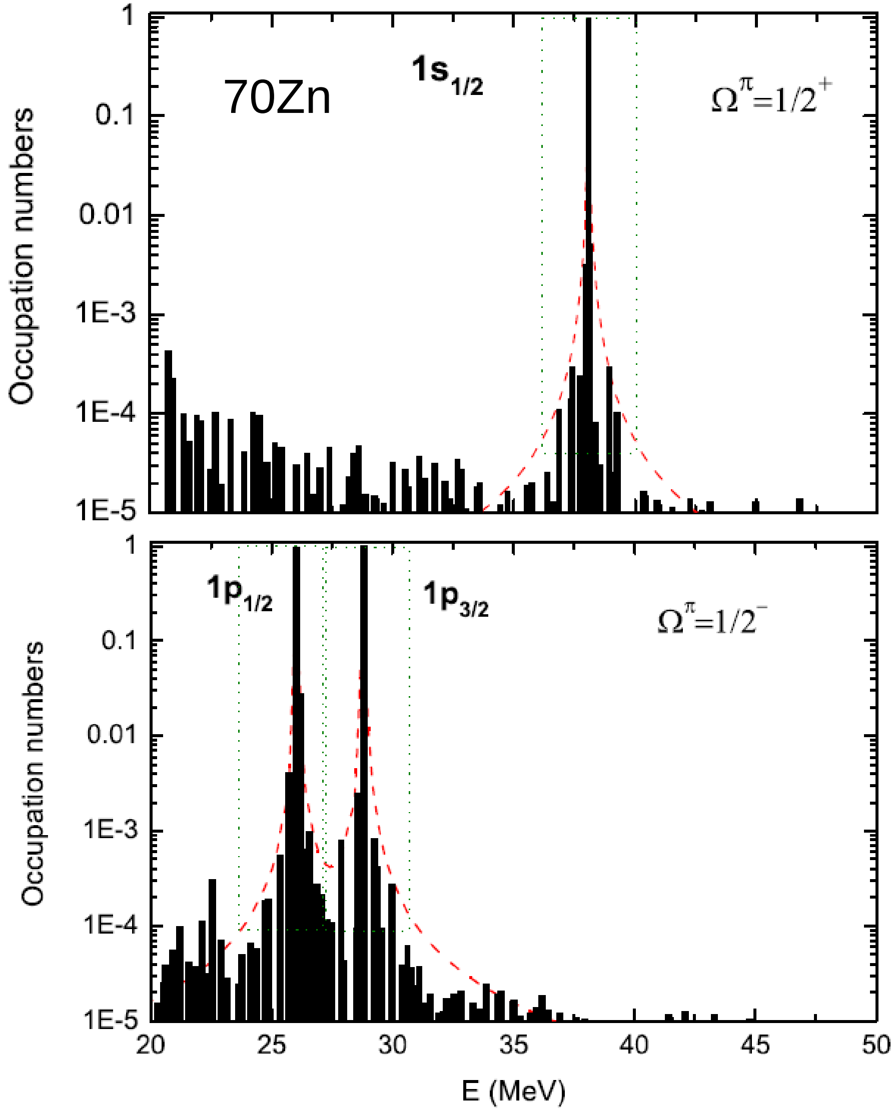



M. Stoitsov et al, J. Phys. Conf. Ser. 180, 012802 (2009)

# Coordinate-space solutions

- In the box solution, also called *$L^2$* discretization, the continuum is discretized into finite states, with very good accuracy compared to exact treatments.
- Even with this method the resonance widths can be calculated precisely, compared to the complex scaling method.
- HFB-AX generates very dense quasiparticle spectrum, provides a high resolution for continuum and resonance states.

For example, about 7000 states in a 40×40 fm box.

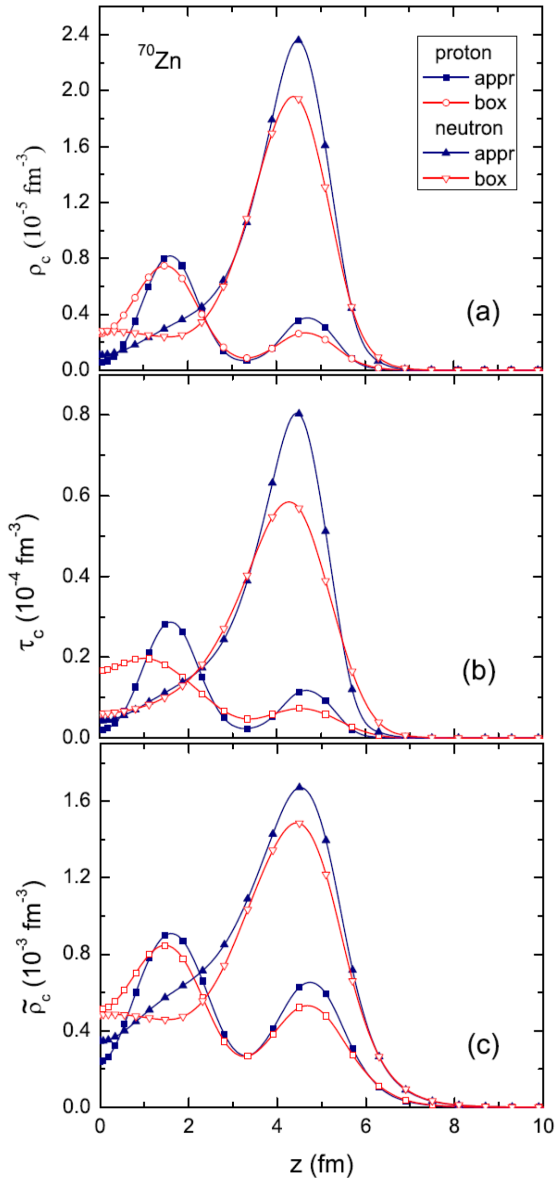


# Quasiparticle continuum contribution

- ❑ Local-density approximation for continuum states works for HFB-popov equation for Bose gas;
  Also works for Bogoliubov de Gennes equations for Fermi gas.

  *J. Reidl, A. Csordas, R. Graham, and P.Szepfalusy, Phys. Rev. A 59, 3816 (1999)*
  *X.J. Liu, H. Hu, P.D. Drummond, Phys. Rev. A 76,043605 (2007)*

- ❑ Continuum contributions from 40 to 60 MeV
  - Local density approximation
  - Box solution from HFB-AX




What we see:

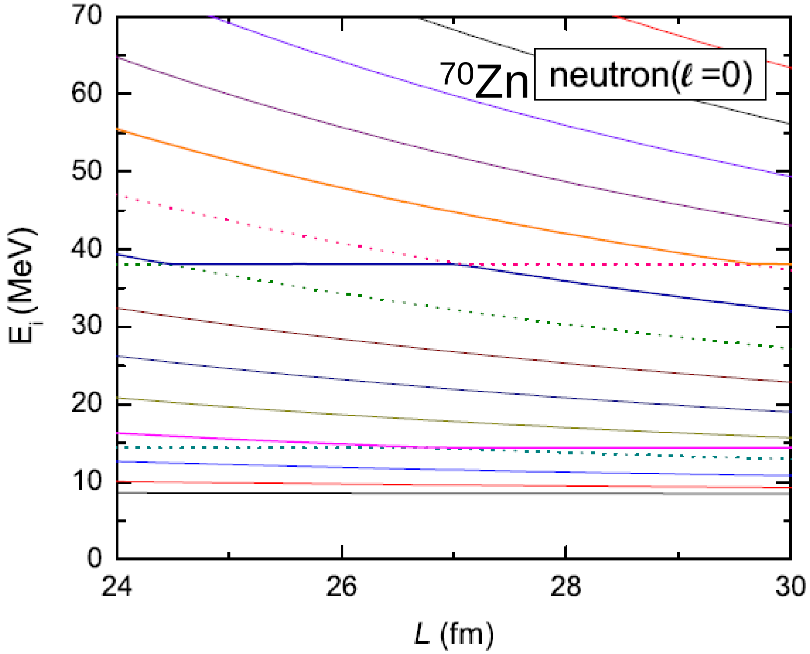
Generally the two methods agrees with each other;

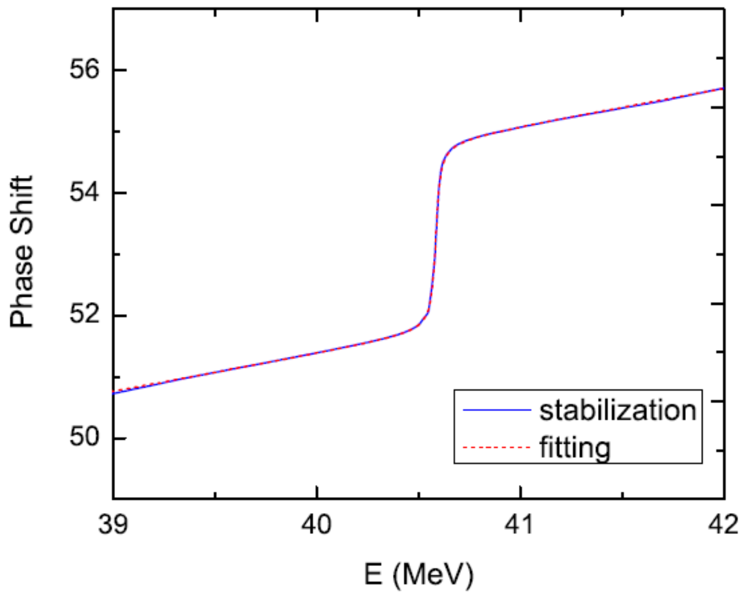
The distributions are very similar for the three kind of densities, and this depends on the pairing potential;

Continuum significantly impacts the *pp* channel.

# Quasiparticle resonances in nuclei

- Stabilization method: the main idea is to get resonance widths from the box-size dependence of quasiparticle energies




In principle, we can get very accurate results, but it is expensive for narrow resonances

Phase shift: $\eta(E) = \pi \int_0^E \Delta(E')dE'$

Continuum level density: $\Delta(E) = Tr[\delta(E-H) - \delta(E-H_0)]$

***V.A. Mandelshtam, H.S. Taylor, V. Ryaboy and N. Moiseyev, PRA 50, 2764 (1994)***

# ASLDA for imbalanced cold Fermions

- ASLDA Equations (A. Bulgac&M. Forbes, 2008):

$$\begin{bmatrix} h_a(\boldsymbol{r}) - \lambda_a & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -h_b(\boldsymbol{r}) + \lambda_b \end{bmatrix} \begin{bmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{bmatrix} = E_i \begin{bmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{bmatrix}$$

$$\rho_a(\boldsymbol{r}) = \sum_i f_i |u_i(\boldsymbol{r})|^2, \; \rho_b(\boldsymbol{r}) = \sum_i (1-f_i)|v_i(\boldsymbol{r})|^2$$

$$\kappa(\boldsymbol{r}) = \sum_i f_i u_i(\boldsymbol{r}) v_i^*(\boldsymbol{r}), \; \Delta(\boldsymbol{r}) = g_{eff}(\boldsymbol{r})\kappa(\boldsymbol{r}) \qquad f_i = 1/(1+\exp(E_i/kT))$$

ASLDA energy density functional:

$$\mathcal{E} = \alpha_a(x)\frac{\tau_a}{2} + \alpha_b(x)\frac{\tau_b}{2} + \frac{(3\pi^2(\rho_a+\rho_b))^{5/3}}{10\pi^2}\beta(x) - \Delta\kappa$$

$x$ refers to polarization

$$g_{eff}(\boldsymbol{r}) = \frac{\gamma(x)}{(\rho_a+\rho_b)^{1/3} + \Lambda(\boldsymbol{r})\gamma(x)}$$

Pairing regularization

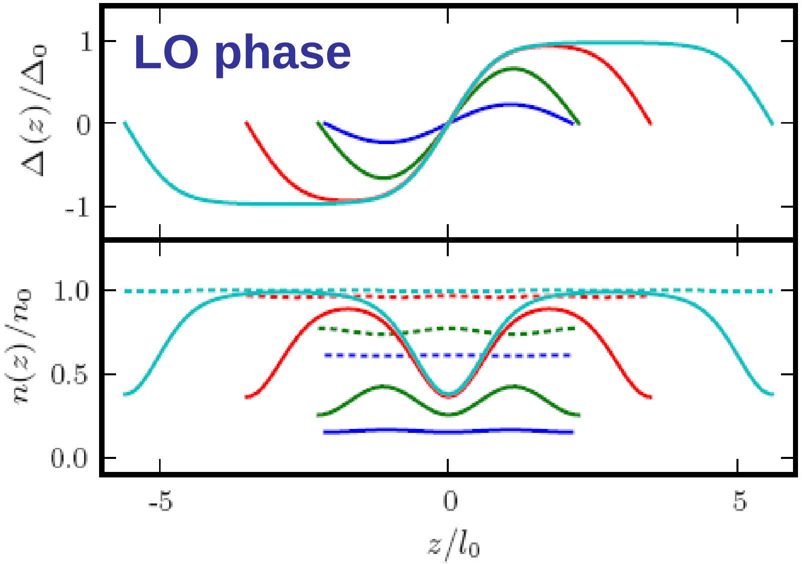
- Becomes SLDA when effective mass of spin-up and spin-down is the same.

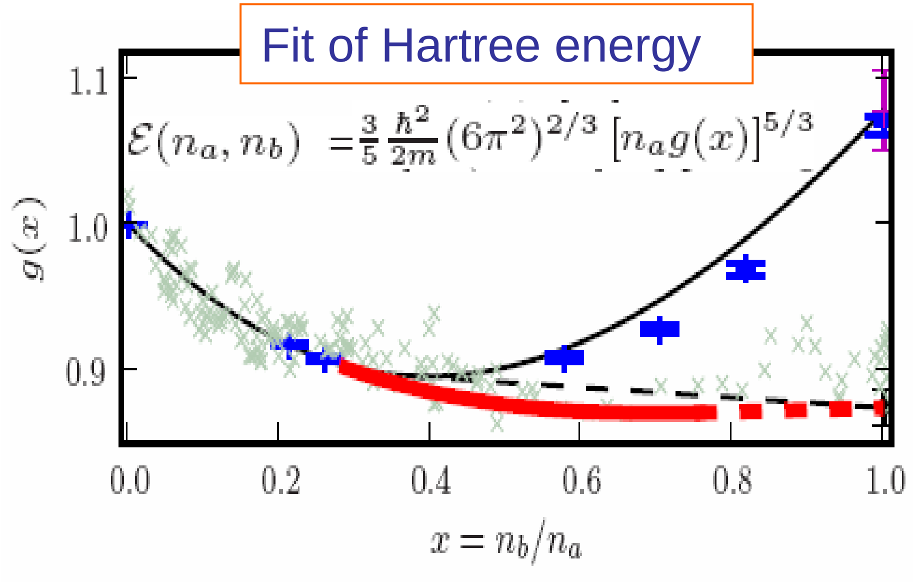
# ASLDA for imbalanced cold Fermions

- Parameters are fitted according to experiments and QMC calculations (effective mass; energy density) as functions of polarizations, close to SLDA at small polarizations

- ASLDA predicted FFLO phase: with periodic boundary conditions

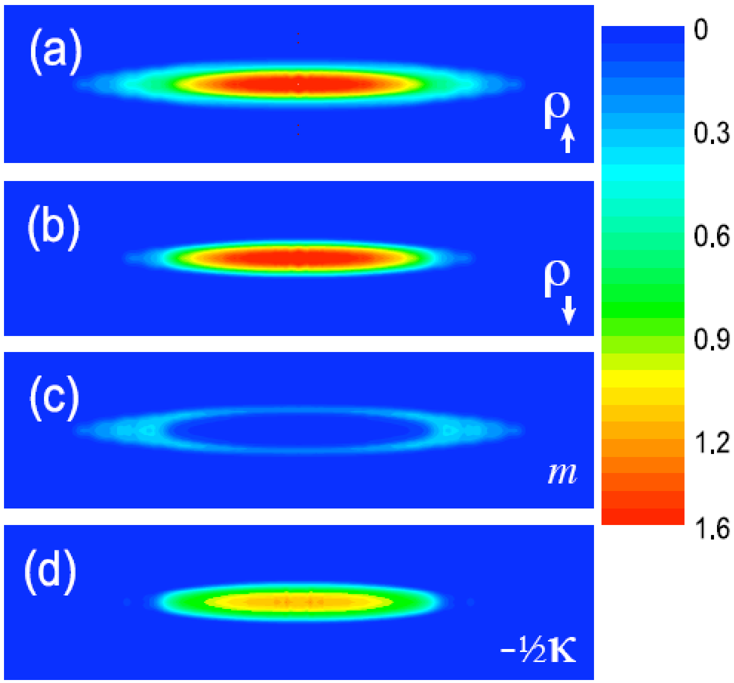
A.Bulgac, M.Forbes, PRL101:215301,2008



# Phase separation

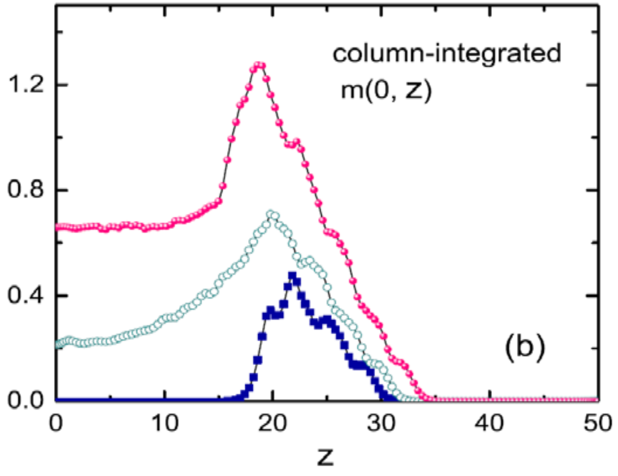
- SLDA calculations( η =10):



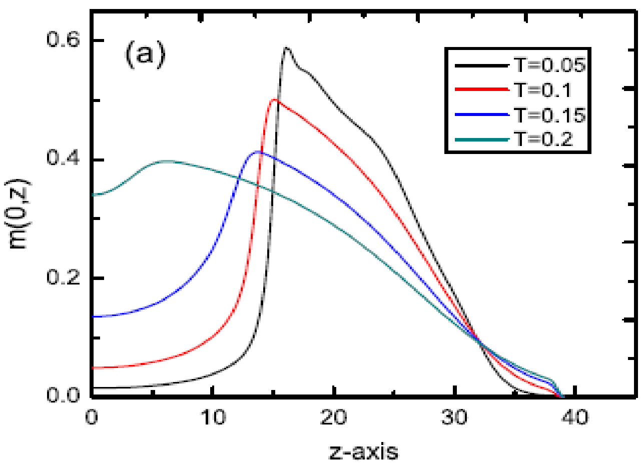

$$P = (N_a - N_b)/(N_a + N_b)$$

Pei, Nazarewicz, Stoitsov, EPJA42,595 2009

**Polarization effects**

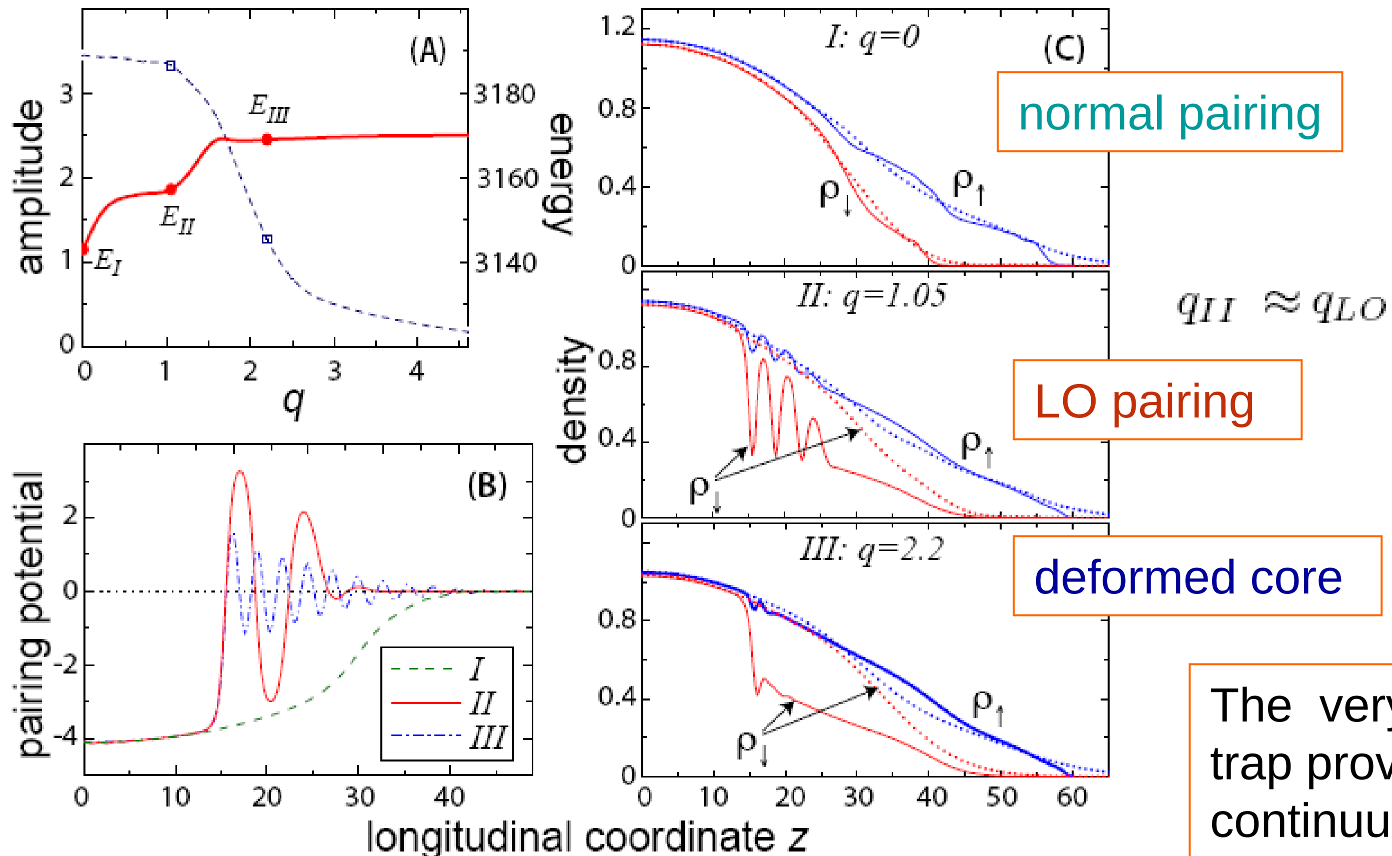



**Temperature effects**



# Coexistence of difference phases

- SLDA calculations start with different initial pairing $\sin(\boldsymbol{q}z)\exp(-(z-z_c)/a)$




$$q_{II} \approx q_{LO} = \sqrt{2\lambda_\uparrow} - \sqrt{2\lambda_\downarrow}$$

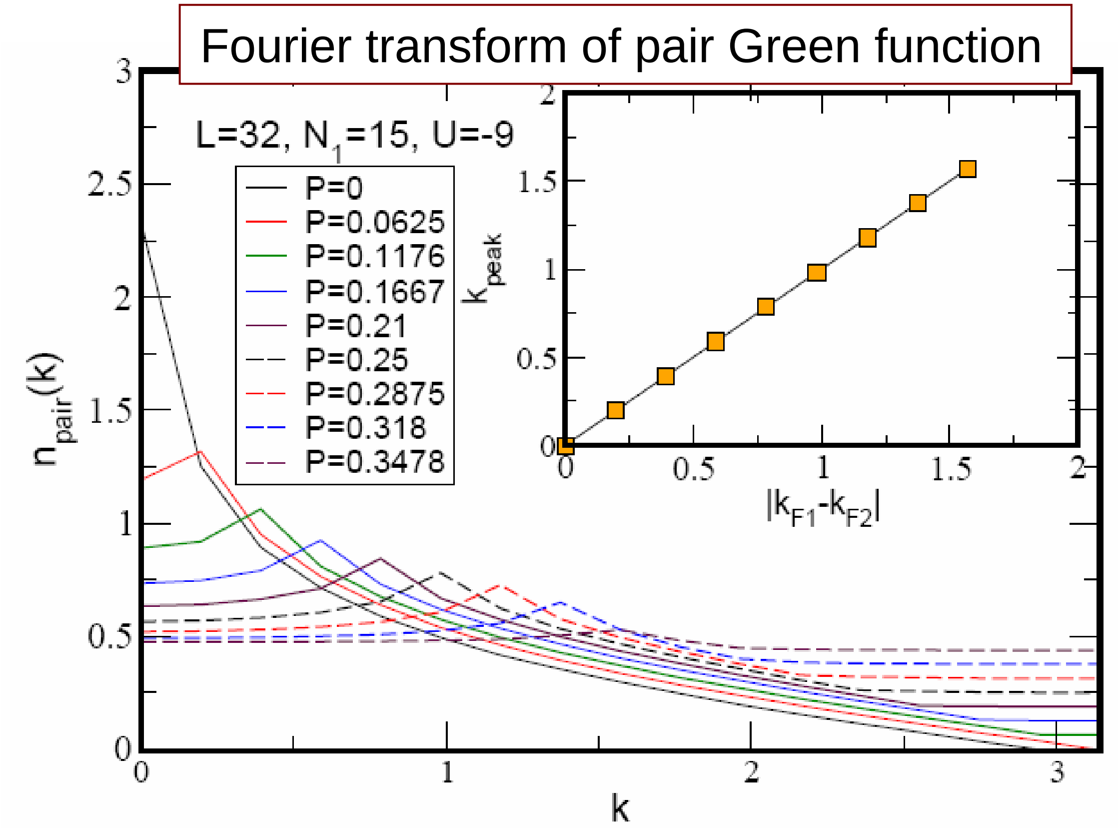
The very elongated trap provides a qusi-continuum background, pairing becomes the most important term

L.O. Baksmaty *et al.*, arXiv:1003.4488 (2010).

Pei, Dukelsky, Nazarewicz, PRA 82, 021603(R) (2010)

# Perspectives from QMC

- Not a pure cos(qx) function in a 1D trap with Hubbard Hamiltonian




G.G. Batrouni *et al.*, Phys. Rev. Lett. **100**, 116405 (2008).

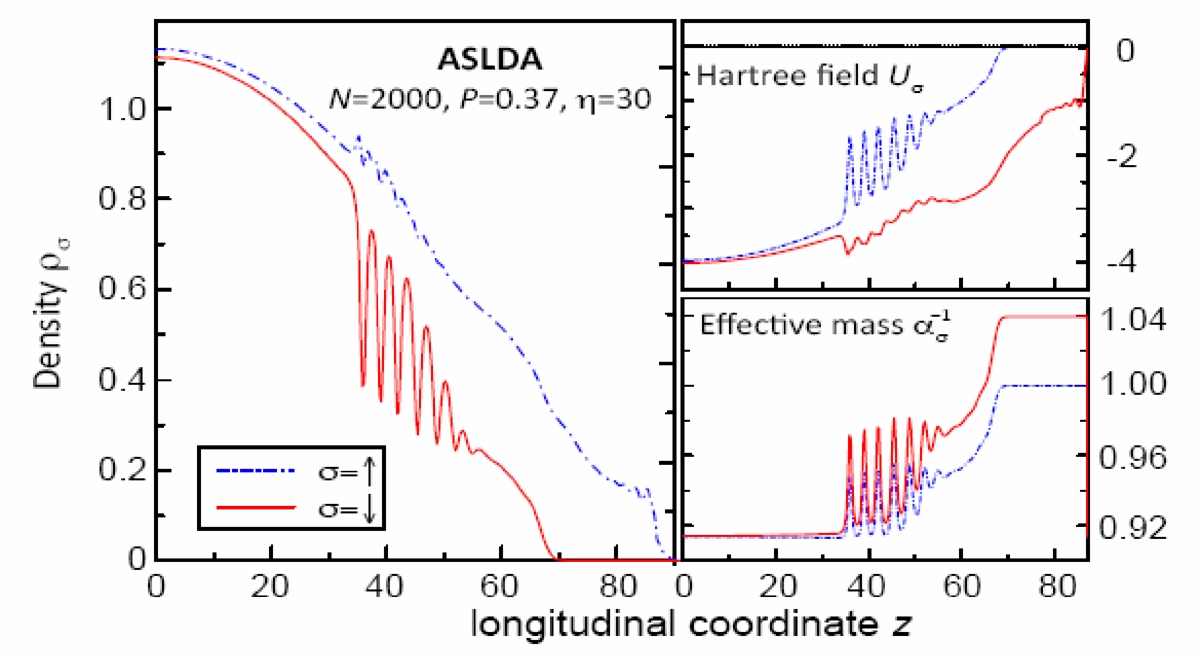
FFLO is a superposition of different momentum states

Superposition can be considered by a generator-coordinate DFT / multi-reference DFT

Elongated trap is an interface to such one dimensional system

# SLDA and ASLDA difference

- The Hartree term and effective mass in ASLDA



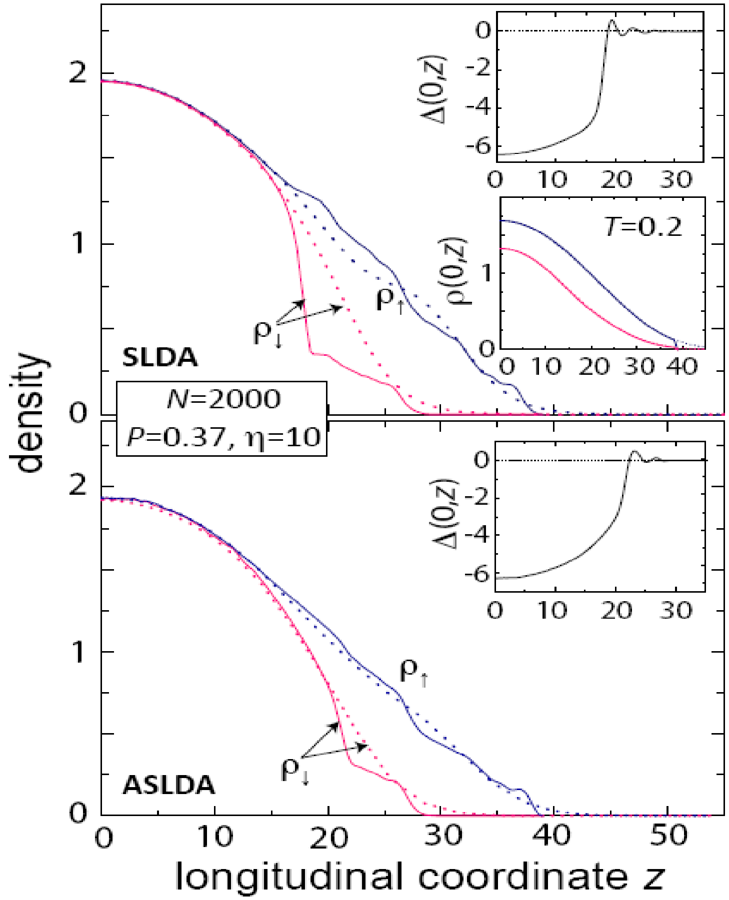

- Compare with the Mean-Field approximation: M*=1

$$\begin{pmatrix} H_\uparrow + g n_\downarrow(r) & \Delta \\ \Delta^* & -H_\downarrow - g n_\uparrow(r) \end{pmatrix} \begin{pmatrix} u_i \\ v_i \end{pmatrix} = E_i \begin{pmatrix} u_i \\ v_i \end{pmatrix}$$

**Tezuka, et al. arXiv:0811.1650**

# SLDA and ASLDA difference

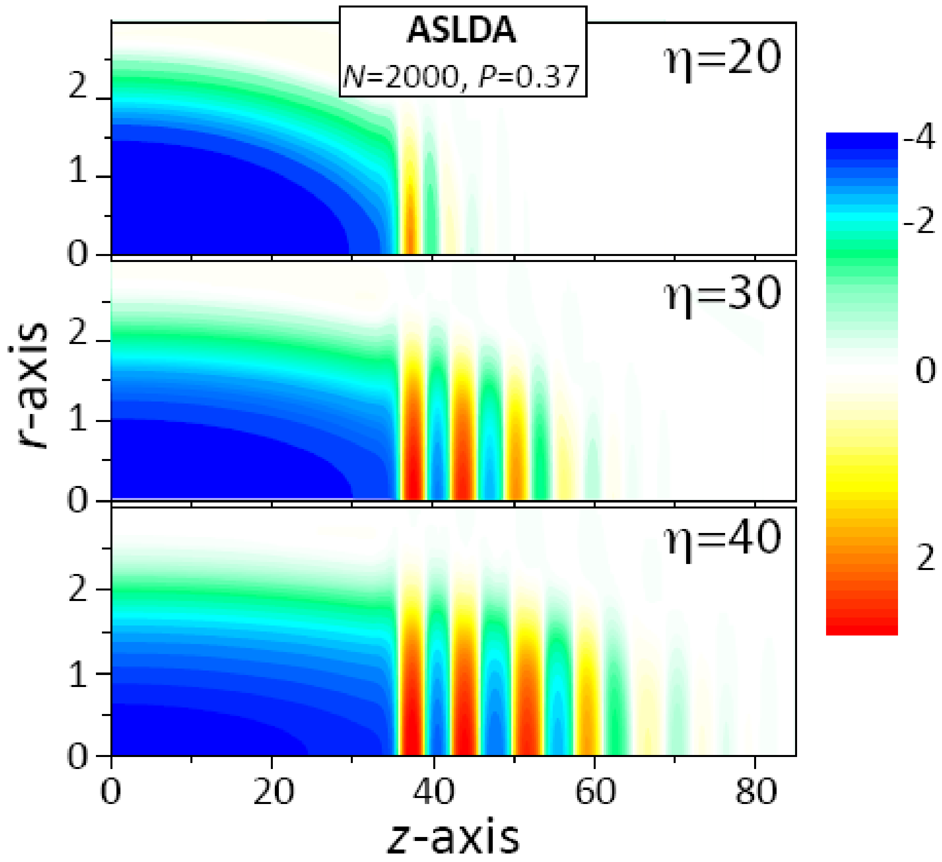
- Ground-state solution starting with smooth pairing




- Small pairing oscillation in g.s. is predicated in less elongated trap.
- Deformed core solution is washed out in ASLDA, because of different Hartree potential.
- Deformation effect disappears at high temperatures

# Propose to access LO states

- Pairing oscillations become remarkable as trap aspect ratio increase
- The oscillations are perpendicular to the long axis
- Oscillation periods are almost the same. Periods are related to the $q_{LO}$




- **Numerical:** evolve the trap from a ground-state solution at a moderate elongated trap to reach an excited state
- **Experiments:** can be accessible by elongate the trap adiabatically.

## Summary

- Cold Fermions have interesting implications for nuclear physics. On the other hand, nuclear physics can contribute to studies of cold Fermions.

- Elongated traps are good for looking for novel superfluid phases: FFLO

  The coordinate-space HFB calculations are useful in the respect.

- ASLDA calculations include local polarizations, i.e., different Hartree potentials for two-spin components, washed out the deformation effect of the superfluid core.

- Both SLDA and ASLDA predicted remarkable oscillating LO phase, coexisting with the normal superfluid phase. And it is accessible by experiments.

Thanks for your attention!