The Incredible Many Facets of the Unitary Fermi Gas

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Outline:

What is a unitary Fermi gas?

Thermodynamic properties

Pairing gap and pseudo-gap

EOS for spin imbalanced systems

P-wave pairing

Small systems in traps and (A)SLDA

Unitary Fermi supersolid: the Larkin-Ovchinnikov phase

Time-dependent phenomena

What else can we expect?

What is the unitary regime?

A gas of interacting fermions is in the unitary regime if the average separation between particles is large compared to their size (range of interaction), but small compared to their scattering length.

The system is very dilute, but strongly interacting!

$$n\, r_0^3 \ll 1$$

$$n\, |a|^3 \gg 1$$

n - number density

$$r_0 \ll n^{-1/3} \approx \lambda_F/2 \ll |a|$$

r_0 - range of interaction

a - scattering length

Bertsch Many-Body X challenge, Seattle, 1999

What are the ground state properties of the many-body system composed of spin ½ fermions interacting via a zero-range, infinite scattering-length contact interaction.

Why? Besides pure theoretical curiosity, this problem is relevant to neutron stars!

In 1999 it was not yet clear, either theoretically or experimentally, whether such fermion matter is stable or not! A number of people argued that under such conditions fermionic matter is unstable.

- ***systems of bosons are unstable (Efimov effect)***
- ***systems of three or more fermion species are unstable (Efimov effect)***

- **Baker (winner of the MBX challenge) concluded that the system is stable. See also Heiselberg (entry to the same competition)**

- **Carlson et al (2003) Fixed-Node Green Function Monte Carlo and Astrakharchik et al. (2004) FN-DMC provided the best theoretical estimates for the ground state energy of such systems.**

- **Thomas' Duke group (2002) demonstrated experimentally that such systems are (meta)stable.**

Superconductivity and superfluidity in Fermi systems

20 orders of magnitude over a century of (low temperature) physics

- ✓ Dilute atomic Fermi gases $T_c \approx 10^{-12} - 10^{-9}$ eV
- ✓ Liquid ^3He $T_c \approx 10^{-7}$ eV
- ✓ Metals, composite materials $T_c \approx 10^{-3} - 10^{-2}$ eV
- ✓ Nuclei, neutron stars $T_c \approx 10^{5} - 10^{6}$ eV
- • QCD color superconductivity $T_c \approx 10^{7} - 10^{8}$ eV

units (1 eV $\approx 10^4$ K)

Thermodynamic properties

Finite Temperatures

Grand Canonical Path-Integral Monte Carlo

$$\hat{H} = \hat{T} + \hat{V} = \int d^3x \left[\psi_\uparrow^\dagger(\vec{x}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \psi_\uparrow(\vec{x}) + \psi_\downarrow^\dagger(\vec{x}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \psi_\downarrow(\vec{x}) \right] - g \int d^3x \; \hat{n}_\uparrow(\vec{x}) \hat{n}_\downarrow(\vec{x})$$

$$\hat{N} = \int d^3x \; \left[\hat{n}_\uparrow(\vec{x}) + \hat{n}_\downarrow(\vec{x}) \right], \qquad \hat{n}_s(\vec{x}) = \psi_s^\dagger(\vec{x}) \psi_s(\vec{x}), \qquad s = \uparrow, \downarrow$$

Trotter expansion (*trotterization* of the propagator)

$$Z(\beta) = \mathrm{Tr} \; \exp\left[-\beta \left(\hat{H} - \mu \hat{N} \right) \right] = \mathrm{Tr} \; \left\{ \exp\left[-\tau \left(\hat{H} - \mu \hat{N} \right) \right] \right\}^{N_\tau}, \qquad \beta = \frac{1}{T} = N_\tau \tau$$

$$E(T) = \frac{1}{Z(T)} \mathrm{Tr} \; \hat{H} \exp\left[-\beta \left(\hat{H} - \mu \hat{N} \right) \right]$$

$$N(T) = \frac{1}{Z(T)} \mathrm{Tr} \; \hat{N} \exp\left[-\beta \left(\hat{H} - \mu \hat{N} \right) \right]$$

No approximations so far, except for the fact that the interaction is not well defined!

Recast the propagator at each time slice and put the system on a 3d-spatial lattice, in a cubic box of side $L=N_s l$, with periodic boundary conditions

$$\exp\left[-\tau\left(\hat{H}-\mu\hat{N}\right)\right] \approx \exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]\exp(-\tau\hat{V})\exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]+O(\tau^3)$$

Discrete Hubbard-Stratonovich transformation

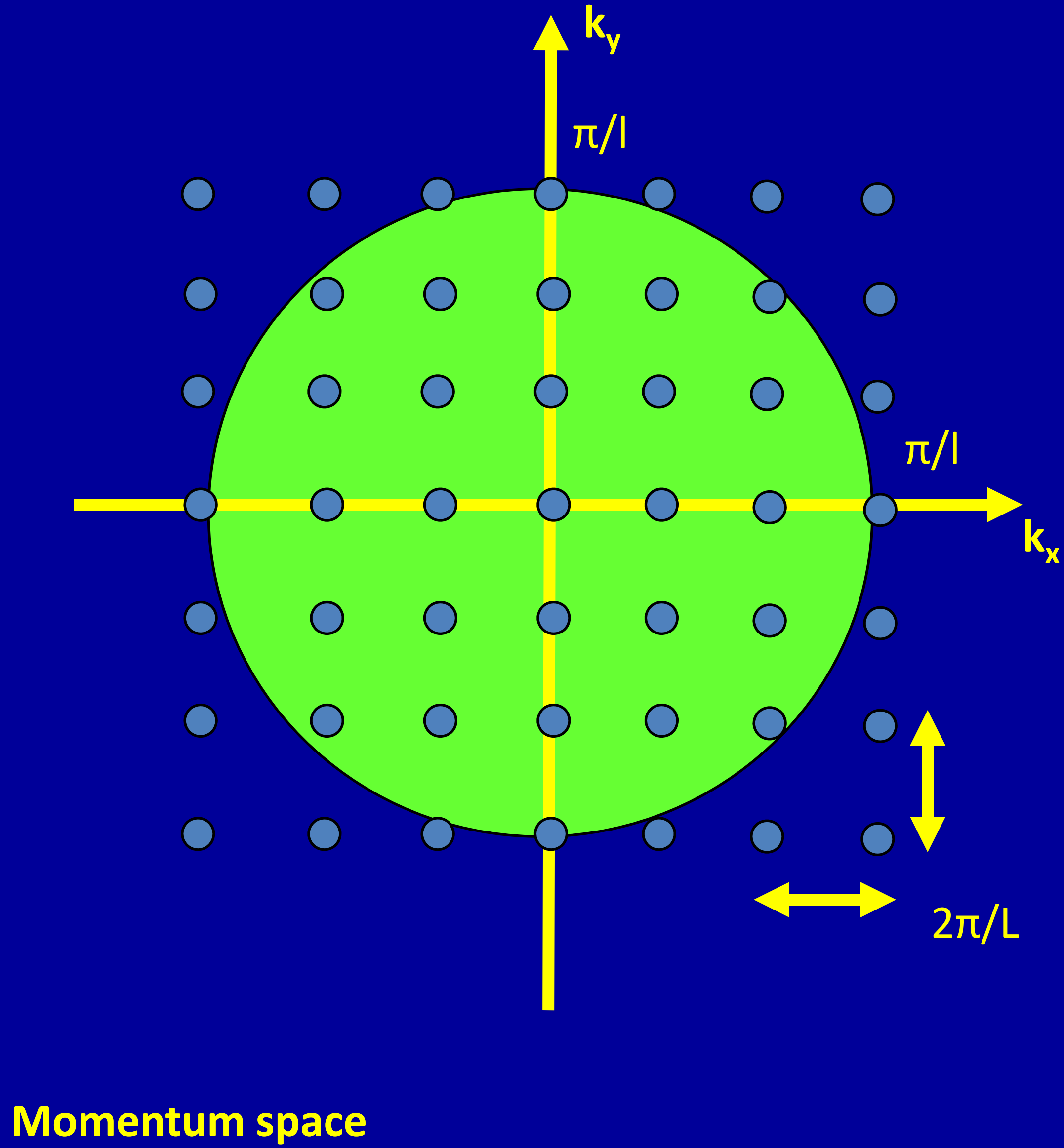
$$\exp(-\tau\hat{V}) = \prod_{\vec{x}} \sum_{\sigma_\pm(\vec{x})=\pm 1} \frac{1}{2}\left[1+\sigma_\pm(\vec{x})A\hat{n}_\uparrow(\vec{x})\right]\left[1+\sigma_\pm(\vec{x})A\hat{n}_\downarrow(\vec{x})\right], \qquad A=\sqrt{\exp(\tau g)-1}$$

σ-fields fluctuate both in space and imaginary time

$$\frac{m}{4\pi\hbar^2 a} = -\frac{1}{g} + \frac{m k_c}{2\pi^2\hbar^2}, \qquad k_c < \frac{\pi}{l}$$

Running coupling constant g defined by lattice

How to choose the lattice spacing and the box size?



$$\varepsilon_F,\ \Delta,\ T \ll \frac{\hbar^2\pi^2}{2ml^2}$$

$$\delta\varepsilon > \frac{2\hbar^2\pi^2}{mL^2}$$

$$\varepsilon_F,\ \Delta \gg \frac{2\hbar^2\pi^2}{mL^2}$$

$$\xi \ll L = N_s l$$

$$\delta p > \frac{2\pi\hbar}{L}$$

$$Z(T) = \int \prod_{\vec{x},\tau} D\sigma(\vec{x},\tau)\ \mathrm{Tr}\,\hat{U}(\{\sigma\})$$

$$\hat{U}(\{\sigma\}) = T_\tau \prod_\tau \exp\{-\tau[\hat{h}(\{\sigma\}) - \mu]\}$$

One-body evolution operator in imaginary time

$$E(T) = \int \frac{\prod_{\vec{x},\tau} D\sigma(\vec{x},\tau)\mathrm{Tr}\,\hat{U}(\{\sigma\})}{Z(T)} \frac{\mathrm{Tr}\left[\hat{H}\hat{U}(\{\sigma\})\right]}{\mathrm{Tr}\,\hat{U}(\{\sigma\})}$$

$$\mathrm{Tr}\,\hat{U}(\{\sigma\}) = \{\det[1+\hat{U}(\{\sigma\})]\}^2 = \exp[-S(\{\sigma\})] > 0$$

No sign problem!

$$n_\uparrow(\vec{x},\vec{y}) = n_\downarrow(\vec{x},\vec{y}) = \sum_{k,l<k_c} \varphi_{\vec{k}}(\vec{x}) \left[\frac{\hat{U}(\{\sigma\})}{1+\hat{U}(\{\sigma\})}\right]_{\vec{k}\ \vec{l}} \varphi_{\vec{l}}^*(\vec{y}), \qquad \varphi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k}\cdot\vec{x})}{\sqrt{V}}$$

All traces can be expressed through these single-particle density matrices

More details of the calculations:

- **Typical lattice sizes used from $\underline{8^3 \times 300}$ (high Ts) to $\underline{8^3 \times 1800}$ (low Ts)**

- **Effective use of FFT(W) makes all imaginary time propagators diagonal (either in real space or momentum space) and there is no need to store large matrices**

- **Update field configurations using the Metropolis importance sampling algorithm**

- **Change randomly at a fraction of all space and time sites the signs the auxiliary fields $\sigma(x,\tau)$ so as to maintain a running average of the acceptance rate between 0.4 and 0.6**

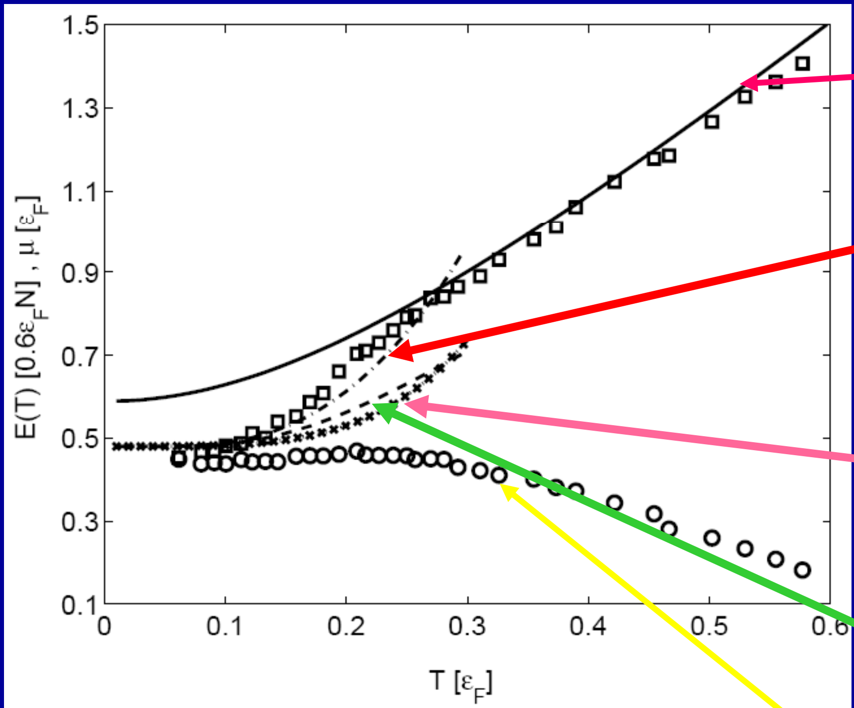
- **Thermalize for 50,000 – 100,000 MC steps or/and use as a start-up field configuration a $\sigma(x,\tau)$-field configuration from a different T**

- **At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics**

- **Use 100,000-2,000,000 $\sigma(x,\tau)$- field configurations for calculations**

- **MC correlation "time" ≈ 250 – 300 time steps at $T \approx T_c$**

a = ±∞



Normal Fermi Gas
(with vertical offset, solid line)

Bogoliubov-Anderson phonons and quasiparticle contribution (dot-dashed lien)

Bogoliubov-Anderson phonons contribution only

Quasi-particles contribution only (dashed line)

μ - chemical potential (circles)

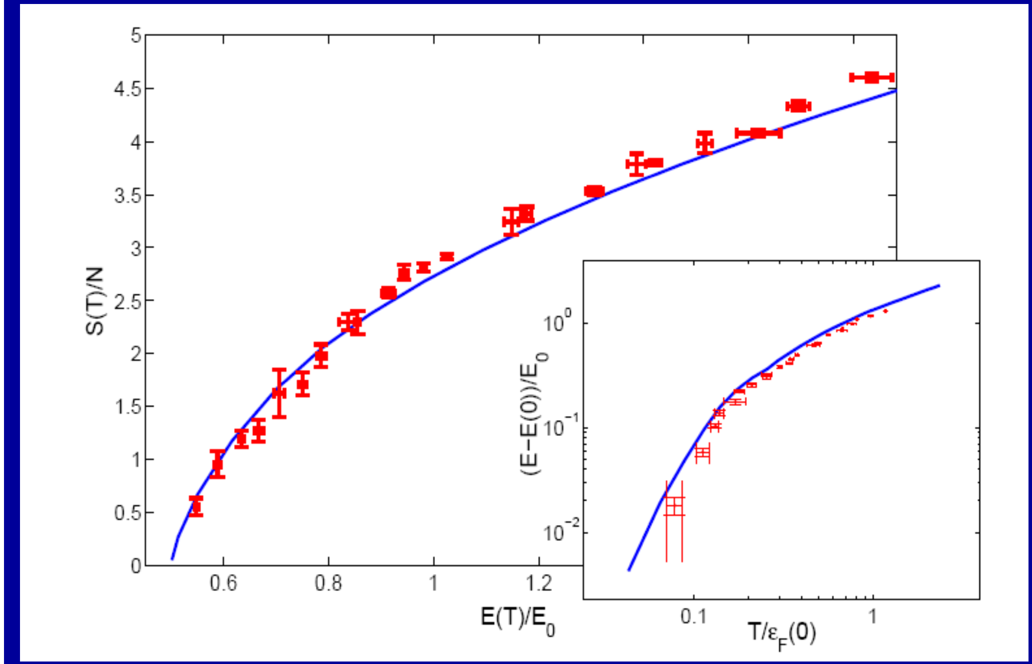
$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.44$$

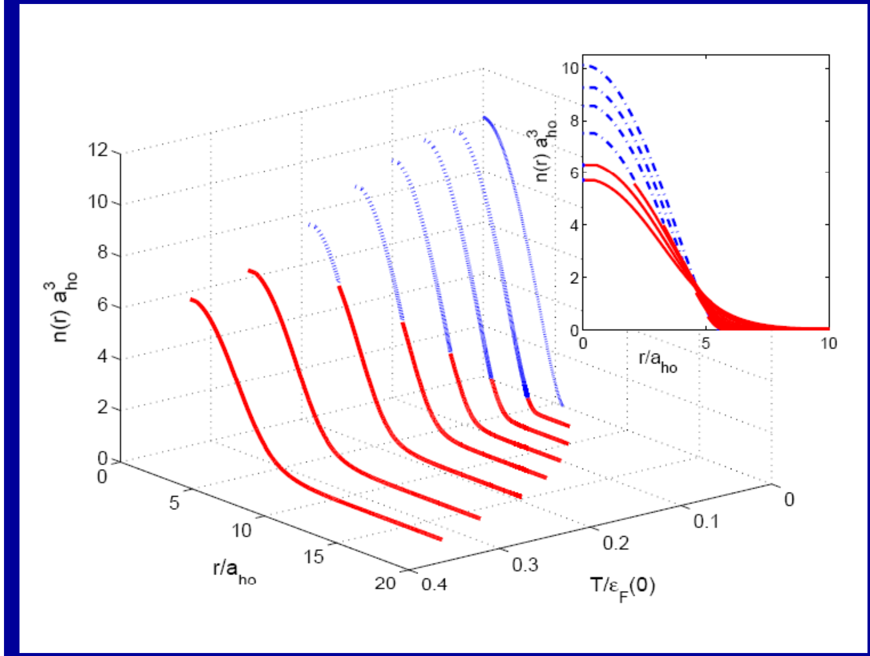
$$E_{\text{quasi-particles}}(T) = \frac{3}{5}\varepsilon_F N \frac{5}{2}\sqrt{\frac{2\pi\Delta^3 T}{\varepsilon_F^4}}\exp\left(-\frac{\Delta}{T}\right)$$

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

Bulgac, Drut, and Magierski
PRL 96, 090404 (2006)

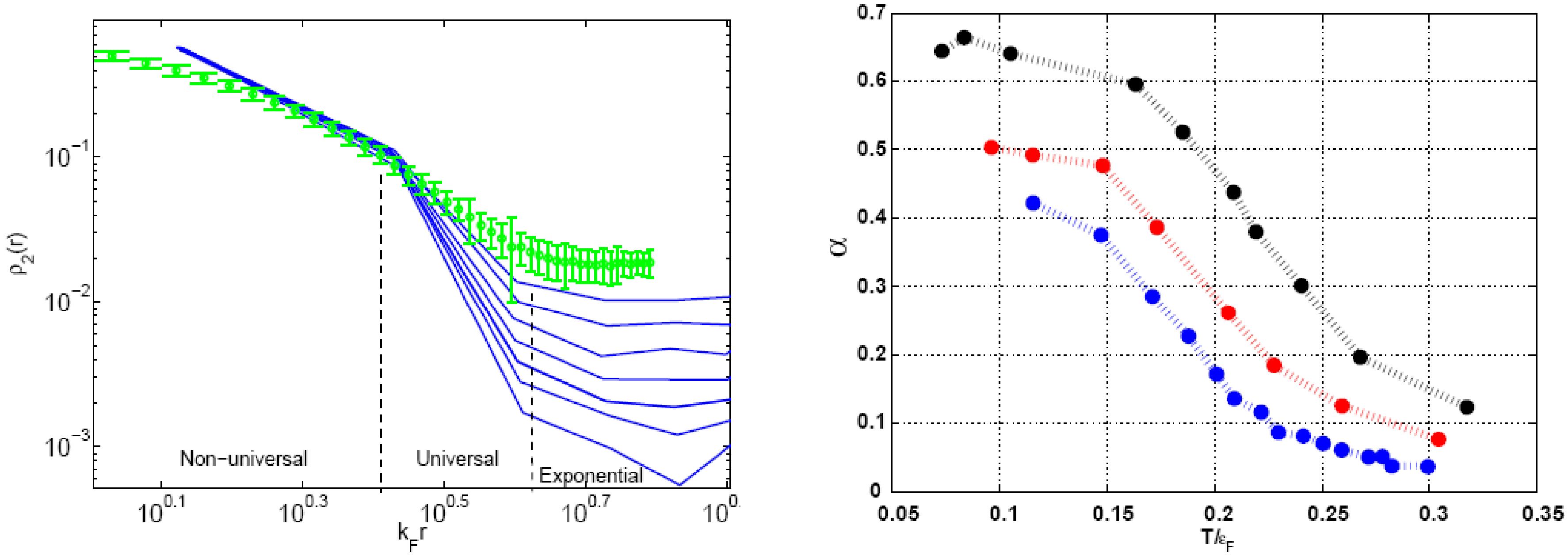
Measurement of the Entropy and Critical Temperature of a Strongly Interacting Fermi Gas, Luo, Clancy, Joseph, Kinast, and Thomas, PRL 98, 080402 (2007)





Bulgac, Drut, and Magierski
PRL 99, 120401 (2007)

Long range order and condensate fraction

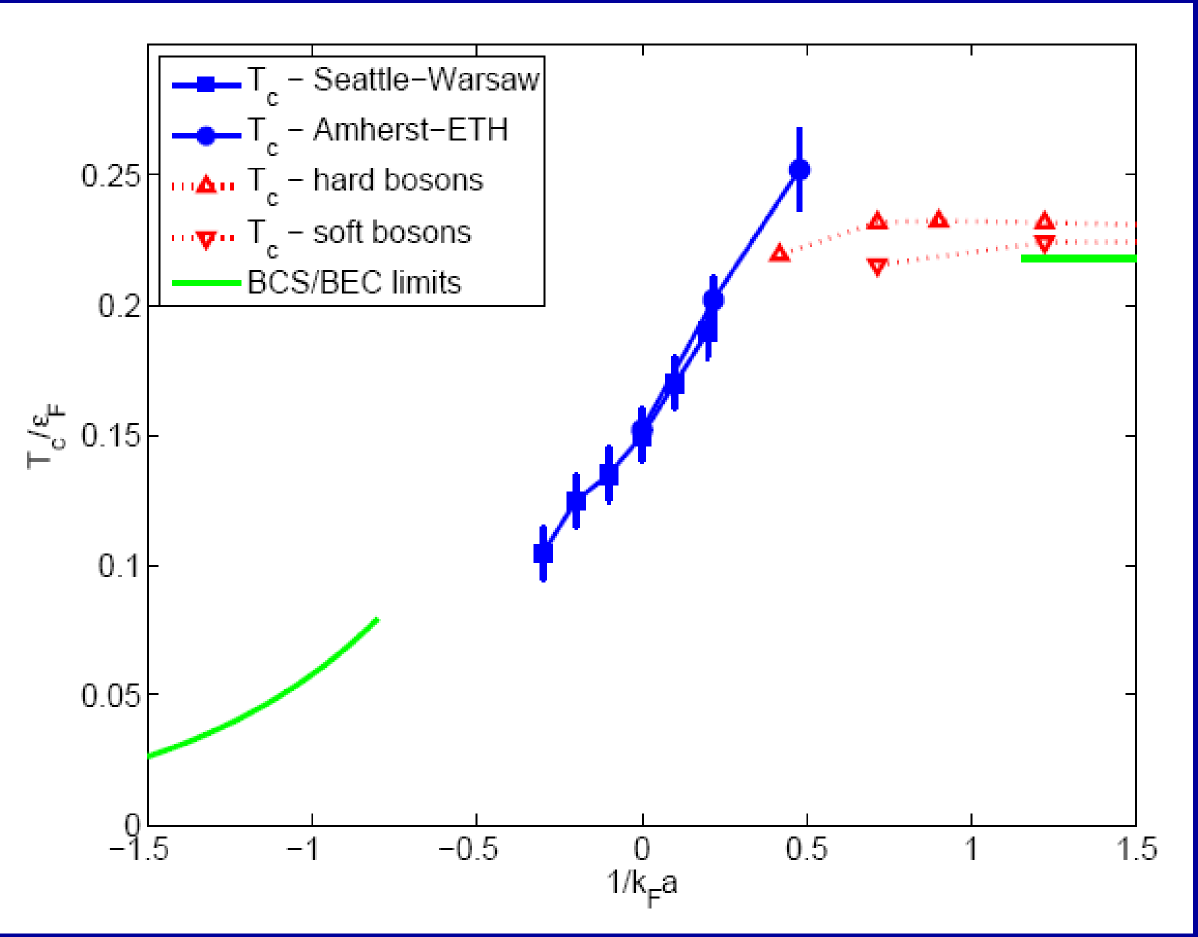


$$g_2(\vec{r}) = \left(\frac{2}{N}\right)^2 \int d^3\vec{r}_1 \int d^3\vec{r}_2 \left\langle \psi_\uparrow^\dagger(\vec{r}_1+\vec{r})\psi_\downarrow^\dagger(\vec{r}_2+\vec{r})\psi_\downarrow(\vec{r}_2)\psi_\uparrow(\vec{r}_2)\right\rangle$$

$$\alpha = \lim_{r\to\infty} \frac{N}{2} g_2(\vec{r}) - n(\vec{r})^2, \qquad n(\vec{r}) = \frac{2}{N}\int d^3\vec{r}_1 \left\langle \psi_\uparrow^\dagger(\vec{r}_1+\vec{r})\psi_\uparrow(\vec{r}_1)\right\rangle$$

Bulgac, Drut, and Magierski, arXiv:0803:3238

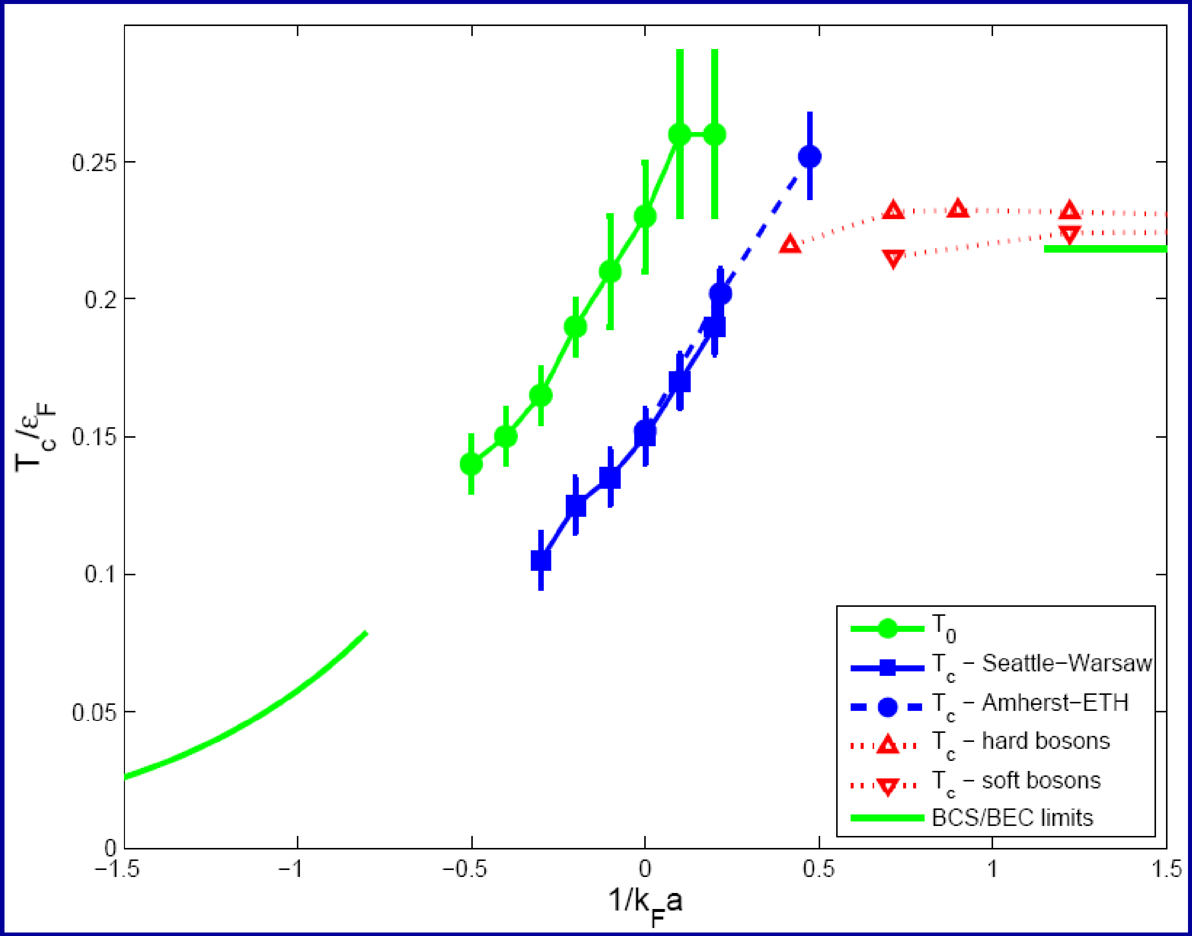
Critical temperature for superfluid to normal transition



Amherst-ETH: Burovski et al. arXiv:0805:3047
Hard and soft bosons: Pilati et al. PRL 100, 140405 (2008)

Bulgac, Drut, and Magierski, arXiv:0803:3238

Critical temperature for superfluid to normal transition

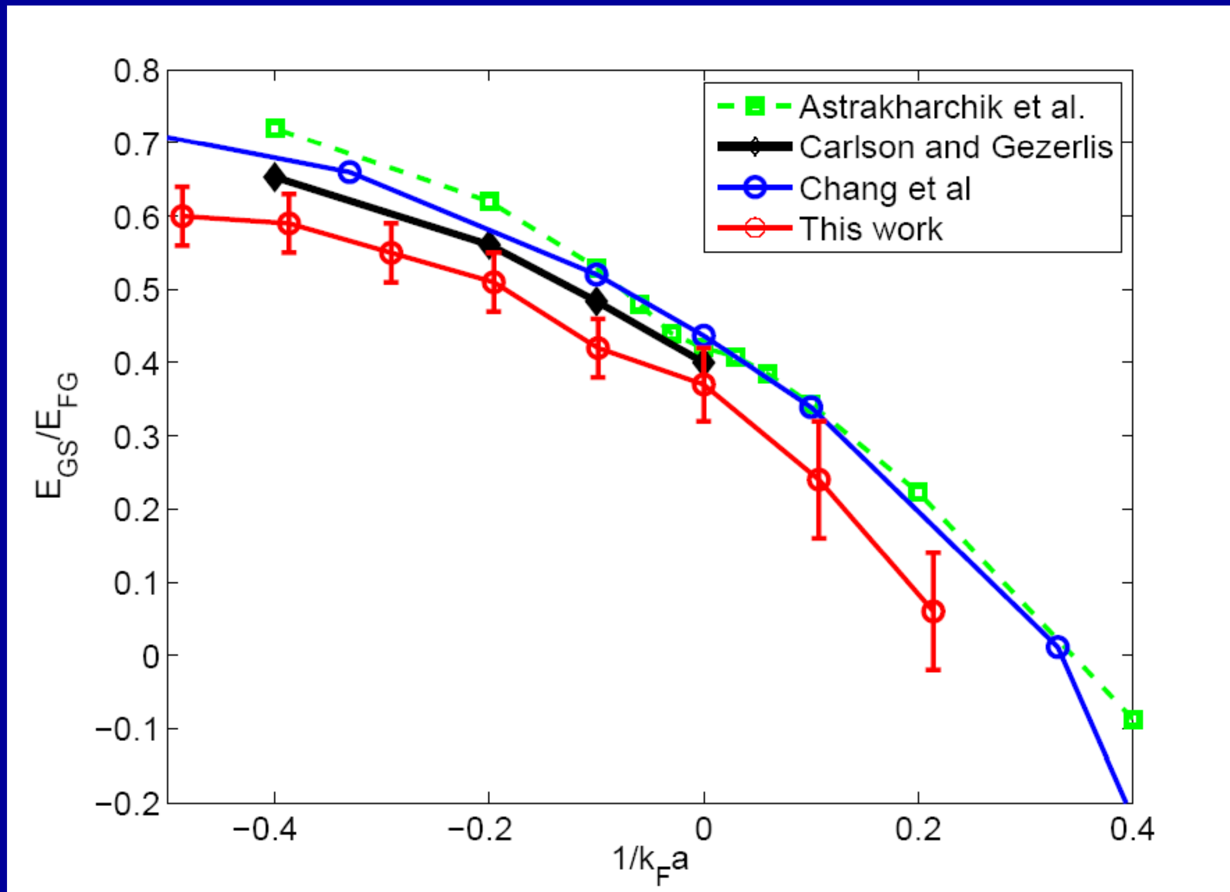


Amherst-ETH: Burovski et al. arXiv:0805:3047

Hard and soft bosons: Pilati et al. PRL 100, 140405 (2008)

Bulgac, Drut, and Magierski, arXiv:0803:3238

Ground state energy



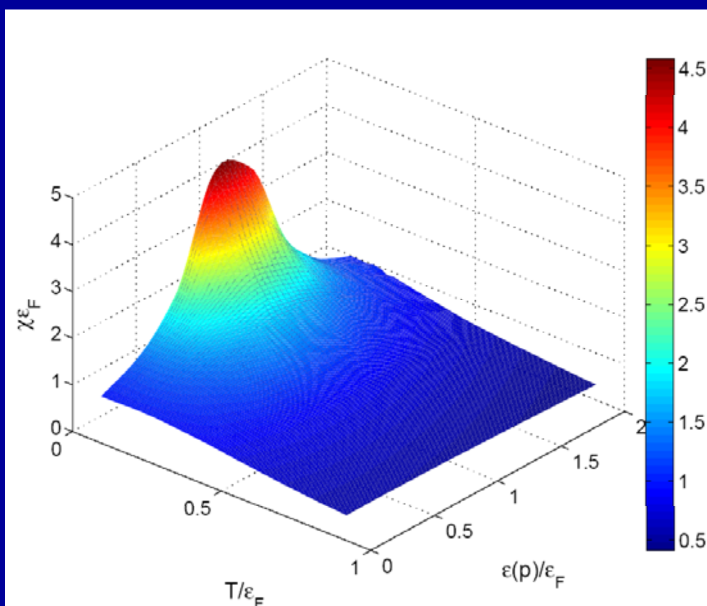
Bulgac, Drut, Magierski, and Wlazowski, arXiv:0801:1504
Bulgac, Drut, and Magierski, arXiv:0803:3238

Pairing Gap and Pseudo-gap

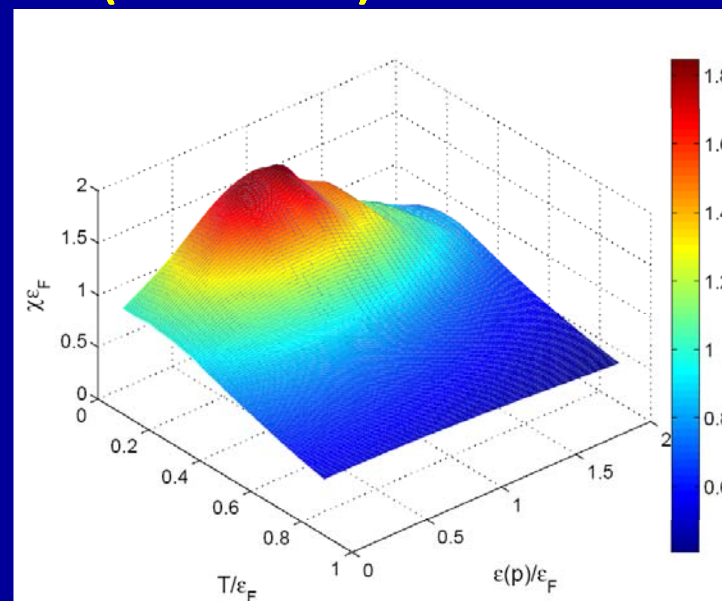
Response of the two-component Fermi gas in the unitary regime

$$\chi(\vec{p}) = -T\frac{d}{dg}\frac{\mathrm{Tr}\{\exp[-\beta(\mathrm{H}-\mu\mathrm{N}+\mathrm{g}\,\psi(\vec{\mathrm{p}}))]\,\psi^{\dagger}(\vec{\mathrm{p}})\}}{\mathrm{Tr}\{\exp[-\beta(\mathrm{H}-\mu\mathrm{N}+\mathrm{g}\,\psi(\vec{\mathrm{p}}))]\}}\Bigg|_{g=0} = -\int_0^{\beta} d\tau\,\mathrm{G}(\vec{p},\tau)$$

One-body temperature (Matsubara) Green's function



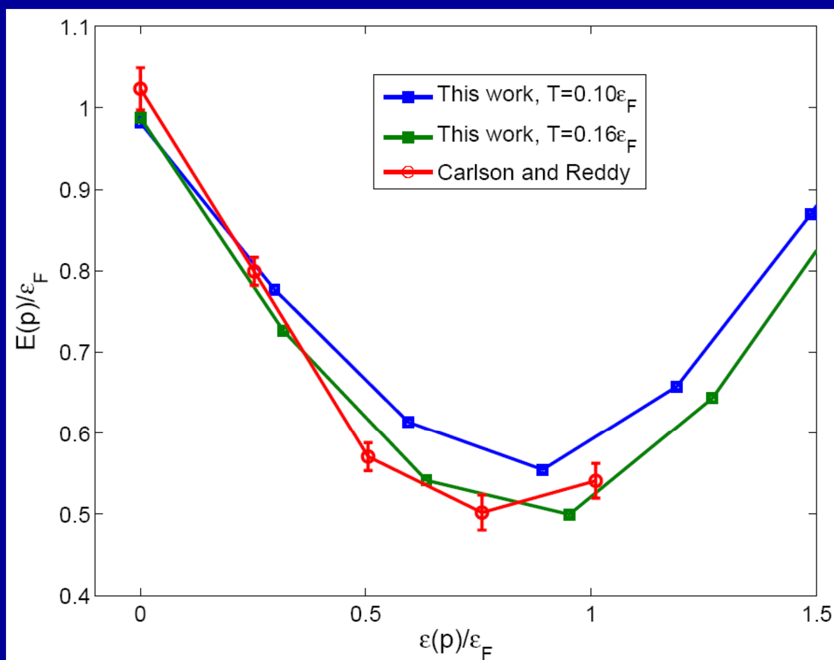
$$\frac{1}{k_F a} = -2$$

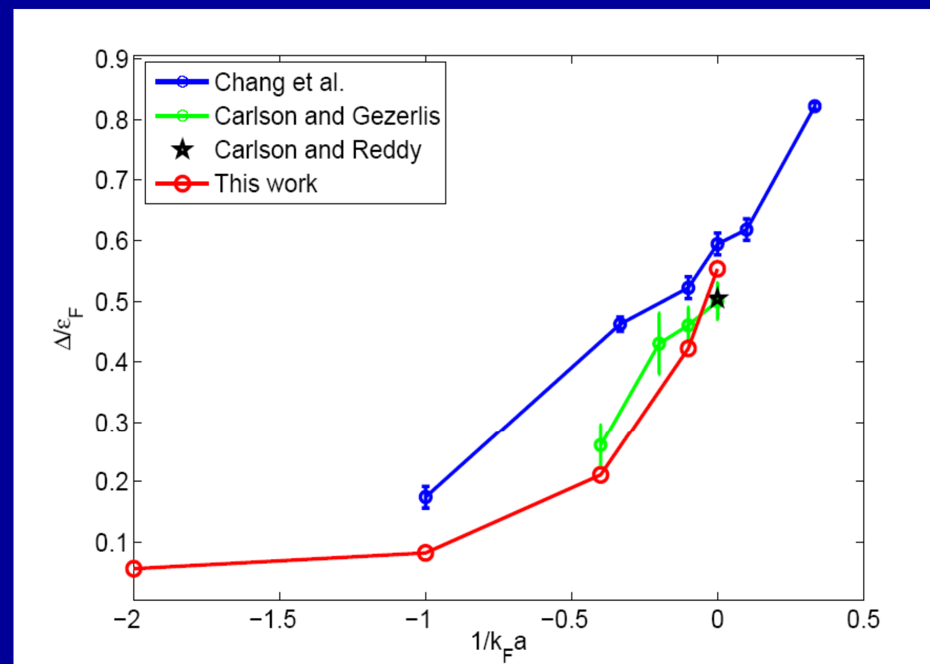


$$\frac{1}{k_F a} = 0$$

Bulgac, Drut, and Magierski, arXiv:0801:1504

Quasi-particle spectrum and pairing gap

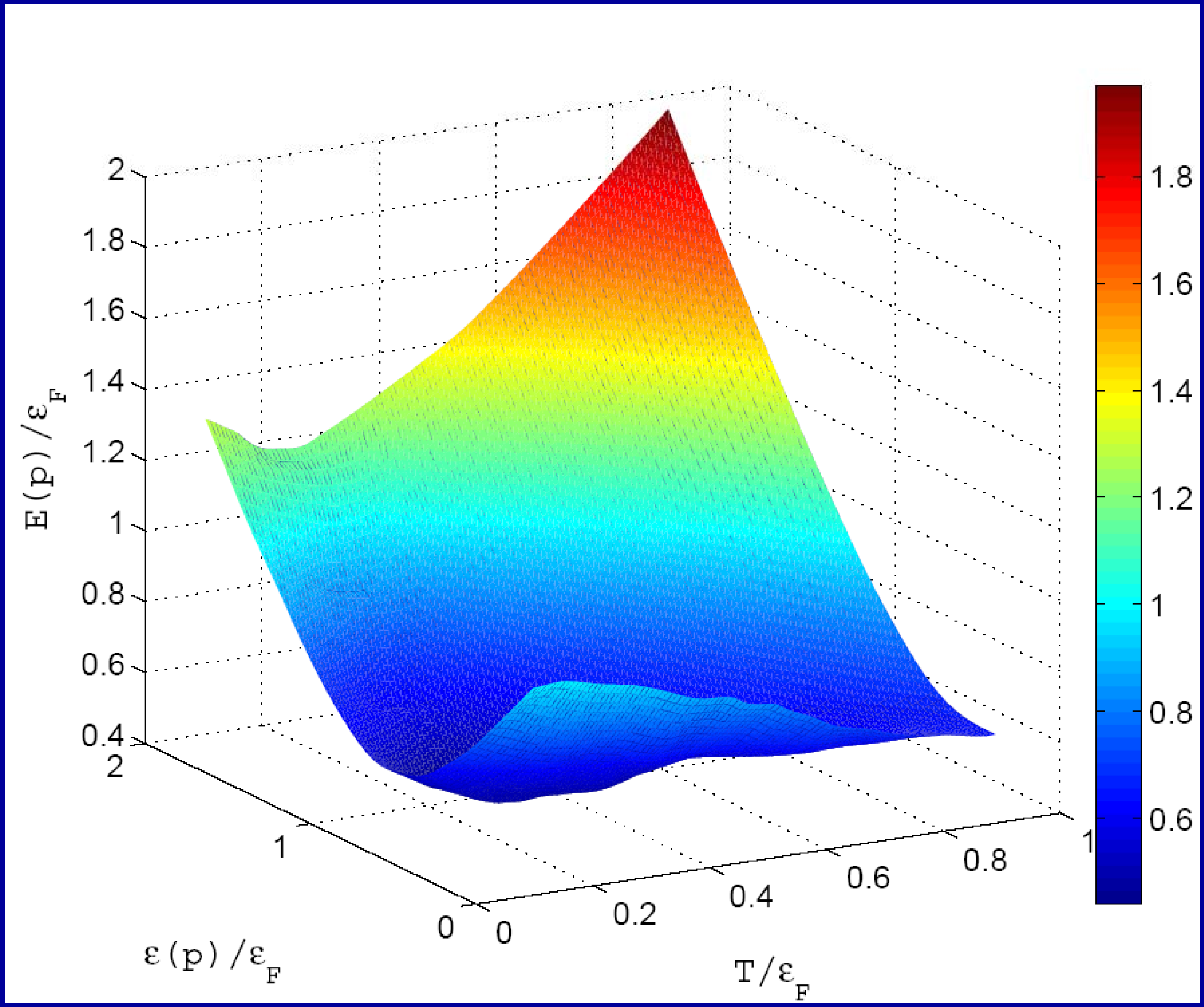




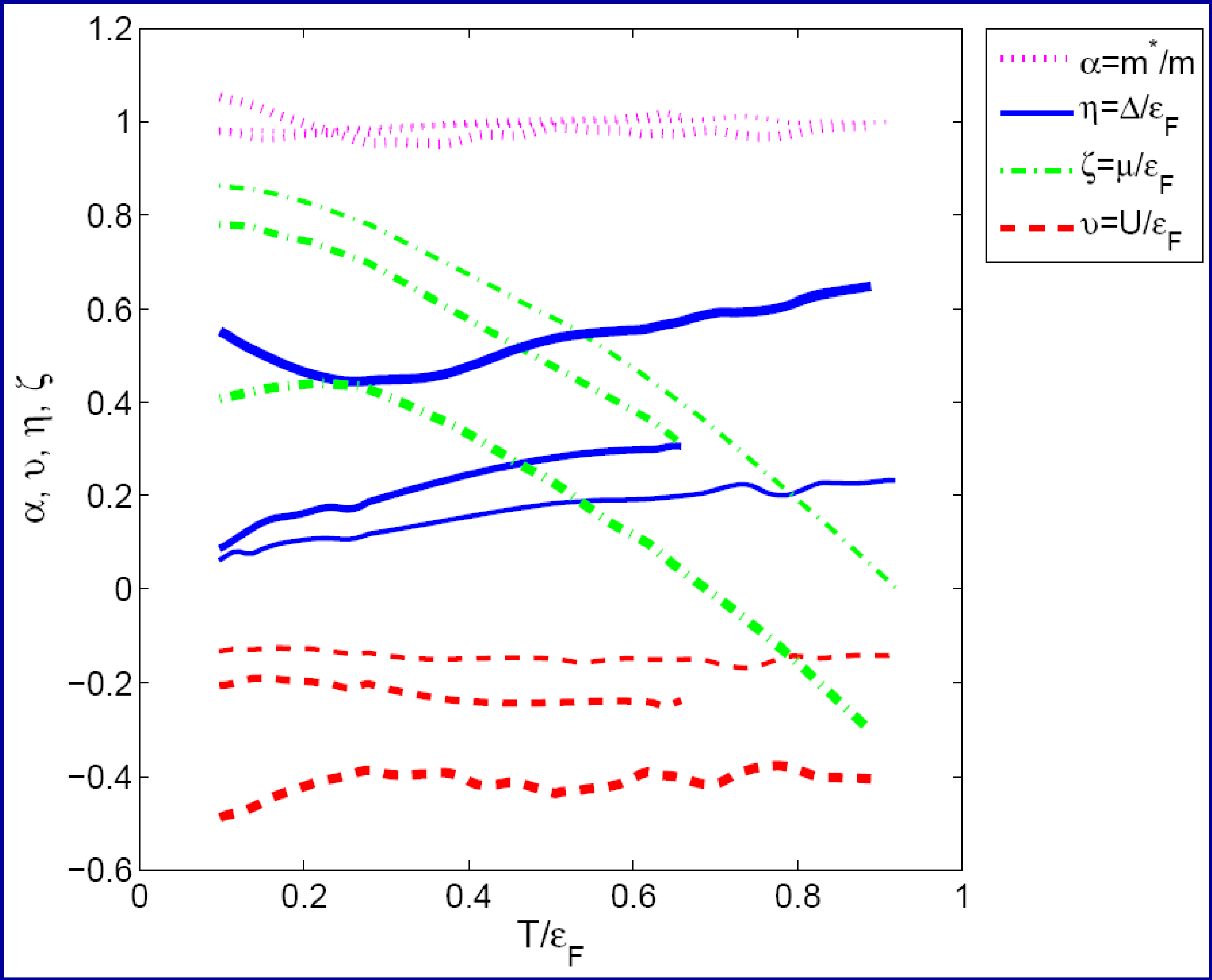
$$\chi(\vec{p}) = -\int_0^\beta d\tau \mathrm{G}(\vec{p},\tau) = \frac{1}{E(\vec{p})}\frac{\exp[\beta E(\vec{p})]-1}{\exp[\beta E(\vec{p})]+1}$$

Bulgac, Drut, and Magierski, arXiv:0801:1504

Quasi-particle spectrum at unitarity



Bulgac, Drut, and Magierski, arXiv:0801:1504

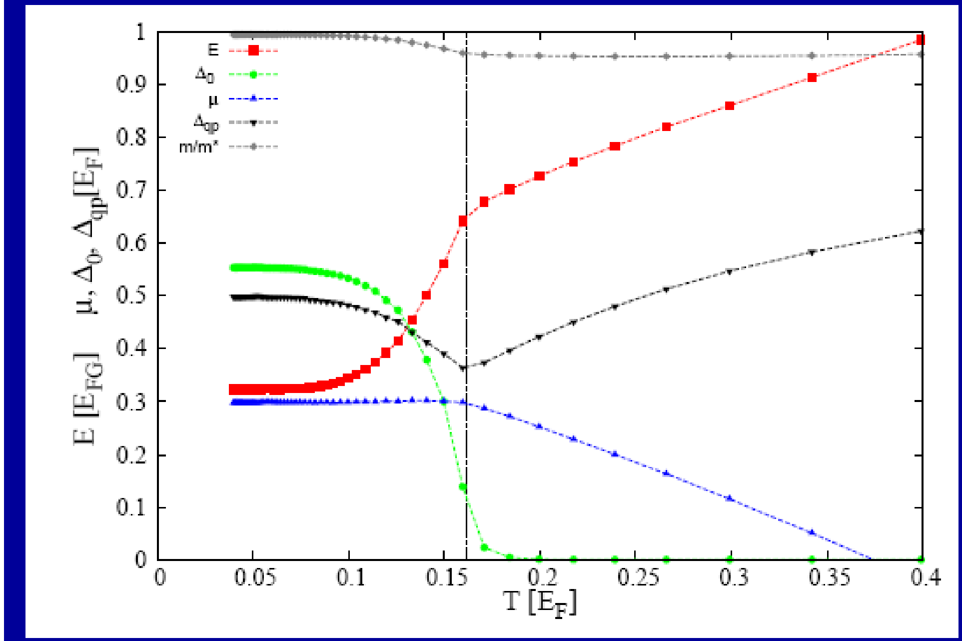


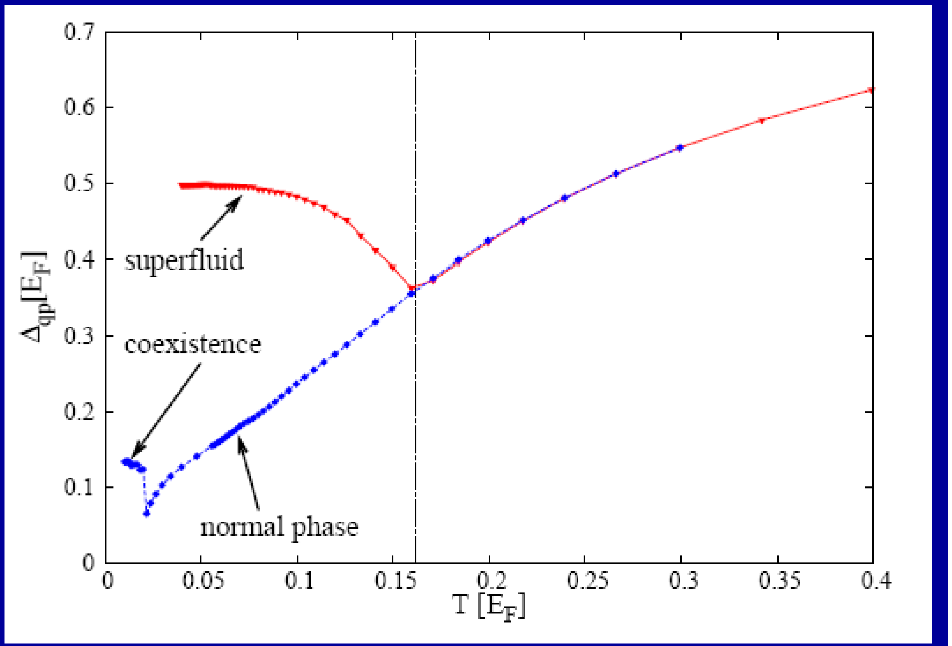
$$\frac{1}{k_F a} = -2, \ \ -1, \ \ 0$$

$$E(p) = \sqrt{\left(\frac{\alpha p^2}{2} + U - \mu\right)^2 + \Delta^2}$$

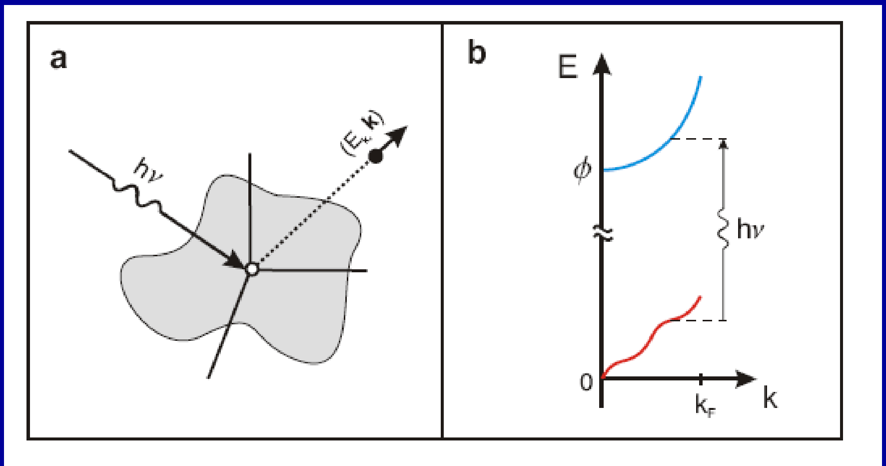
Bulgac, Drut, and Magierski, arXiv:0801:1504

Dynamical Mean-Field Theory applied to a Unitary Fermi gas (exact in infinite number of dimensions)



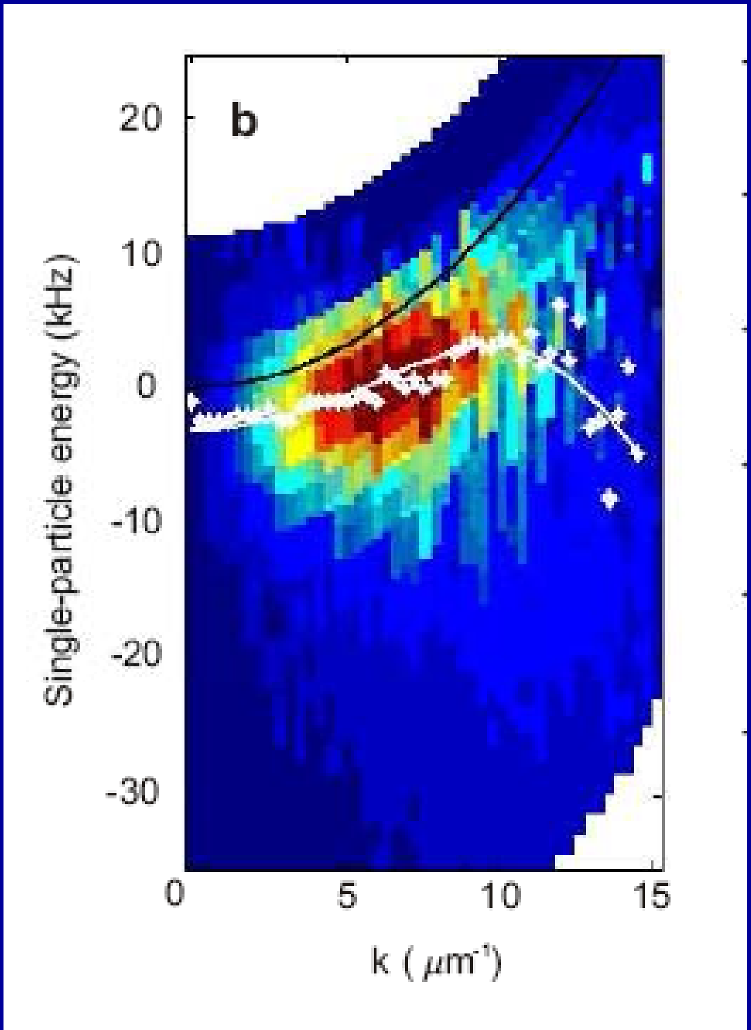


Superfluid to insulator phase transition in a unitary Fermi gas
Barnea, arXiv:0803:2293



$$-E_s + h\nu = \frac{\hbar^2 k^2}{2m} + \phi$$

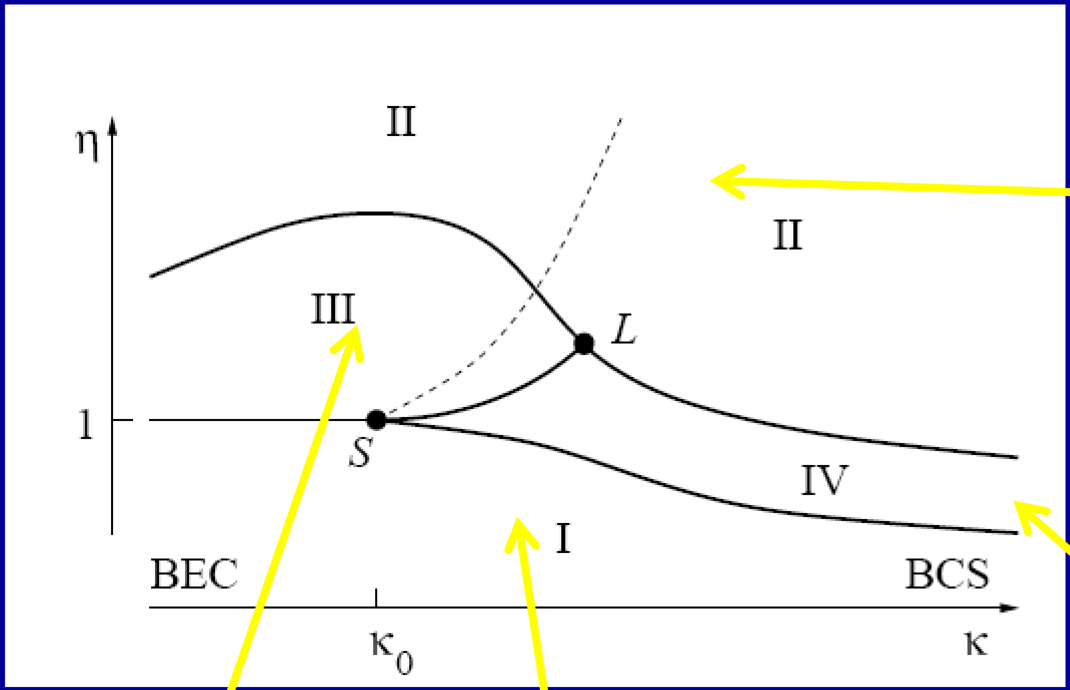
$$E(N) = E(N-1) + E_s$$



Using photoemission spectroscopy to probe a strongly interacting Fermi gas

Stewart, Gaebler and Jin, arXiv:0805:0026

EOS for spin imbalanced systems



Normal phase
(unpaired spin-up fermions)

Fully symmetric phase

LOFF phases

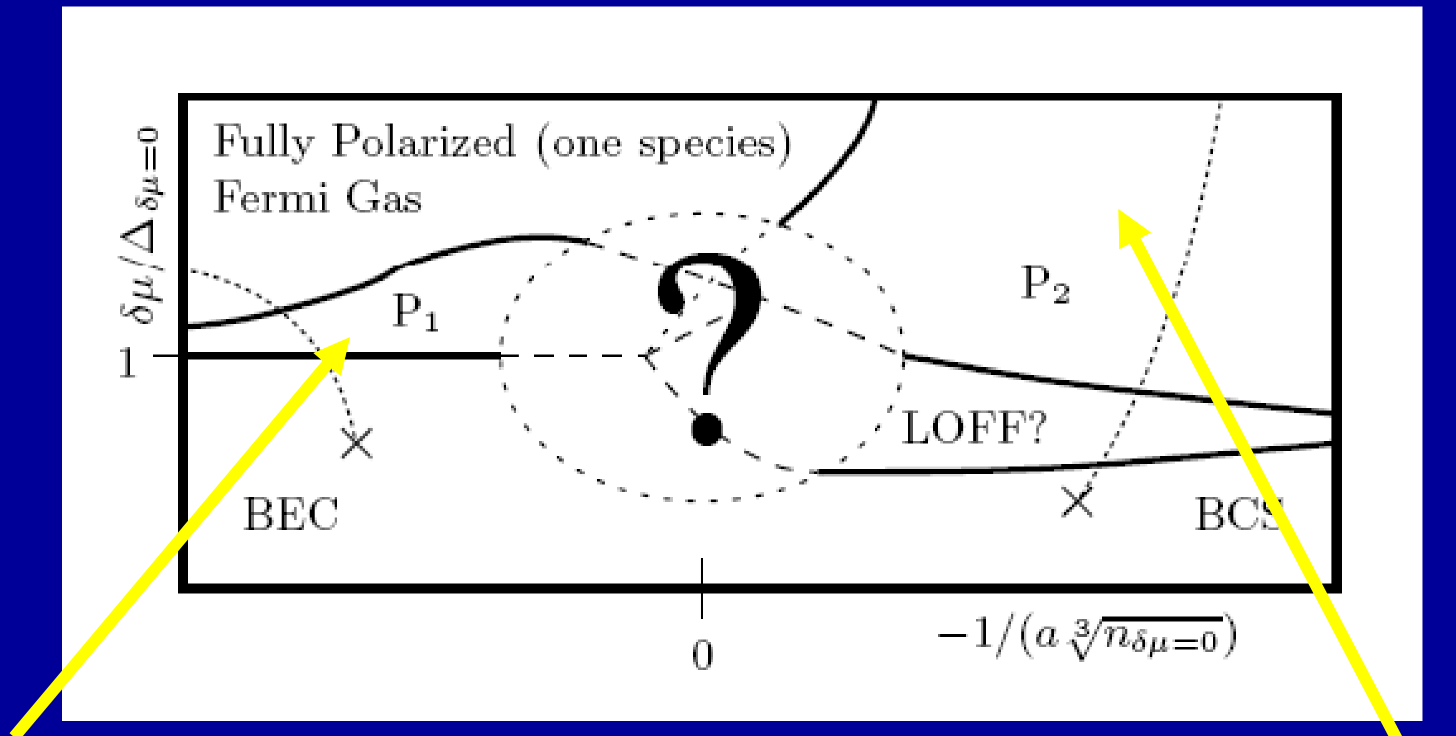
Gapless BEC superfluid
(BEC of dimers + unpaired spin-up fermions)

Son and Stephanov, PRA 74, 013614 (2006)

What we think is happening in spin imbalanced systems?

Induced P-wave superfluidity

Two new superfluid phases where before they were not expected

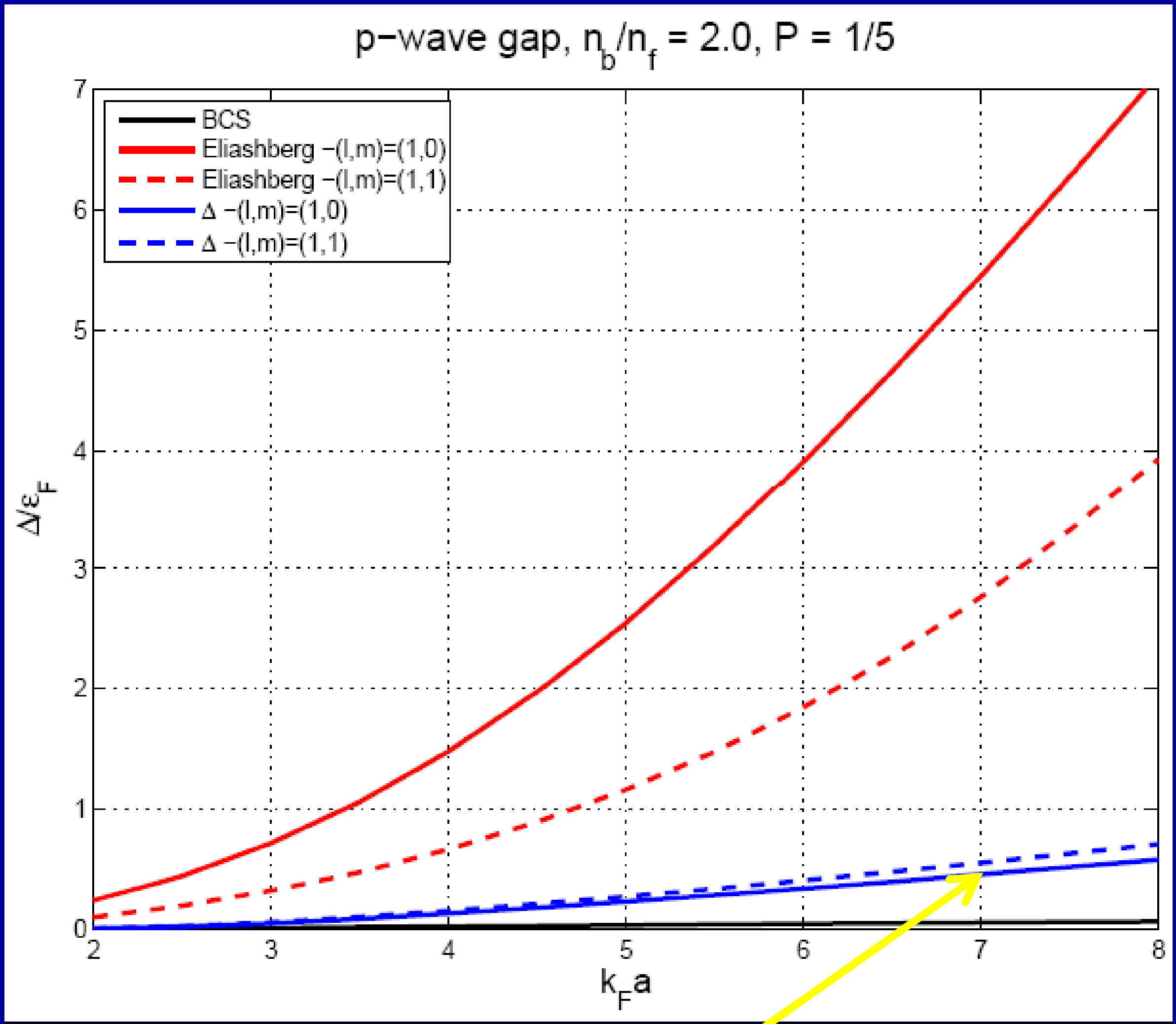


One Bose superfluid coexisting with one P-wave Fermi superfluid

Two coexisting P-wave Fermi superfluids

Bulgac, Forbes, Schwenk, PRL 97, 020402 (2006)

Going beyond the naïve BCS approximation



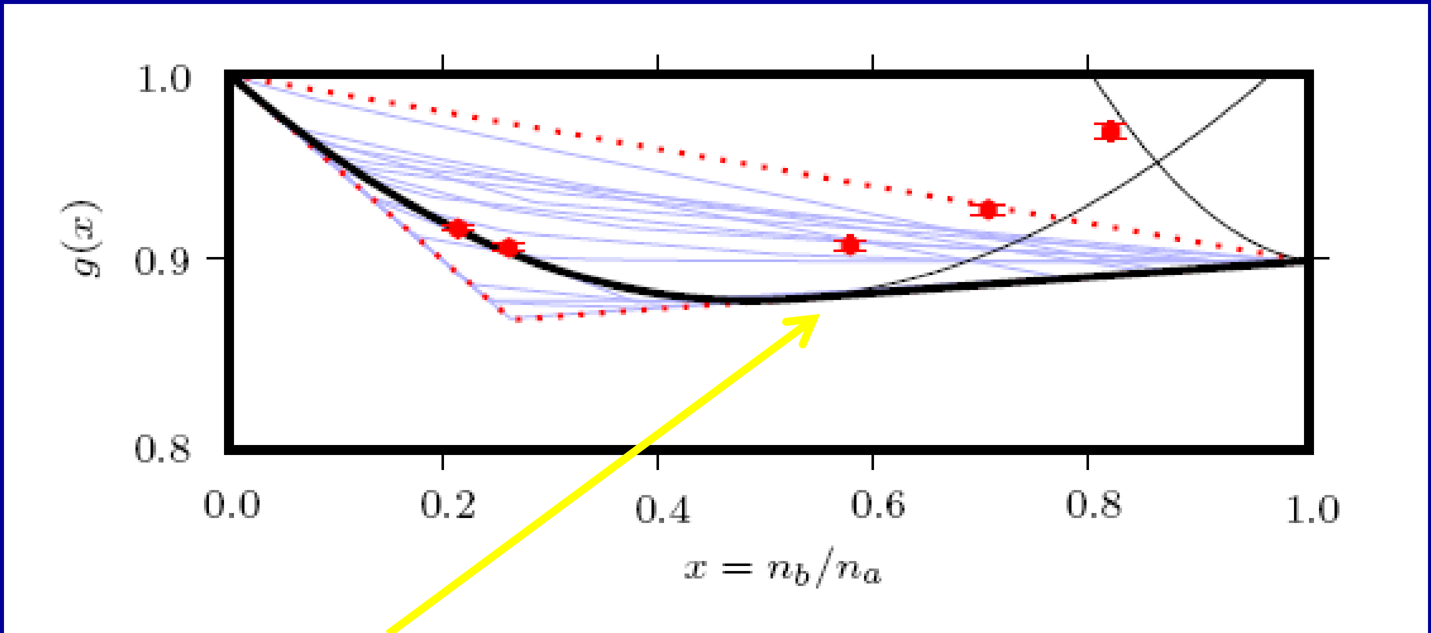
Eliashberg approx. (red)

BCS approx. (black)

Full momentum and frequency dependence of the self-consistent equations (blue)

Bulgac and Yoon, unpublished (2007)

What happens at unitarity?



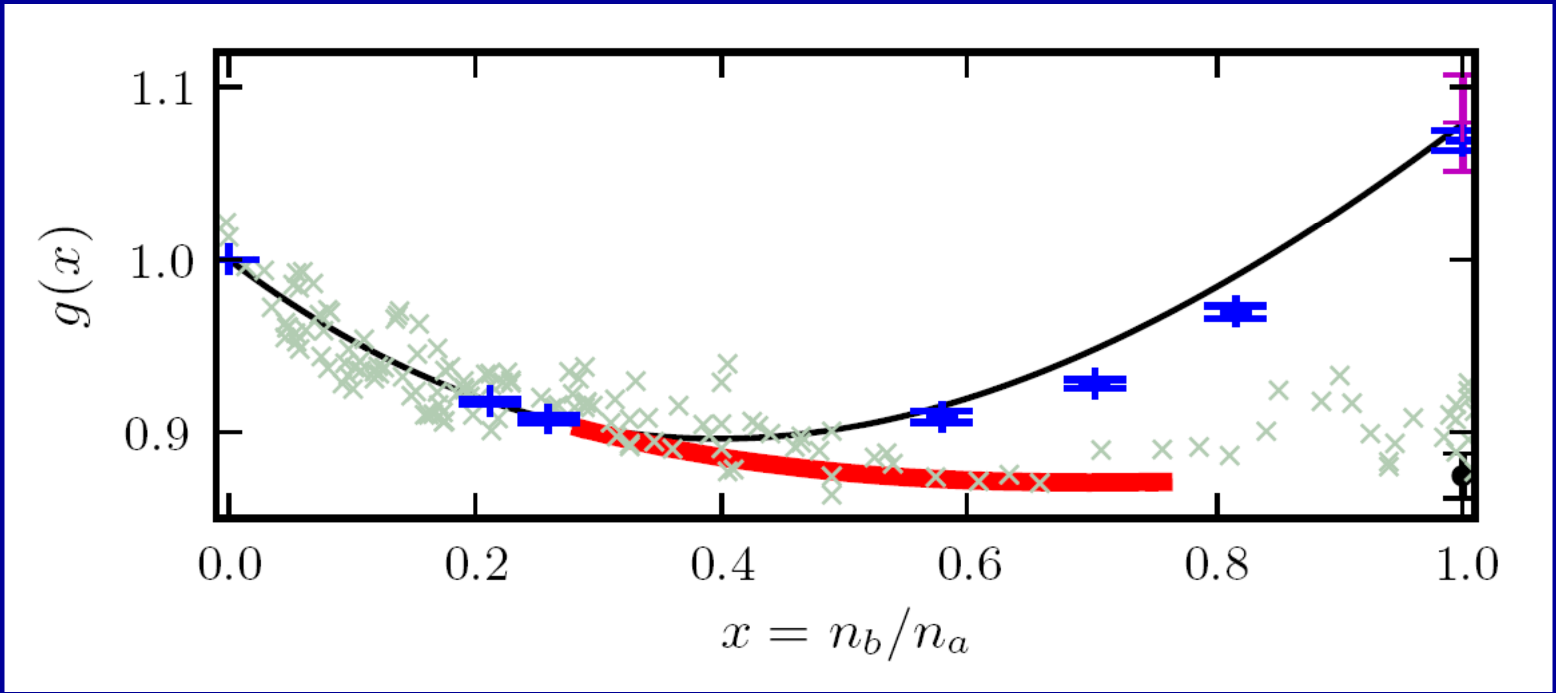
Predicted quantum first phase order transition, subsequently observed in MIT experiment , Shin *et al*. arXiv:0709:3027

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

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

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 density
Blue points: DMC calculations for normal state, Lobo et al, PRL 97, 200403 (2006)
Gray crosses: experimental EOS due to Shin, arXiv :0801:1523

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

Bulgac and Forbes, arXiv:0804:3364

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

How to construct and validate an *ab initio* Energy Density Functional (EDF)?

- ❑ **Given a many body Hamiltonian determine the properties of the infinite homogeneous system as a function of density**
- ❑ **Extract the 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!**

The SLDA energy density functional at unitarity for equal numbers of spin-up and spin-down fermions

Only this combination is cutoff independent

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

$$n(\vec{r}) = 2 \sum_{0<E_k<E_c} \left| \mathrm{v}_k(\vec{r}) \right|^2, \quad \tau_c(\vec{r}) = 2 \sum_{0<E_k<E_c} \left| \vec{\nabla} \mathrm{v}_k(\vec{r}) \right|^2,$$

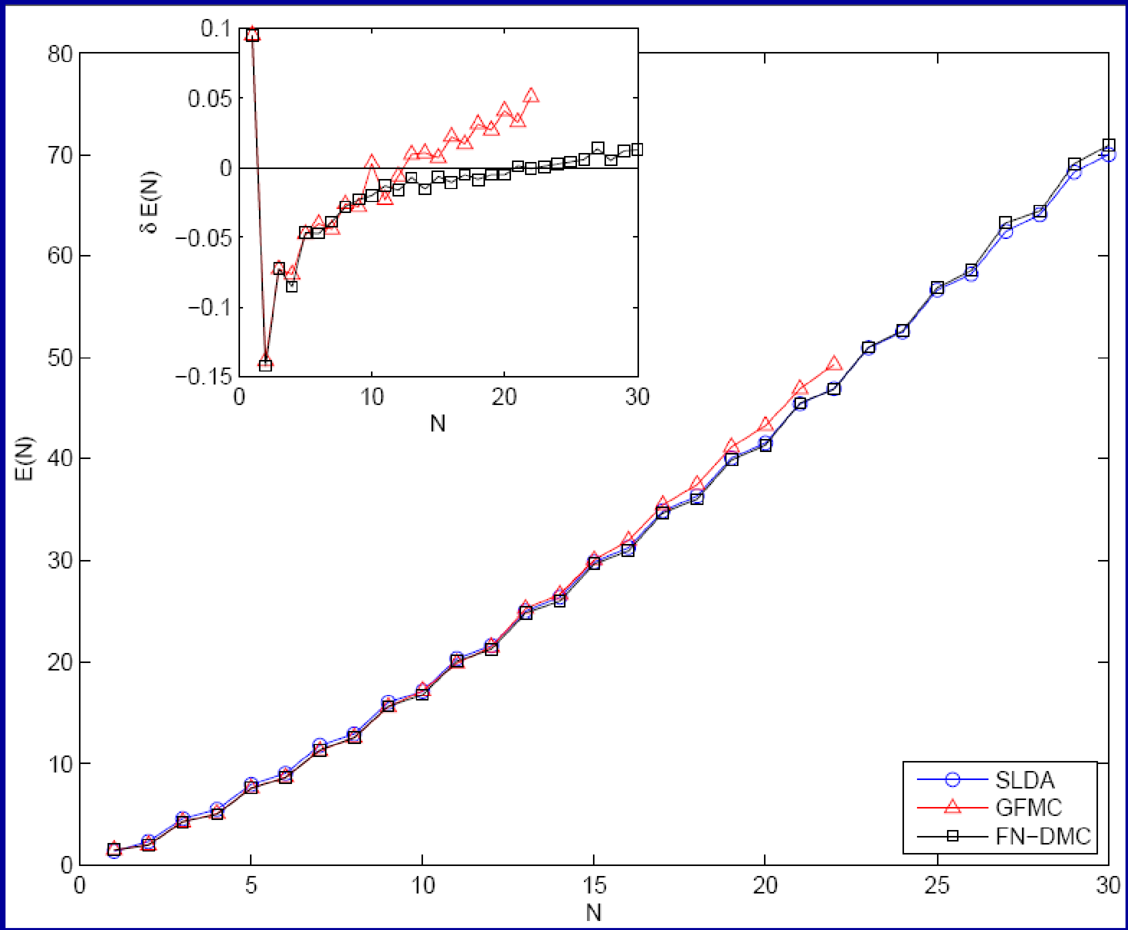
$$\nu_c(\vec{r}) = \sum_{0<E<E_c} \mathrm{u}_k(\vec{r}) \mathrm{v}_k^*(\vec{r})$$

$$U(\vec{r}) = \beta \frac{(3\pi^2)^{2/3} n^{2/3}(\vec{r})}{2} - \frac{\left| \Delta(\vec{r}) \right|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r}) + \text{small correction}$$

$$\Delta(\vec{r}) = -g_{eff}(\vec{r}) \nu_c(\vec{r})$$

α can take any positive value,
but the best results are obtained when α is fixed by the qp-spectrum

Fermions at unitarity in a harmonic trap
Total energies E(N)



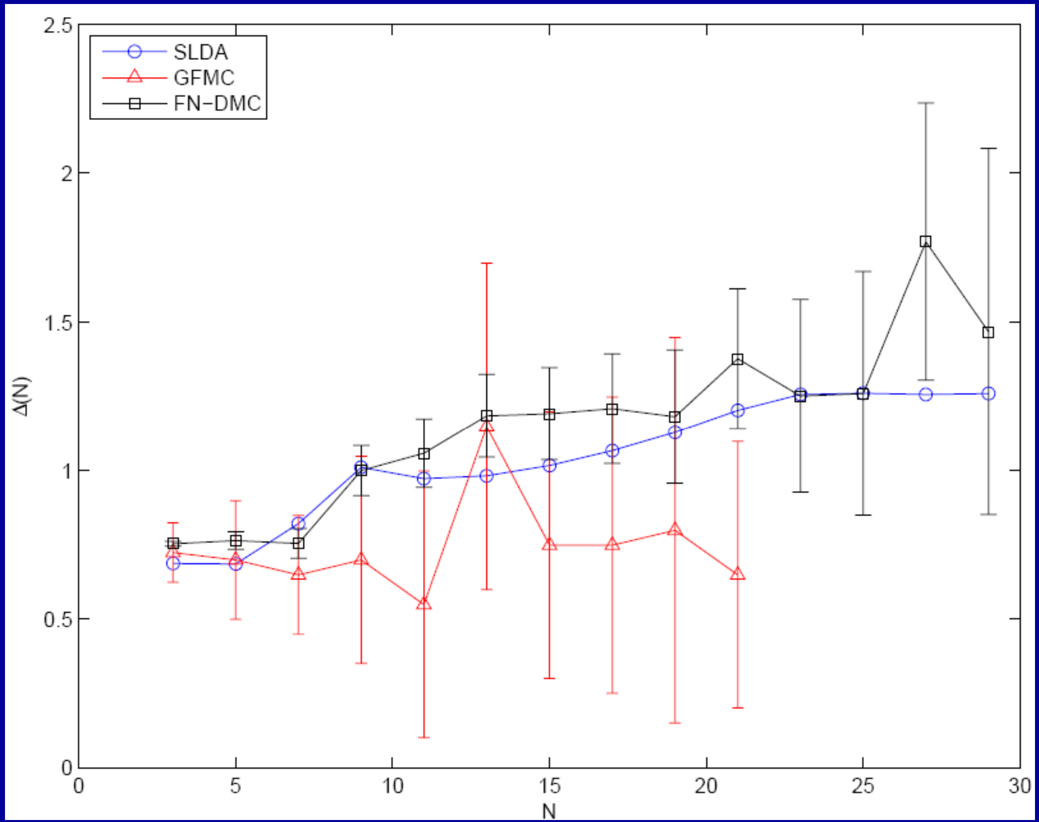
GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

FN-DMC - von Stecher, Greene and Blume, PRL <u>99</u>, 233201 (2007)

PRA <u>76</u>, 053613 (2007)

Bulgac, PRA 76, 040502(R) (2007)

Fermions at unitarity in a harmonic trap
Pairing gaps



$$\Delta(N) = \frac{E(N+1) - 2E(N) + E(N-1)}{2}, \quad \text{for odd } N$$

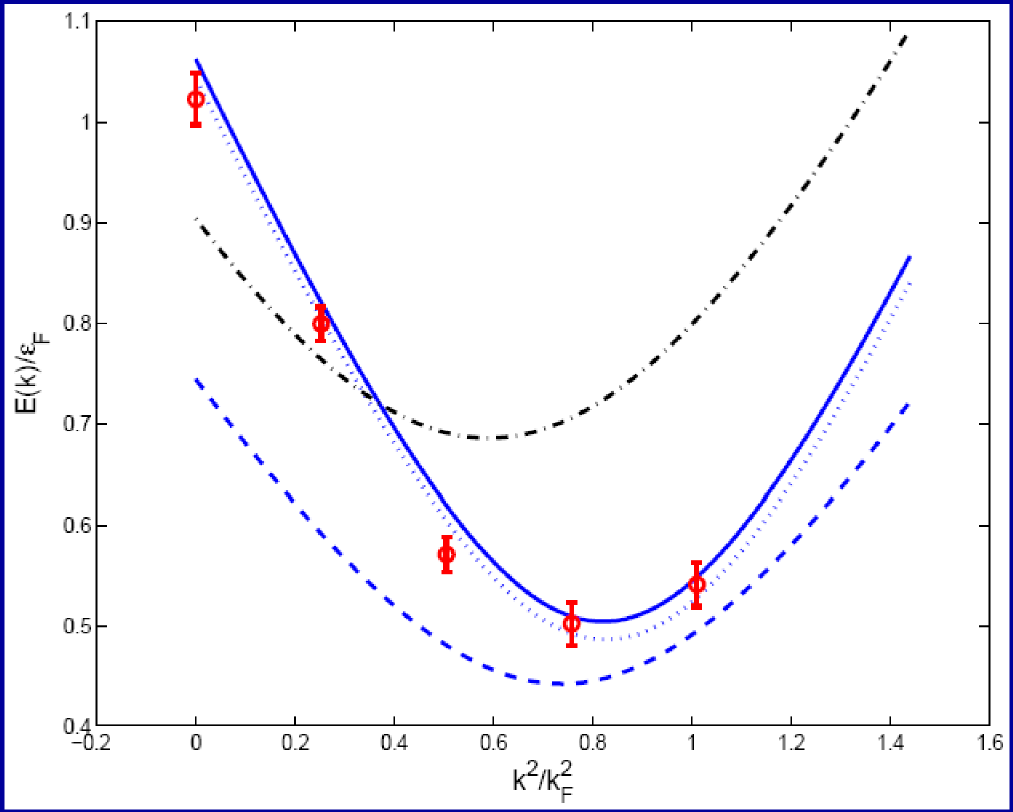
GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)

PRA 76, 053613 (2007)

Bulgac, PRA 76, 040502(R) (2007)

Quasiparticle spectrum in homogeneous matter



solid/dotted blue line	**- SLDA, homogeneous GFMC due to Carlson et al**
red circles	**- GFMC due to Carlson and Reddy**
dashed blue line	**- SLDA, homogeneous MC due to Juillet**

black dashed-dotted line – meanfield at unitarity

Two more universal parameter characterizing the unitary Fermi gas and its excitation spectrum:
effective mass, meanfield potential

Bulgac, PRA 76, 040502(R) (2007)

Asymmetric SLDA (ASLDA)

$$n_a(\vec r) = \sum_{E_n<0} \left|u_n(\vec r)\right|^2, \qquad n_b(\vec r) = \sum_{E_n>0} \left|v_n(\vec r)\right|^2,$$

$$\tau_a(\vec r) = \sum_{E_n<0} \left|\vec\nabla u_n(\vec r)\right|^2, \qquad \tau_b(\vec r) = \sum_{E_n>0} \left|\vec\nabla v_n(\vec r)\right|^2,$$

$$\nu(\vec r) = \frac{1}{2}\sum_{E_n} \mathrm{sign}(E_n) u_n(\vec r) v_n^*(\vec r),$$

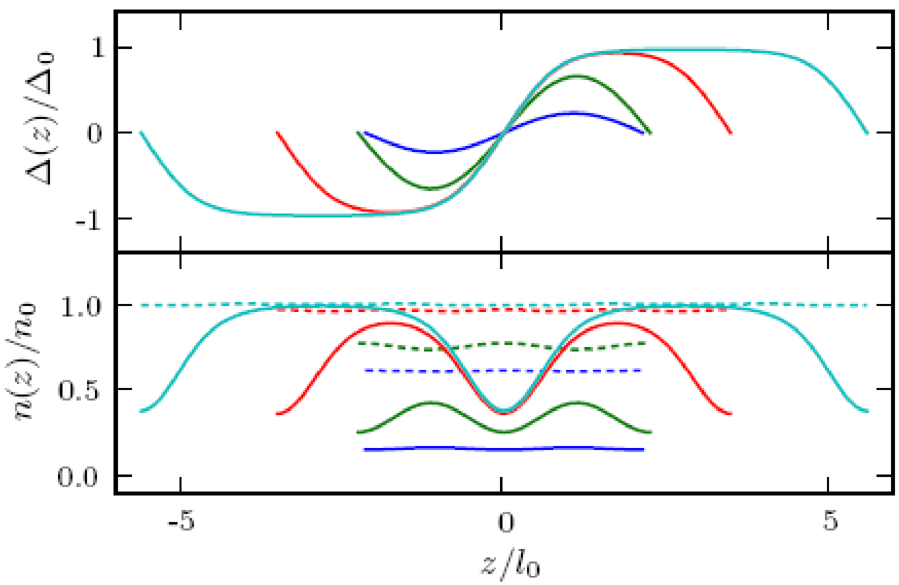
$$\mathrm{E}(\vec r) = \frac{\hbar^2}{2m}\left[\alpha_a(\vec r)\tau_a(\vec r) + \alpha_b(\vec r)\tau_b(\vec r)\right] - \Delta(\vec r)\nu(\vec r) + \\ + \frac{3\left(3\pi^2\right)^{2/3}\hbar^2}{10m}\left[n_a(\vec r) + n_b(\vec r)\right]^{5/3}\beta[x(\vec r)],$$

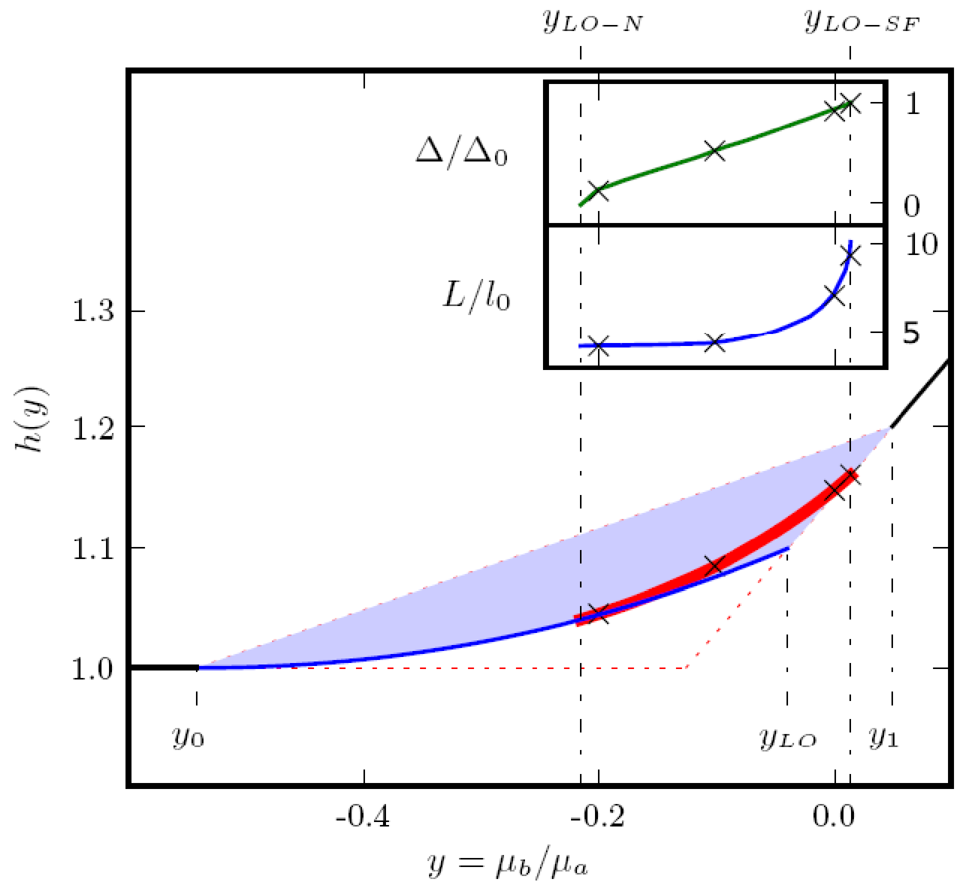
$$\alpha_a(\vec r) = \alpha\left[x(\vec r)\right], \qquad \alpha_b(\vec r) = \alpha\left[1/x(\vec r)\right], \qquad x(\vec r) = n_b(\vec r)/n_a(\vec r),$$

$$\Omega = -\int d^3\vec r\ \mathrm{P}(\vec r) = \int d^3\vec r\ \left[\mathrm{E}(\vec r) - \mu_a n_a(\vec r) - \mu_b n_b(\vec r)\right]$$

Bulgac and Forbes, arXiv:0804:3364

Unitary Fermi Supersolid: the Larkin-Ovchinnikov phase





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

Bulgac and Forbes, arXiv:0804:3364

TD ASLDA

Bulgac, Roche, Yoon

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\mathrm{u}_\mathrm{n}(\vec{r},t)\\ \mathrm{v}_\mathrm{n}(\vec{r},t)\end{pmatrix}=\begin{pmatrix}\hat{h}(\vec{r},t)+\hat{V}_\mathrm{ext}(\vec{r},t) & \hat{\Delta}(\vec{r},t)+\hat{\Delta}_\mathrm{ext}(\vec{r},t)\\ \hat{\Delta}^\dagger(\vec{r},t)+\hat{\Delta}^\dagger_\mathrm{ext}(\vec{r},t) & -\hat{h}(\vec{r},t)-\hat{V}_\mathrm{ext}(\vec{r},t)\end{pmatrix}\begin{pmatrix}\mathrm{u}_\mathrm{n}(\vec{r},t)\\ \mathrm{v}_\mathrm{n}(\vec{r},t)\end{pmatrix}$$

$$Q(\omega)=\sum_\sigma\int d^3r\,dt\,Q(\vec{r},\sigma,t)n(\vec{r},\sigma,t)\exp(i\omega t)$$

$$N_x^3\times N_t,\quad N_x\approx 50\ldots100,\quad N_t\approx 10^4\ldots10^5$$

$$\text{number of }\psi_n(\vec{r},\sigma,t)\approx O(N_x^3\times 40)$$

Space-time lattice, use of FFTW for spatial derivative

No matrix operations (unlike (Q)RPA)

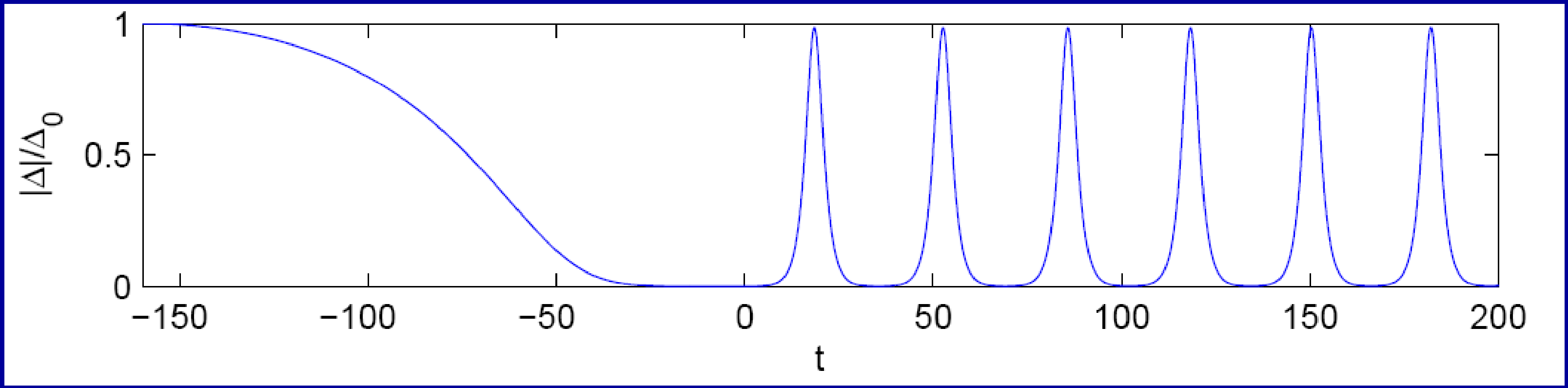
All nuclei (odd, even, spherical, deformed)

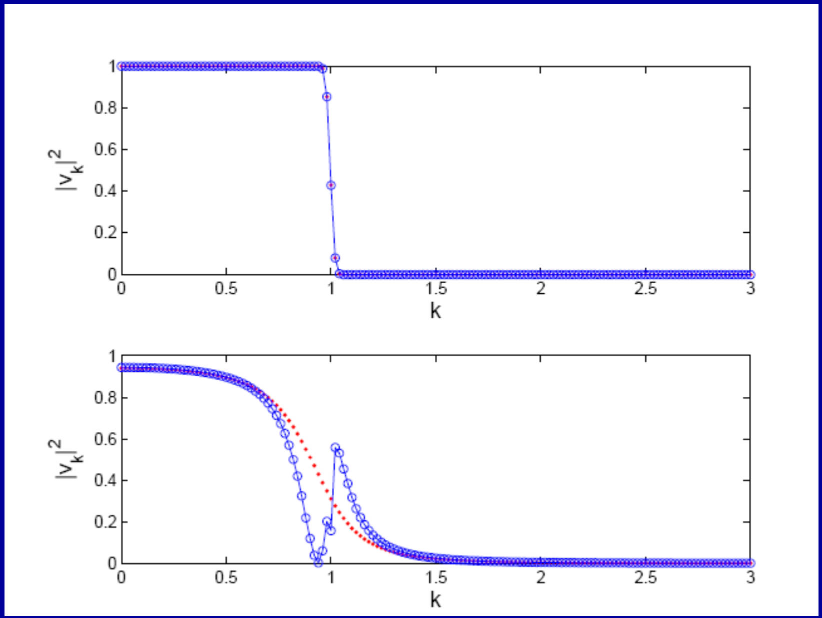
Any quantum numbers of QRPA modes

Fully selfconsistent, no self-consistent symmetries imposed

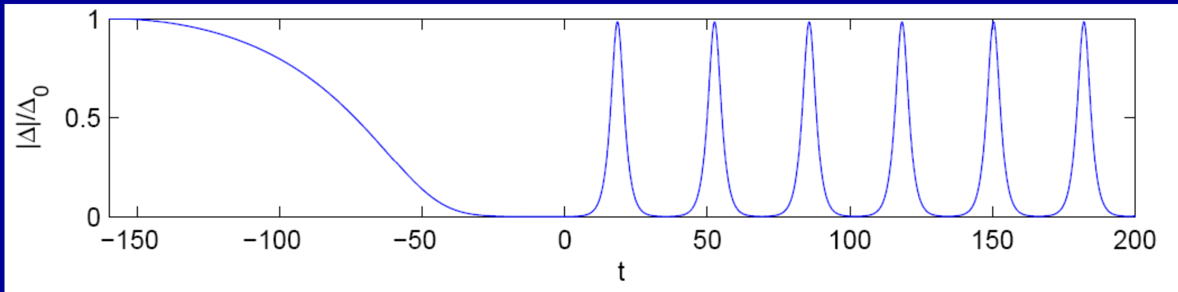
Higgs mode of the pairing field in a homogeneous unitary Fermi gas

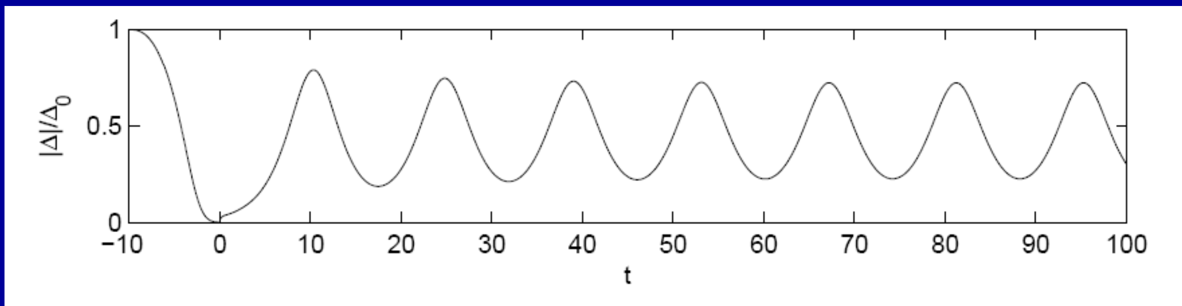
A remarkable example of extreme Large Amplitude Collective Motion

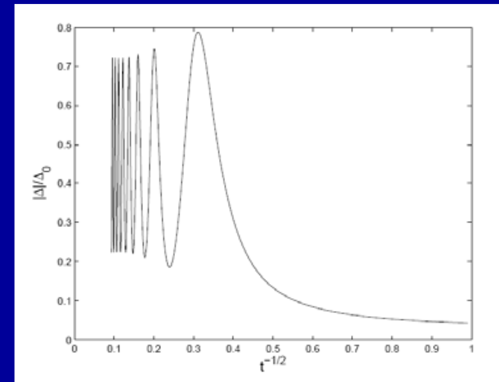


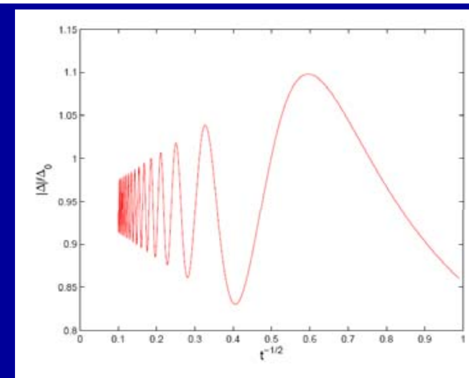


Bulgac and Yoon, unpublished (2007)



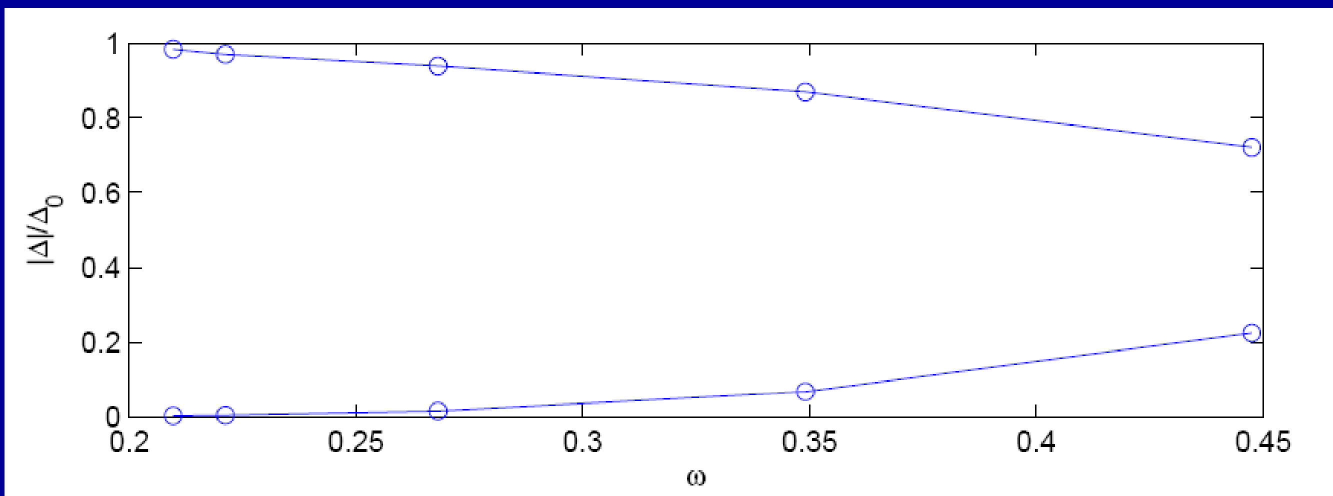






A zoo of Higgs-like pairing modes

<u>The frequency of all these modes is below the 2-qp gap</u>



Maximum and minimum oscillation amplitudes versus frequency

In case you've got lost: *What did I talk about so far?*

What is a unitary Fermi gas?

Thermodynamic properties

Pairing gap and pseudo-gap

EOS for spin imbalanced systems

P-wave pairing

Small systems in traps and (A)SLDA

Unitary Fermi supersolid: the Larkin-Ovchinnikov phase

Time-dependent phenomena

What else can we expect?