Density Functional Theory and Ab Initio Calculations: Cold Atoms (Fermions and Bosons)

Introduction / Motivation

Fermions:

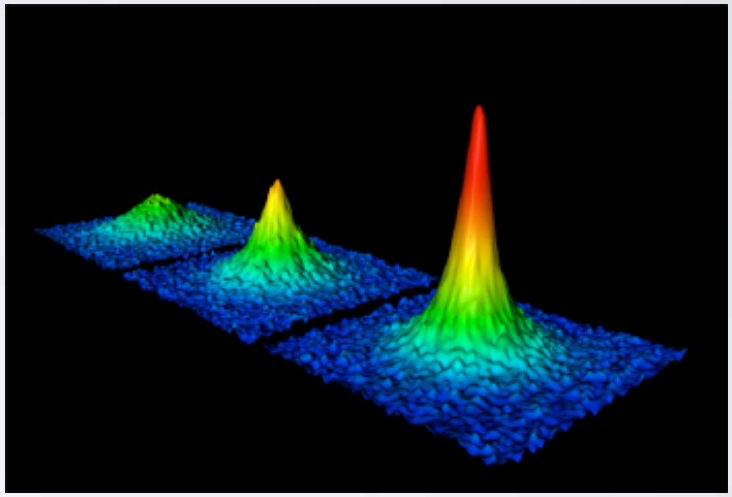
- Homogeneous Fermi Gas
- Inhomogeneous Gas
- Clusters

Bosons:

- Efimov trimers
  - to N-body clusters
- Homogeneous Matter:
  - Energy vs. density
  - 2- and 3-body contacts
  - condensate fraction

Outlooks and challenges

Fermi Condensates



C. Regal et al. PRL 2004

Kevin Schmidt
Shiwei Zhang
Stefano Gandolfi
Silvio Vitiello
Bira v. Kolck
J. Carlson

Density Functionals enormously successful in electronic systems and nuclear physics:

Similarities:

- Homogeneous bulk properties incorporated into DFT
- gradient expansion, …

Differences:

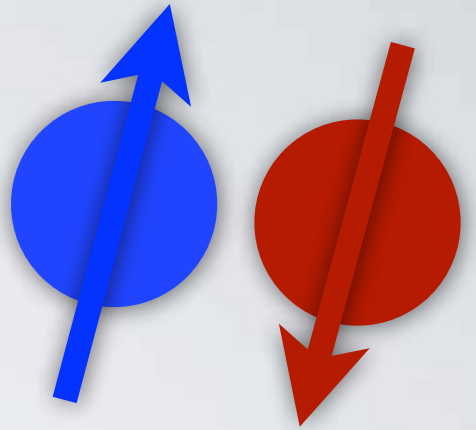
- Nuclei are self-bound
- Nuclei are superfluid - pairing in finite systems

Can we explore these similarities/differences in cold atoms?

- Different challenges
- Scale invariance simplifies the density functional
- ‘Exactly’ solvable

Homogeneous Unitary Fermi Gas

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V_0 \; \delta(\mathbf{r_{ij}})$$

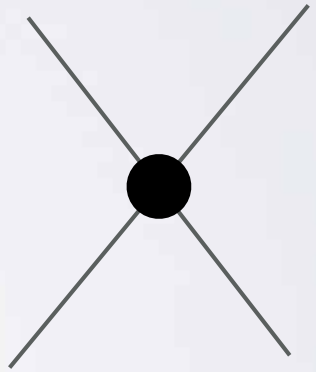


V_0 can be tuned across BCS ($|V_0| \sim 0$) to BEC ($-V_0 >> E_F$)
Concentrate on unitarity : zero energy bound state
infinite scattering length

$$E = \xi \; E_{FG} = \xi \; \frac{3}{5} \; \frac{\hbar^2 k_F^2}{2m}$$

$$\Delta = \delta \; \frac{\hbar^2 k_F^2}{2m}$$

$$T_c = t \; \frac{\hbar^2 k_F^2}{2m}$$



Values of ξ, δ, t are independent of ρ

T=0 Algorithm: Branching random walk (diffusion) using AFMC

exact for unpolarized systems

$$H = \frac{1}{N_k^3} \sum_{\boldsymbol{k},\boldsymbol{j},\boldsymbol{m},s} \psi^\dagger_{\boldsymbol{j}s} \psi_{\boldsymbol{m}s} \epsilon_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r_j}-\boldsymbol{r_m})} + U \sum_{\boldsymbol{i}} n_{\boldsymbol{i}\uparrow} n_{\boldsymbol{i}\downarrow} \,.$$

$$\epsilon_k^{(2)} = \frac{\hbar^2 k^2}{2m}\,, \quad \epsilon_k^{(4)} = \frac{\hbar^2 k^2}{2m}\left[1 - \beta^2 k^2 \alpha^2\right]$$

$$\epsilon_{\boldsymbol{k}}^{(h)} = \frac{\hbar^2}{m\alpha^2}\left[3 - \cos(k_x\alpha) - \cos(k_y\alpha) - \cos(k_z\alpha)\right]$$

Different effective ranges
No sign problem for
attractive interactions

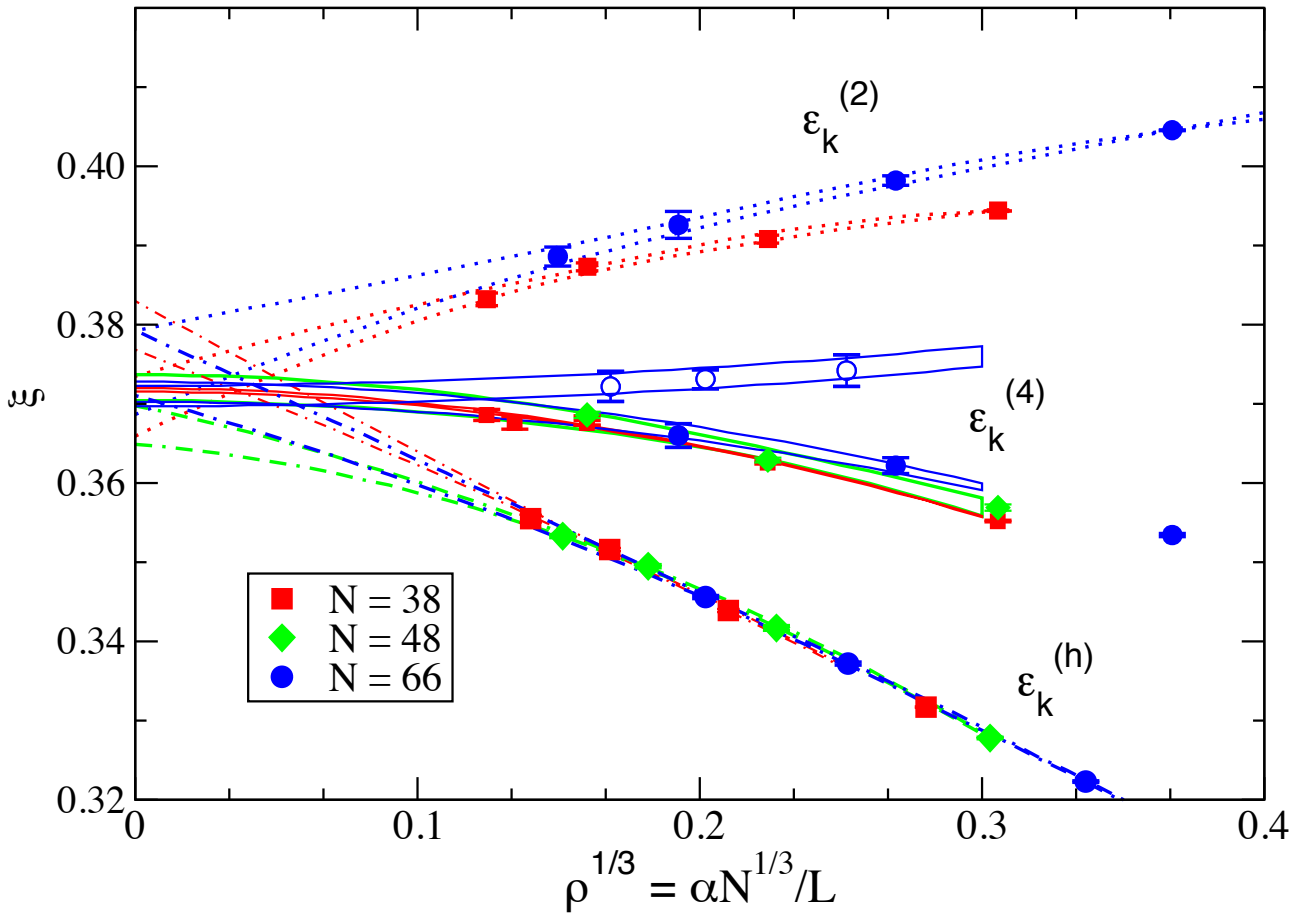
One step of the algorithm:
multiply by exp [-T dt / 2]
momentum space
Auxiliary field for exp [-V dt]
coordinate space
multiply by exp [-T dt /2]
momentum space

Use importance sampling with
BCS wave function

$$|BCS\rangle = \left[\sum_{\boldsymbol{k}} f_k c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}\right]^{N/2} |0\rangle$$

$$\langle W|BCS\rangle = \det A\,,$$

Homogeneous Gas: ξ and effective range $\mathcal{S}$



MIT expt

$\xi = 0.376(0.005)$

arXiv:1110.3309 (Hu, et al)

$$E(k_F r_e)/E_{FG} = \xi + \mathcal{S} k_F r_e + \ldots$$

$\xi = 0.372 \pm 0.005$

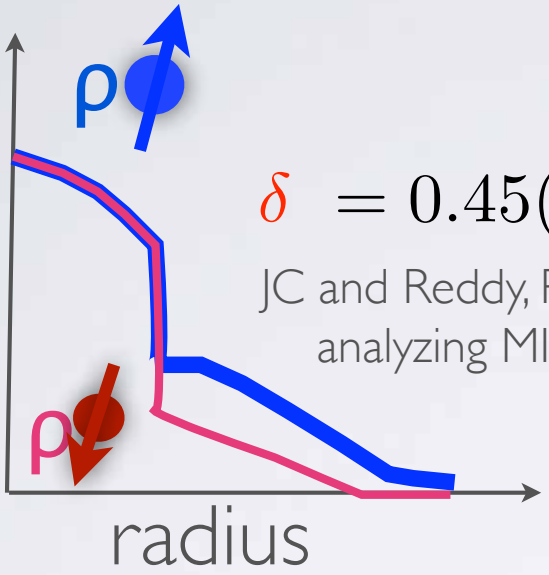
$\mathcal{S} = 0.12 \pm 0.01$

Carlson, Gandolfi, Schmidt, and Zhang, PRA 2011

Carlson, Gandolfi, and Gezerlis, PTEP 2012

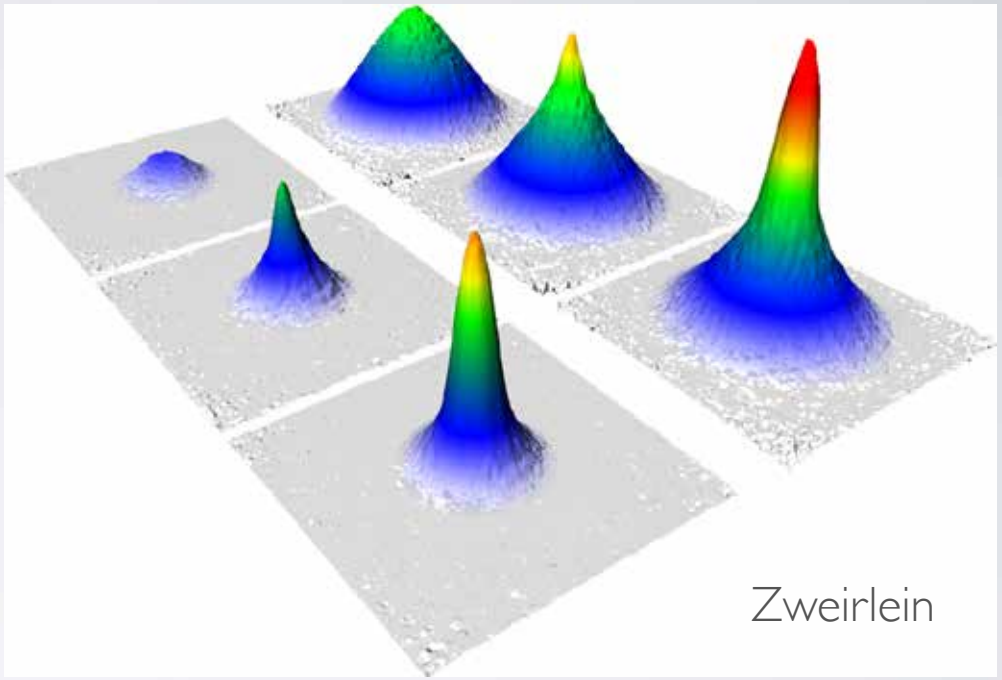
Spin excitations are high energy

Spin up, down densities in a trap

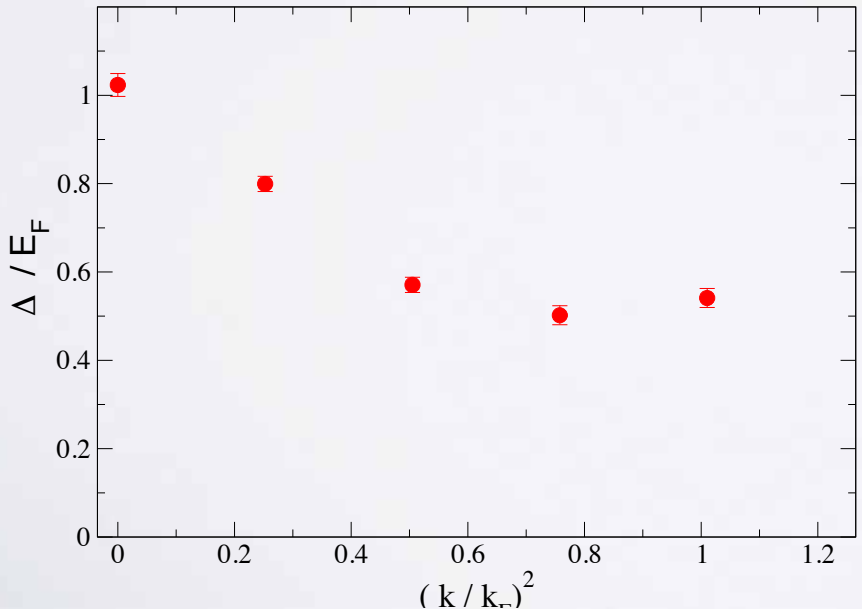


$$\delta = 0.45(05)$$

JC and Reddy, PRL 2007
analyzing MIT data



Zweirlein



$$\Delta = \delta \frac{\hbar^2 k_F^2}{2m}$$

$$\delta = 0.50\ (03)$$

$$(k_{min}/k_f)^2 = 0.80(10)$$

JC and Reddy, PRL 2005

Density Functional for unpolarized systems

$$\mathcal{E}(x) = n(x)V(x) + \frac{3\cdot 2^{2/3}}{5^{5/3} m c_0^{2/3}} n(x)^{5/3} - \frac{4}{45}\frac{2c_1 - 9c_2}{mc_0}\frac{(\nabla n(x))^2}{n(x)} - \frac{12}{5}\frac{c_2}{mc_0}\nabla^2 n(x)\,.$$

Rupak and Schafer Nucl.Phys.A816:52-64,2009
arXiv:0804.2678

Epsilon expansion at unitarity $c_2 \approx 0$

$$\mathcal{E}(x) = n(x)V(x) + 1.364\frac{n(x)^{5/3}}{m} + 0.022\frac{(\nabla n(x))^2}{mn(x)} + O(\nabla^4 n)$$

compare to free fermions

$$\mathcal{E}_{ETF}(x) = n(x)V(x) + 2.871\frac{n(x)^{5/3}}{m} + 0.014\frac{(\nabla n(x))^2}{mn(x)} + 0.167\frac{\nabla^2 n(x)}{m} + O(\nabla^4 n)$$

Note increase in coefficient of gradient term at unitarity compared to free Fermi gas

Change notation:

$$\mathcal{E} \;=\; V(r)\rho(r) \;+\; \xi\,(3\pi^2)^{2/3}\rho^{5/3} \;+ c_2\,\nabla\rho^{1/2}\cdot\nabla\rho^{1/2} + \ldots$$

$$\hbar^2/(2m) \to 1$$

Free fermions (BCS limit) $\quad c_2 \;=\; 0.111$

Free bosons (BEC limit M = 2m) $\quad c_2 \;=\; 0.5$

The gradient term is exactly like
the kinetic term in the Gross–Pitaevskii equation (BEC).
The density functional is scale invariant: 1/length^5

see also M. Forbes arXiv:1211.3779
for treatment with Superfluid Local Density Approximation

We use only bosonic degrees of freedom
no single-particle orbital summation for the density.

Computing the static response from weak external potentials

$$V(r) \;=\; V_0 \; E_F \;\; \cos(\mathbf{k}\cdot\mathbf{r})$$

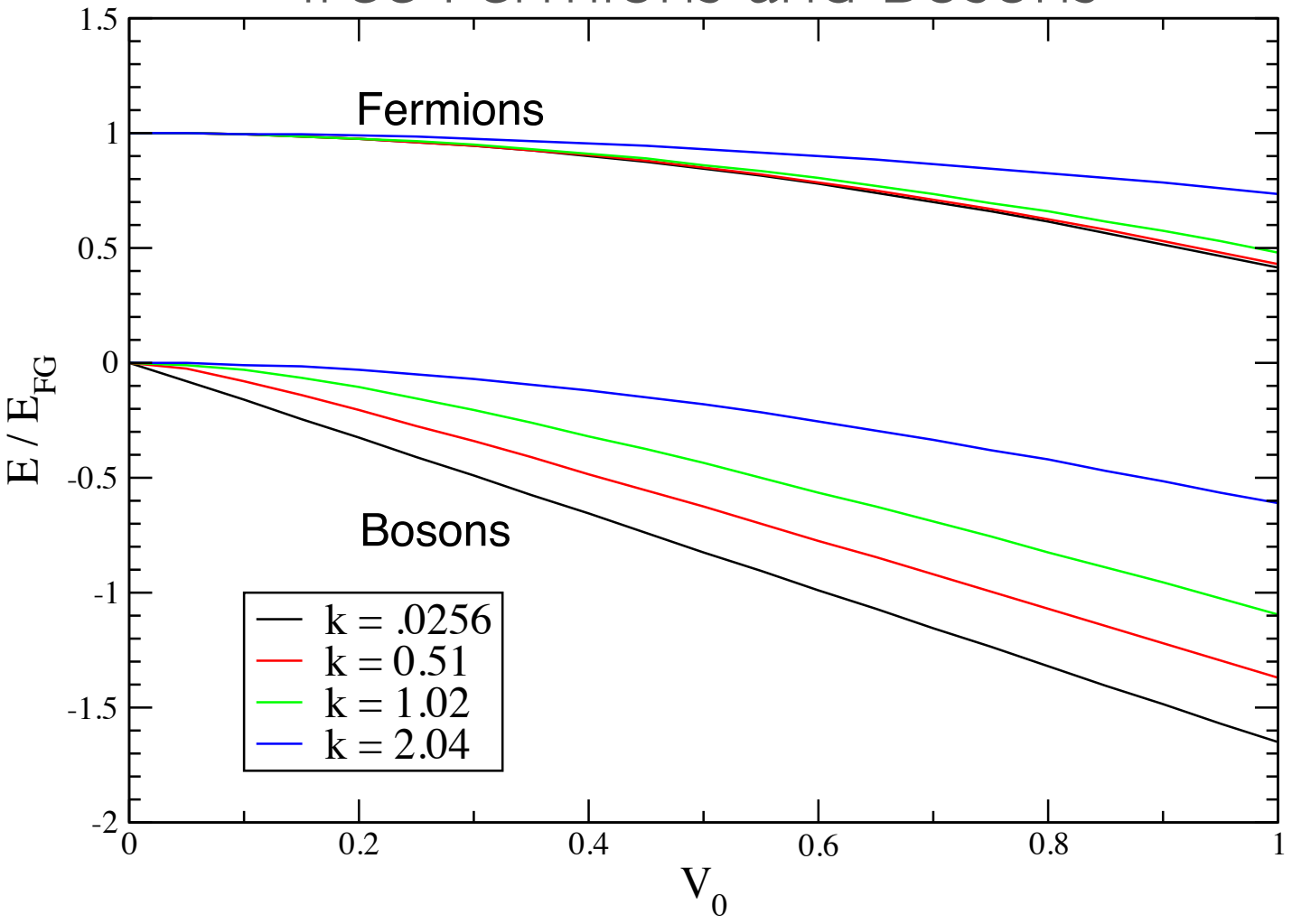
$$E(V_0) \;=\; E_0 - \frac{\sum_f \langle 0|V(r)|f\rangle\langle f|V(r)|0\rangle}{E_f - E_0}$$

$$E(V_0) \;=\; E_0 - \int d\omega \; S(k,\omega)/\omega$$

At low q, E(V0) determined by compressibility (ξ)
Next order in q determined by c_g

Use AFMC to compute the energy for weak external potentials

Static Response for BCS and BEC limits free Fermions and Bosons



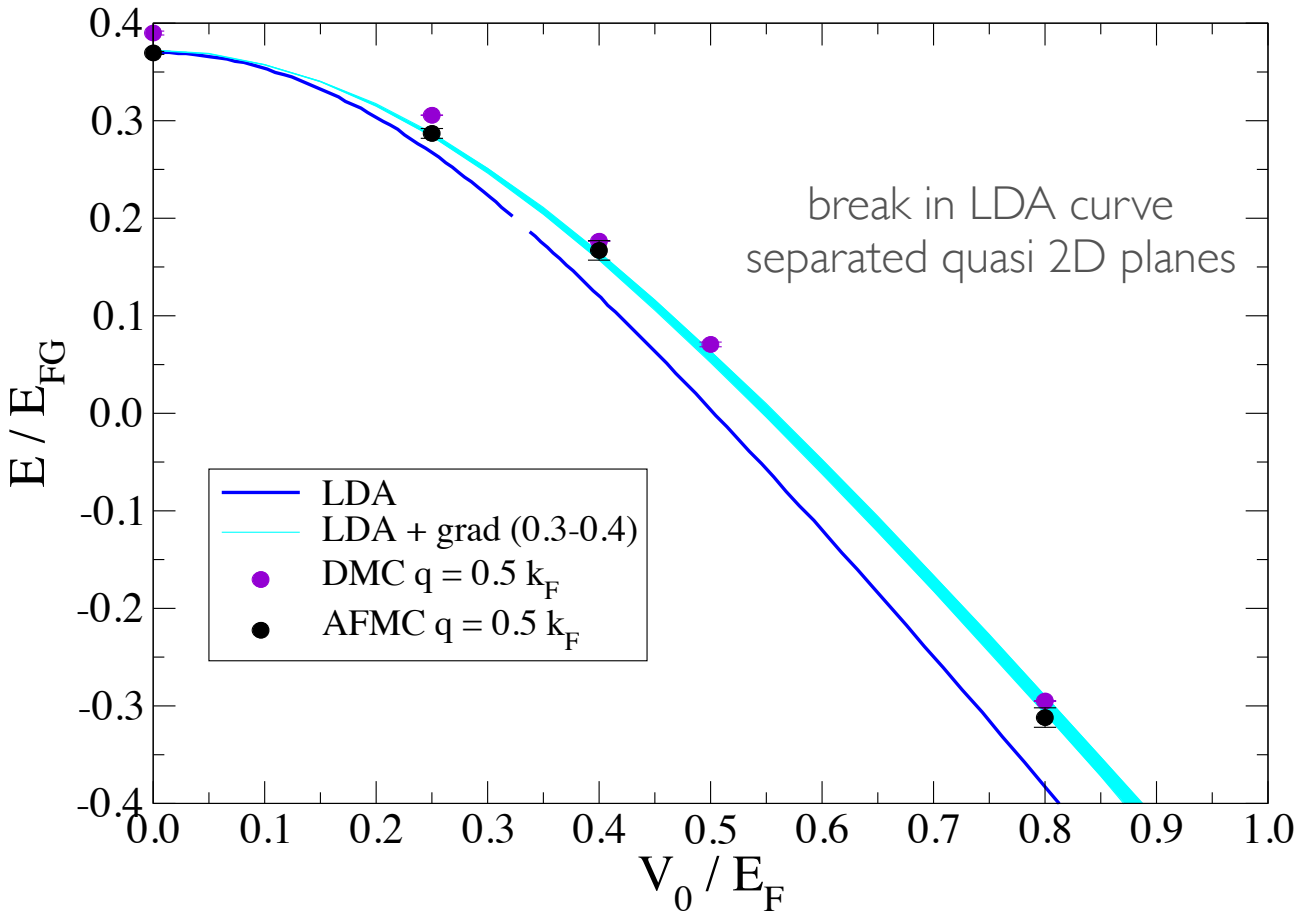
Calculation of c_g from weak external potential

N=66, $k/k_F = 0.5$, $V_0 = 0.25$

AFMC E = 0.291(4) $\Rightarrow$ c_g = 0.37 (0.07)

DMC E = 0.307(1) $\Rightarrow$ c_g = 0.33 (0.02)

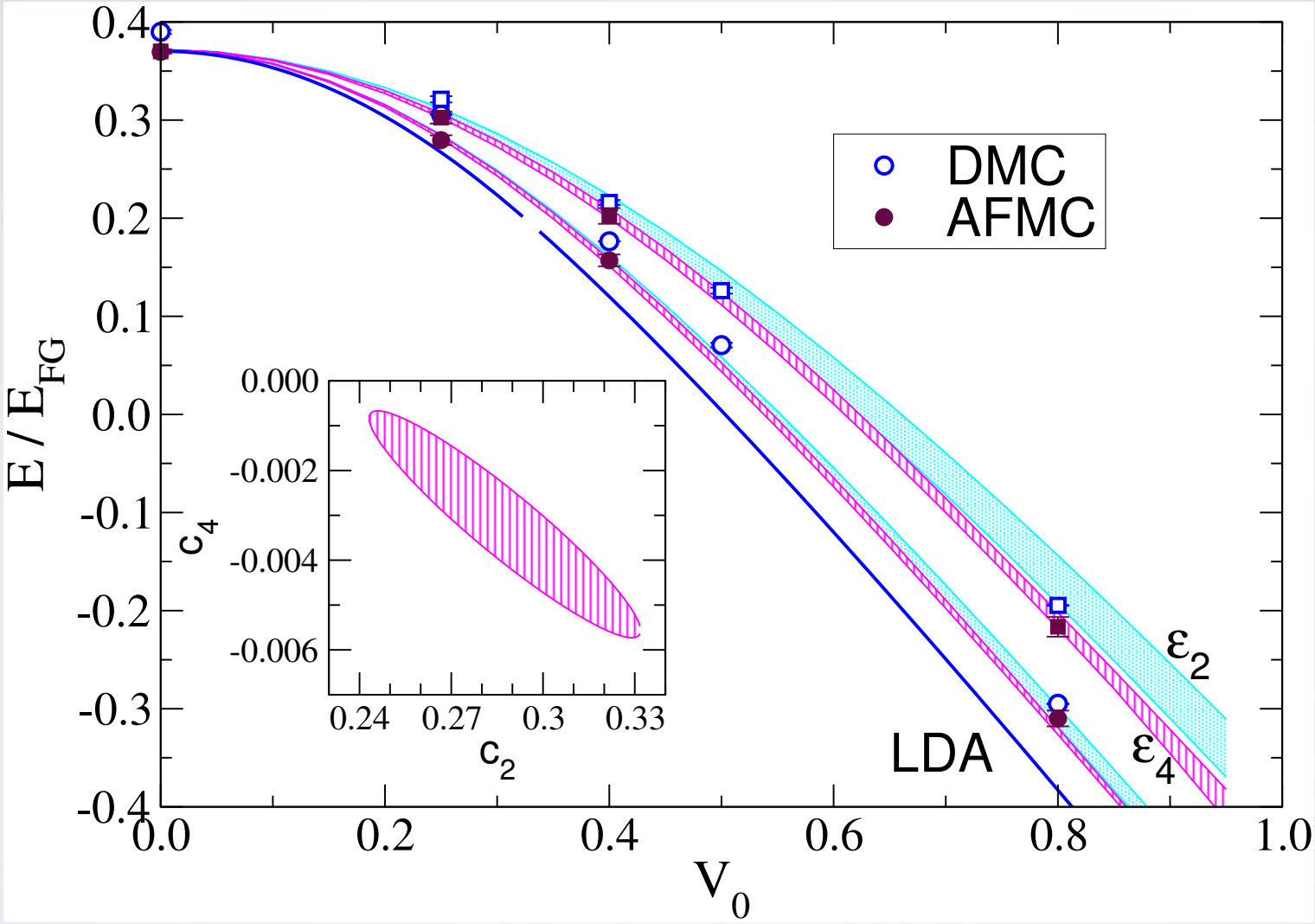
Larger external potentials at $q = k_F / 2$



Carlton and Gandolfi
PRA, 2014

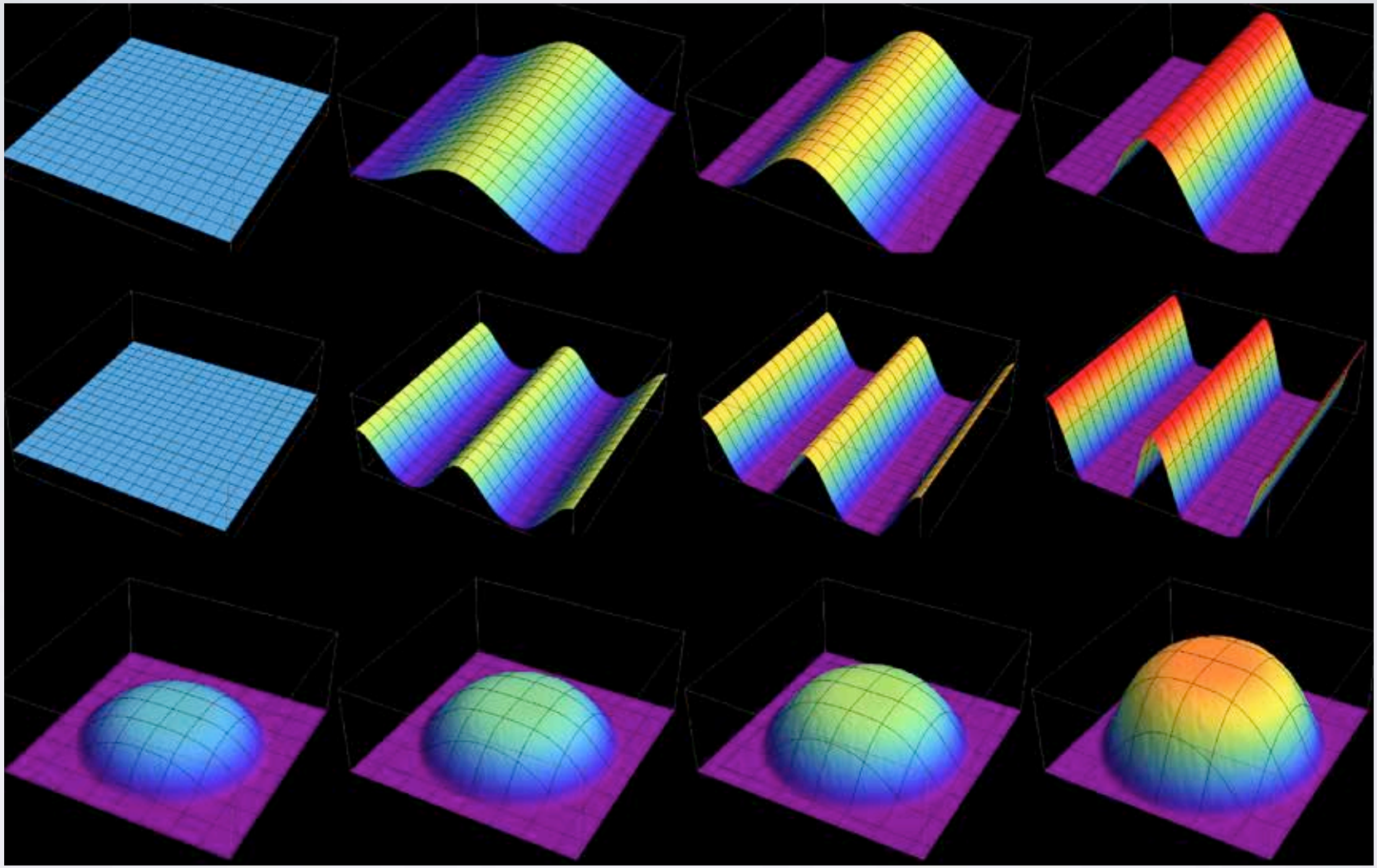
Calculations at higher q: $q/k_F \sim 1$

Lowest order gradient correction no longer sufficient



$$\mathcal{E}_4 = \mathcal{E}_2 + c_4 \frac{\nabla^2 \rho^{1/2} \nabla^2 \rho^{1/2}}{\rho^{2/3}}$$

Can apply density functional to arbitrary external potentials:



What about finite systems?

Consider a small number of particles trapped in a harmonic oscillator:

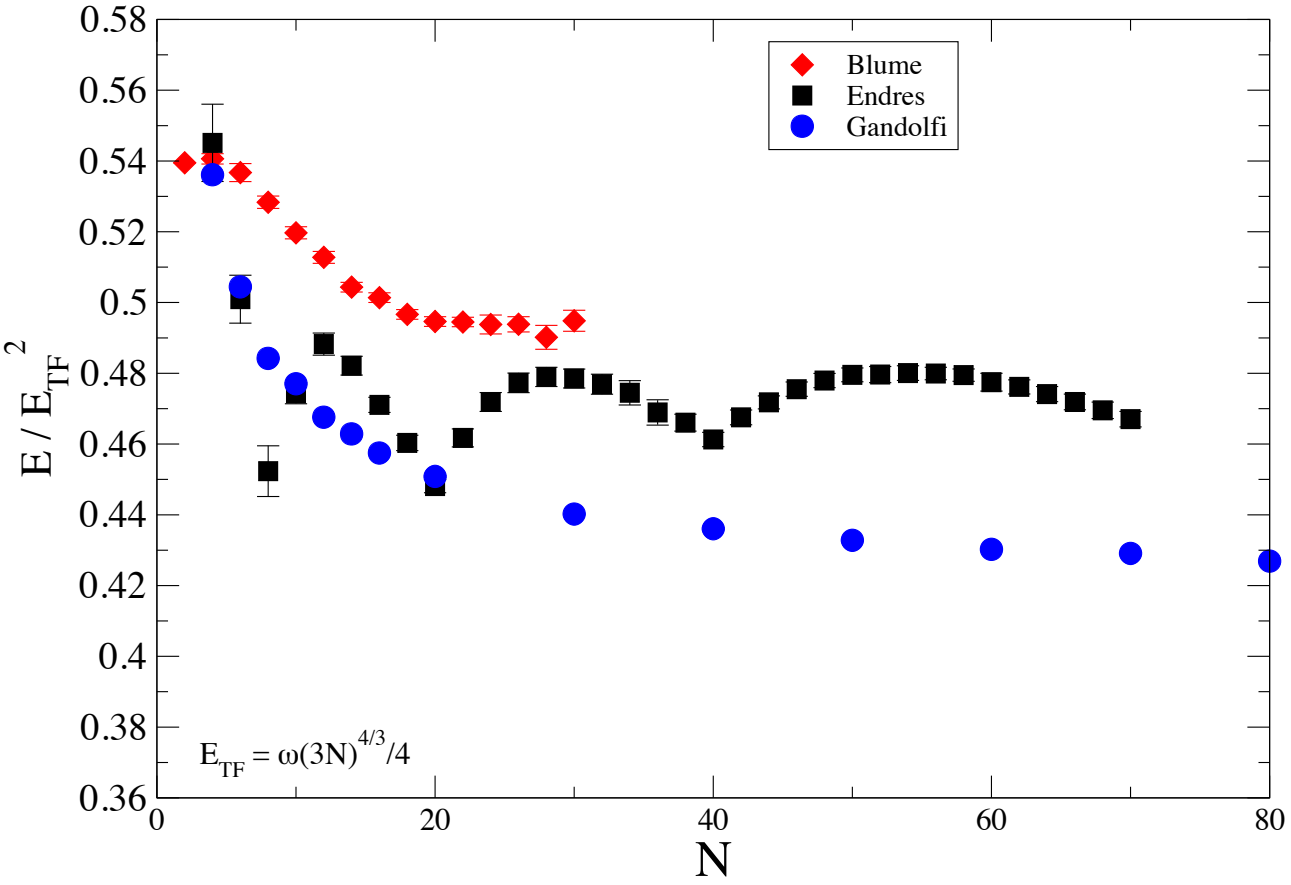
The density functional makes a unique prediction:

No knowledge of (fermionic) shell closures.
Pairing dominates - effectively bosonic DOF only.
Clear approach to the bulk limit.

Does this work and for what N?

Compare DFT prediction to AFMC calculations.
Simple dimensional analysis for large N: $(E/E_{TF})^2 \rightarrow \xi$

Improved DMC results for trapped fermions

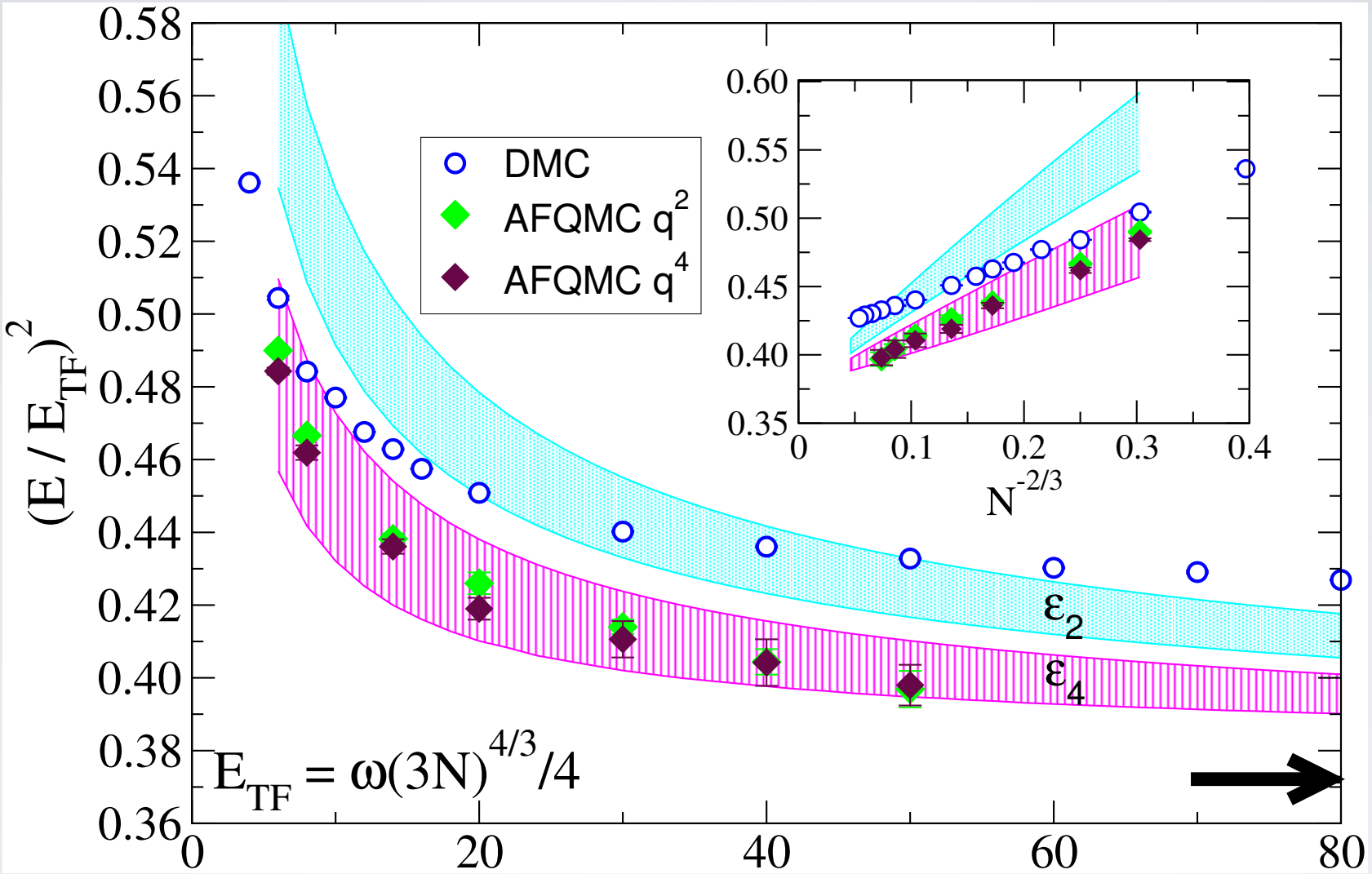


More sophisticated trial wavefunction which includes additional single-particle orbitals & terms which go to SLDA-like pairing.

Approaches FN bulk limit of 0.39

No obvious shell closures

AFMC results for trapped fermions



Fourth order density functional gives excellent predictions for N ~ 10 and larger.

Correct approach to bulk ξ.

No evidence of shell gaps - isolated fermions cannot propagate across the system.

Summary of Fermions at Unitarity

Low-Energy degrees of freedom are phonons in UFG

Scale invariance ties linear response to complete functional

$c_g = 0.3\text{-}0.4$

compared to 0.111 for BCS (free fermions)

0.50 for BEC (free bosons of mass 2m)

Quadratic corrections important for trapped fermions

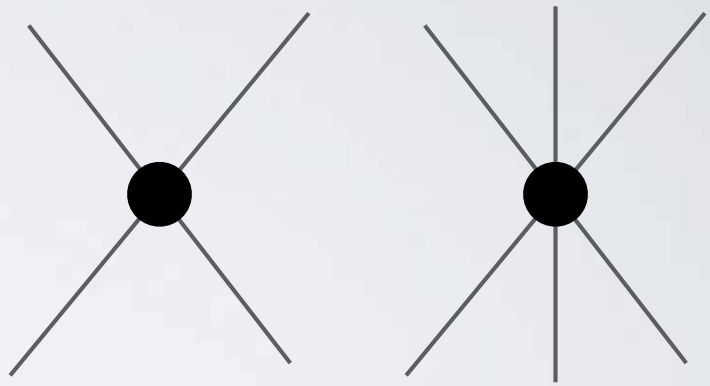
No evidence for shell structure (large pairing gap)
in the unitary Fermi Gas, even for small systems

Unitary Bosons

2-body attractive interaction
tuned to unitarity

3-body repulsive interaction
tuned to very weakly bound
(Efimov) trimer: binding energy E_3

Ground state can be solved for
exactly with DMC



Hamiltonian for Bosons

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk},$$

$$V_{ij} = V_2^0 \frac{\hbar^2}{m}\mu_2^2 \exp[-(\mu_2 r_{ij})^2/2],$$

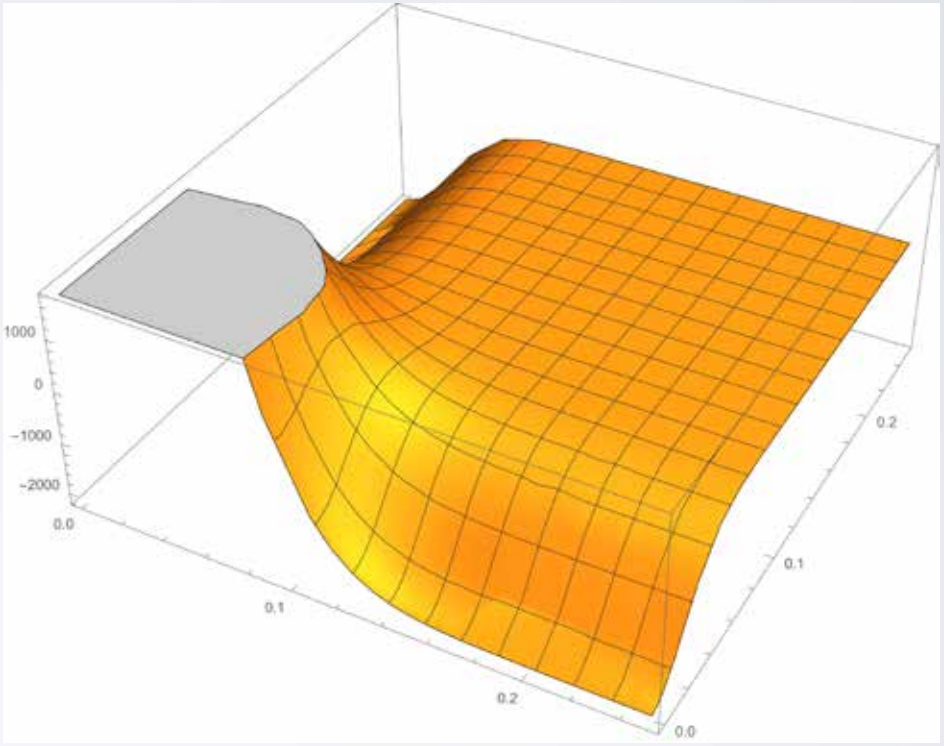
$$V_{ijk} = V_3^0 \frac{\hbar^2}{m}\left(\frac{\mu_3}{2}\right)^2 \exp[-(\mu_3 R_{ijk}/2)^2/2],$$

$$R_{ijk} = (r_{ij}^2 + r_{ik}^2 + r_{jk}^2)^{1/2}.$$

$$X_\mu \equiv \mu_3/\mu_2 = 0.5,\ 0.75 \text{ and } 1.0.$$

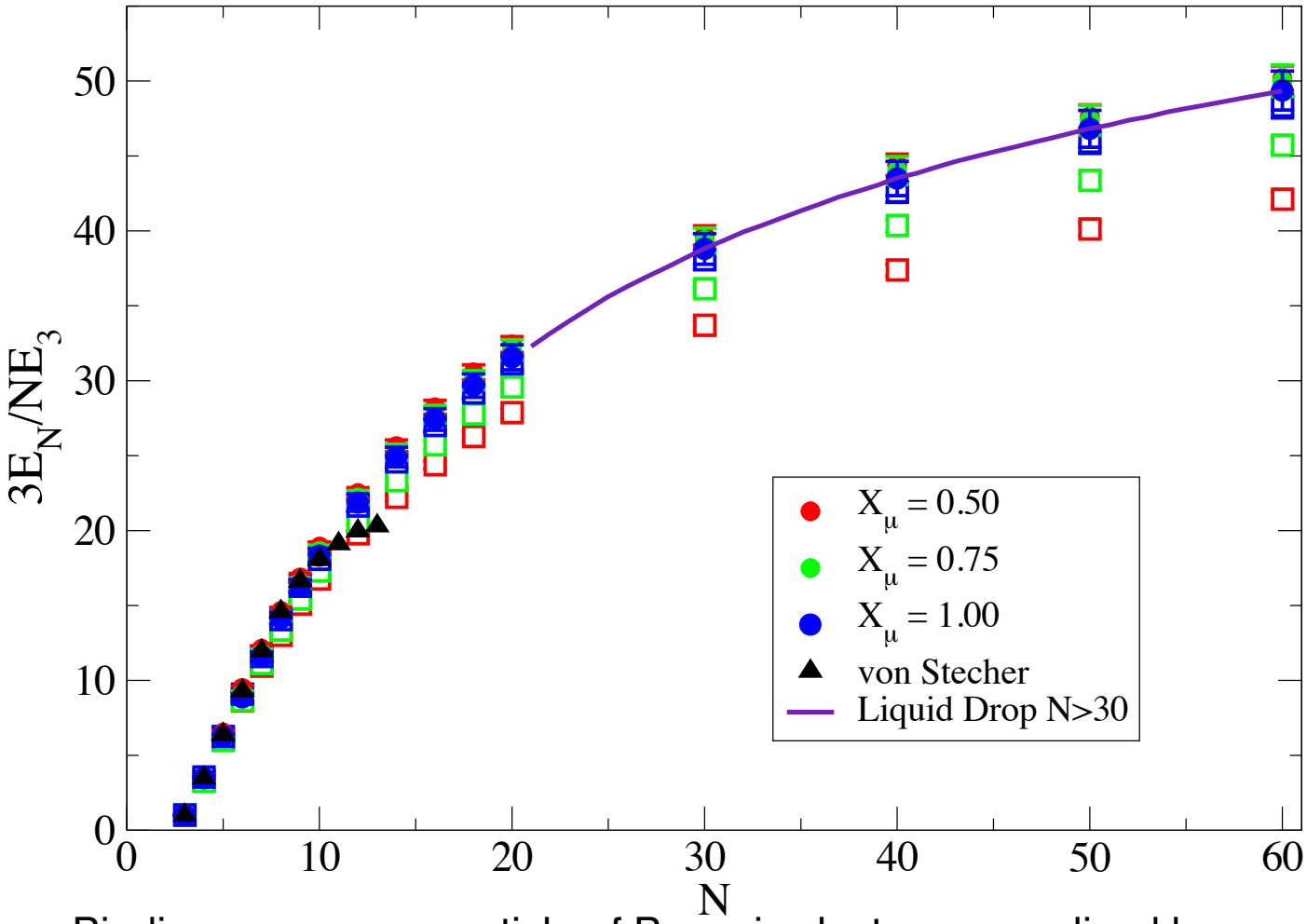
Many previous calculations use a zero-range 2-body interaction plus a hard-core 3-body binding energy: this fixes the trimer binding for a given radius.

The above formulation can be tuned to arbitrarily small 3-body binding energies.

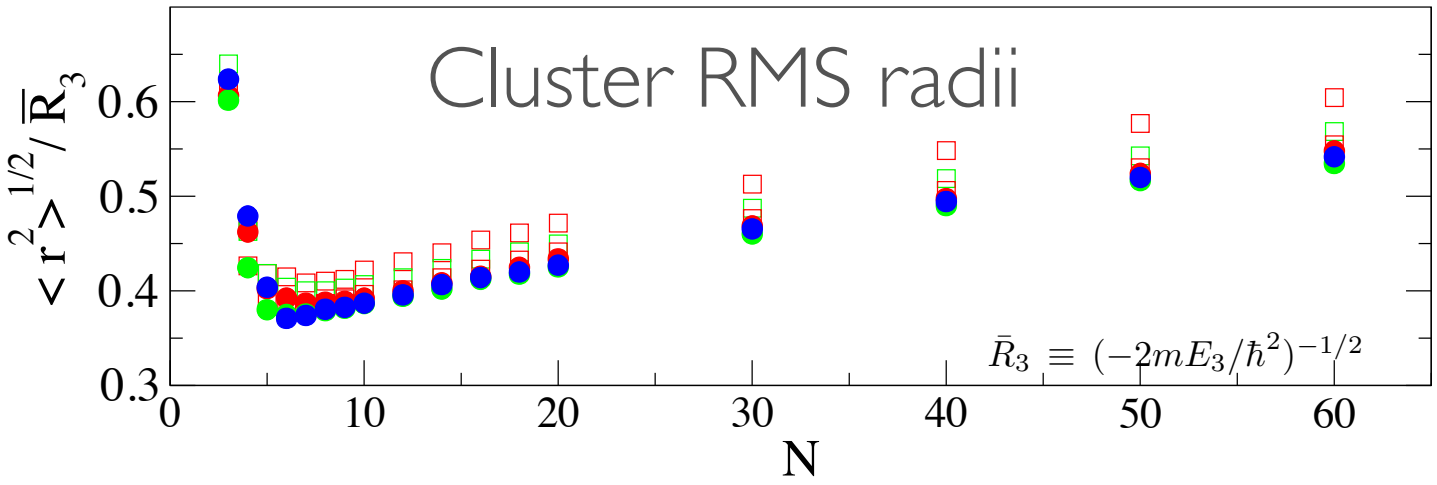


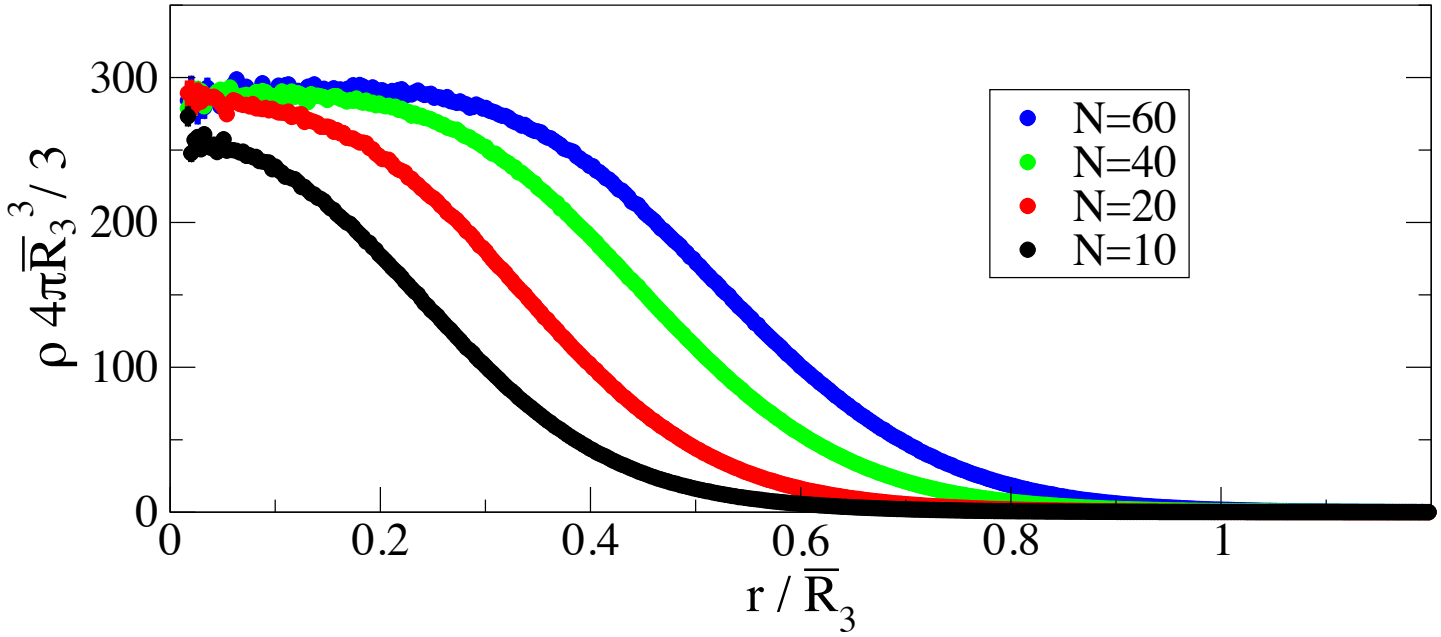
Potential for right angle vs. r12 and r13

Cluster Binding Energy vs. # of Bosons



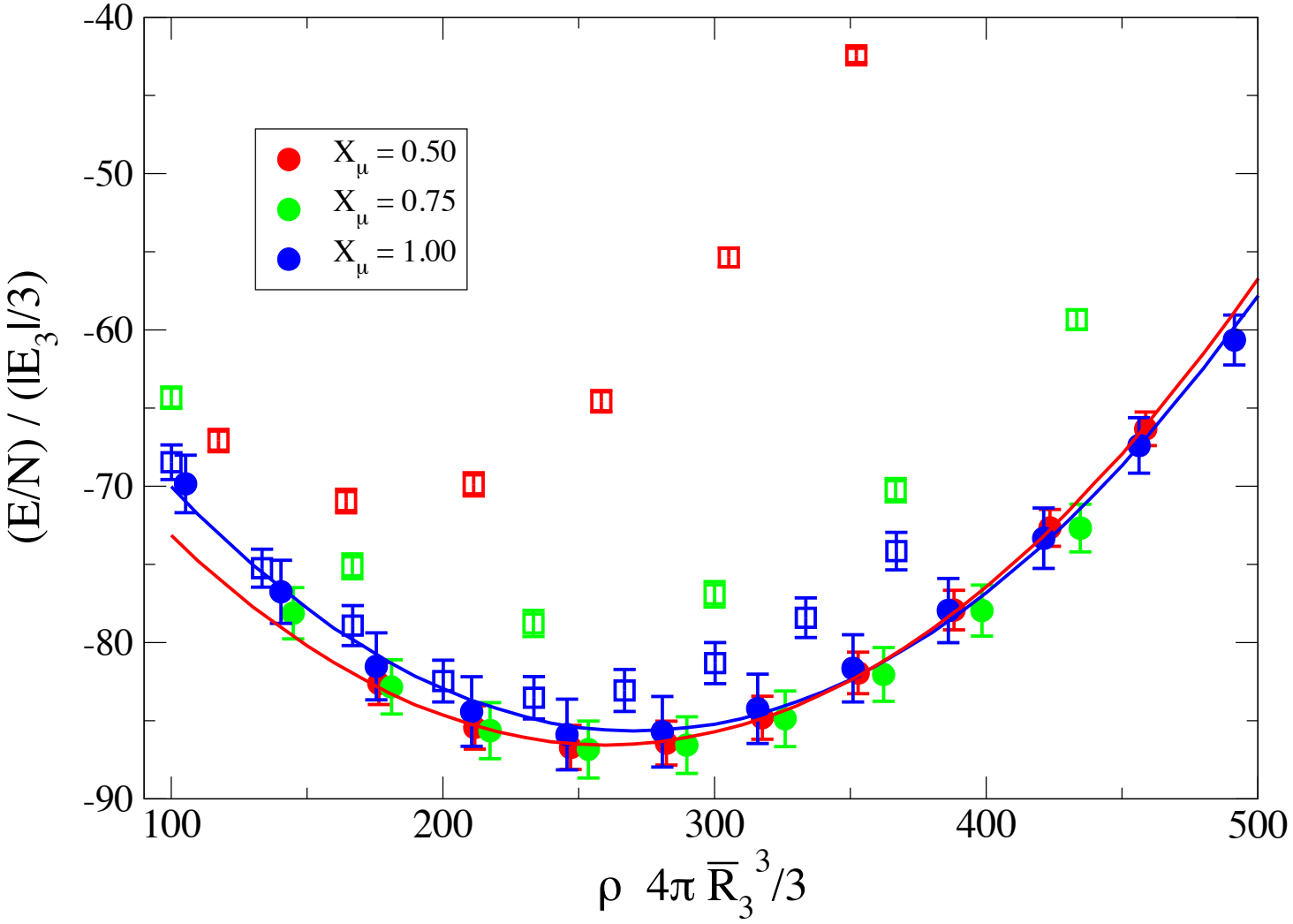
Binding energy per particle of Bosonic clusters normalized by trimer binding per particle



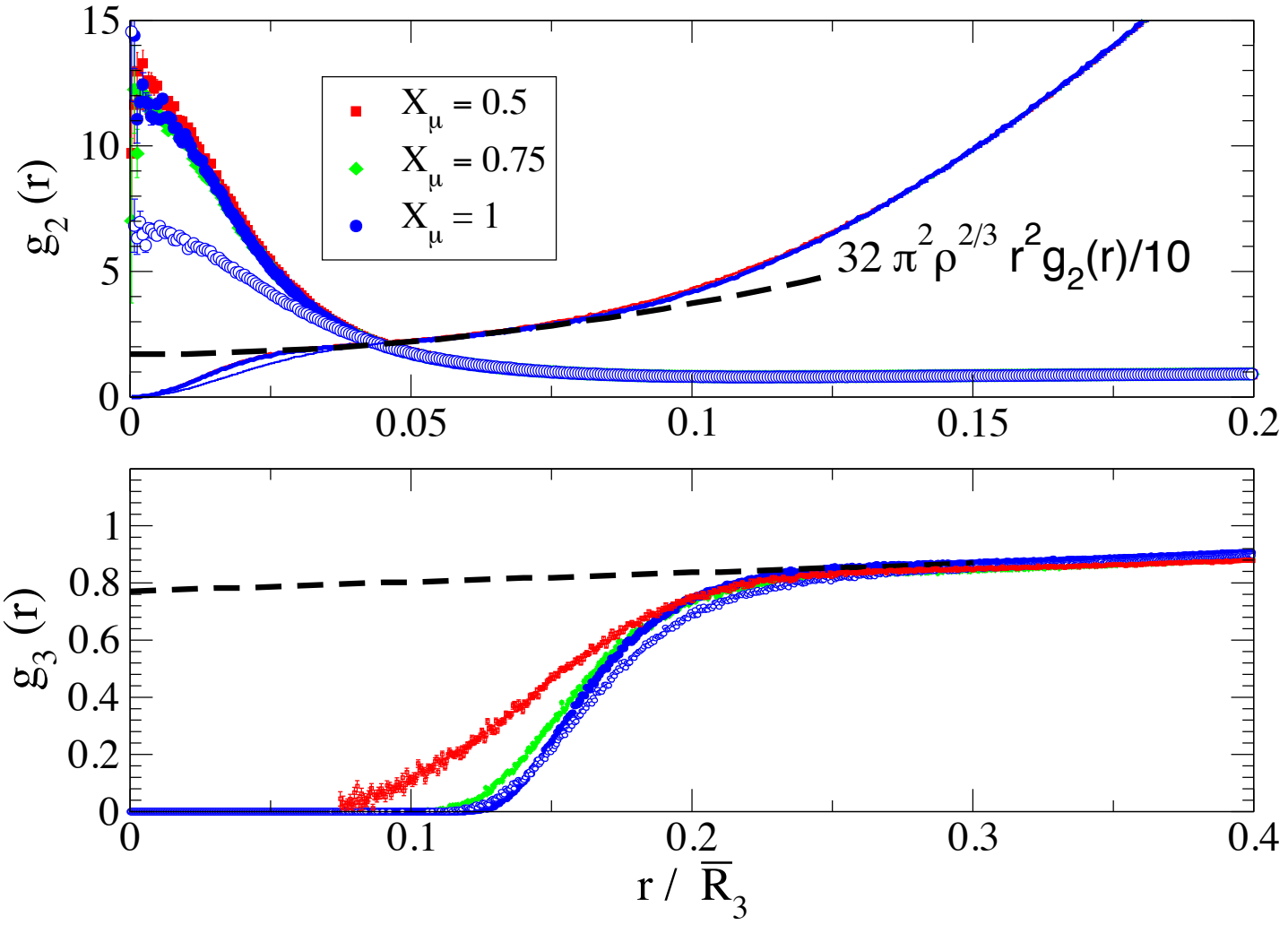


Cluster single-particle densities

Homogeneous Matter Equation of State



2- and 3-body distribution functions



Contacts given by extrapolation to r=0

Contacts:

QMC contacts

$$\alpha_2 = 17(3)$$

$$\beta_3 = 0.9(1)$$

Condensate Fraction

$$\eta = 0.92(1)$$

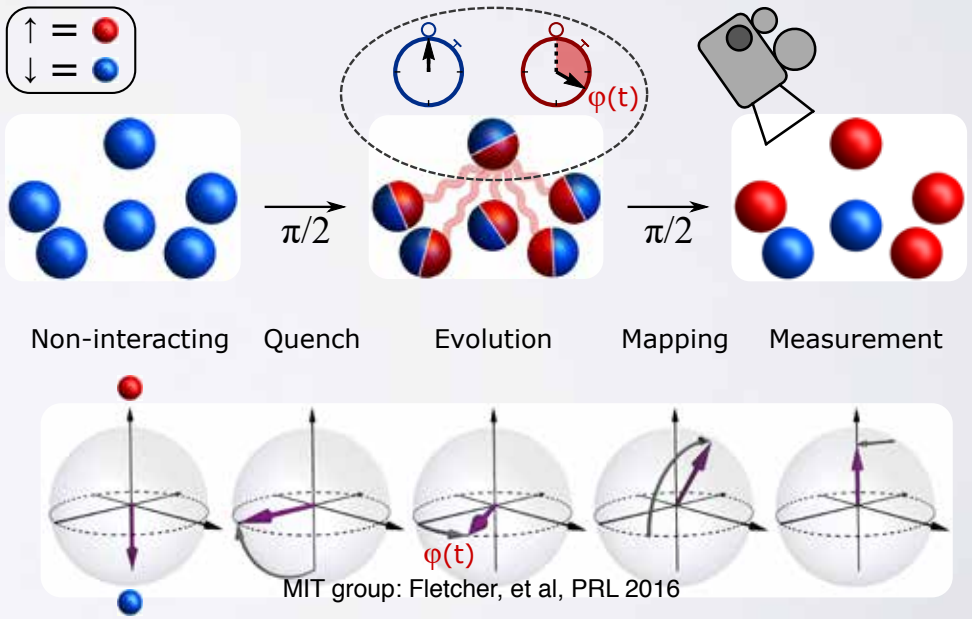
Cluster binding vs. N
roughly similar to
liquid 4He,
but 4He has only
7% condensate

analysis of rapid quench experiments:

$$\alpha_2 = 22(1)$$

$$\beta_3 = 2.1(1)$$

Smith, Braaten, Kang, Platter PRL 2014
analysis of Jin experiment



MIT group: Fletcher, et al, PRL 2016

Conclusions

- Unitary Bosons and Fermions are scale-invariant
- Comparatively simple DFT
- Can predict properties of small finite systems
  from calculations of hom/inhomogeneous matter
- Experimentally testable
  many external potentials will be available

Further tests of DFT

- Test specifically for properties of self-bound systems
  - can test different external potentials
  - comparisons of static/dynamic response

- Test pairing functionals
  - generalize interactions above
    to different scattering length
    and effective range

Can we test dynamics ?

- Significant information on dynamics can be obtained through path integral simulations:
  - density, spin response
  - low-lying collective excitations

- Contacts are interesting, relate EOS to high-momentum tails: EOS can be obtained from a DFT, but high momentum tails?

- At what energies and momenta does DFT start to break down?

What can ab-initio do to inform DFT?

- purely attractive interactions have no sign problem:
  EOS, gradients, static and dynamic response
- Can approach neutron matter much more closely
- Study neutrons with a fixed background proton density
- Real nuclei, ….

Backup Slides

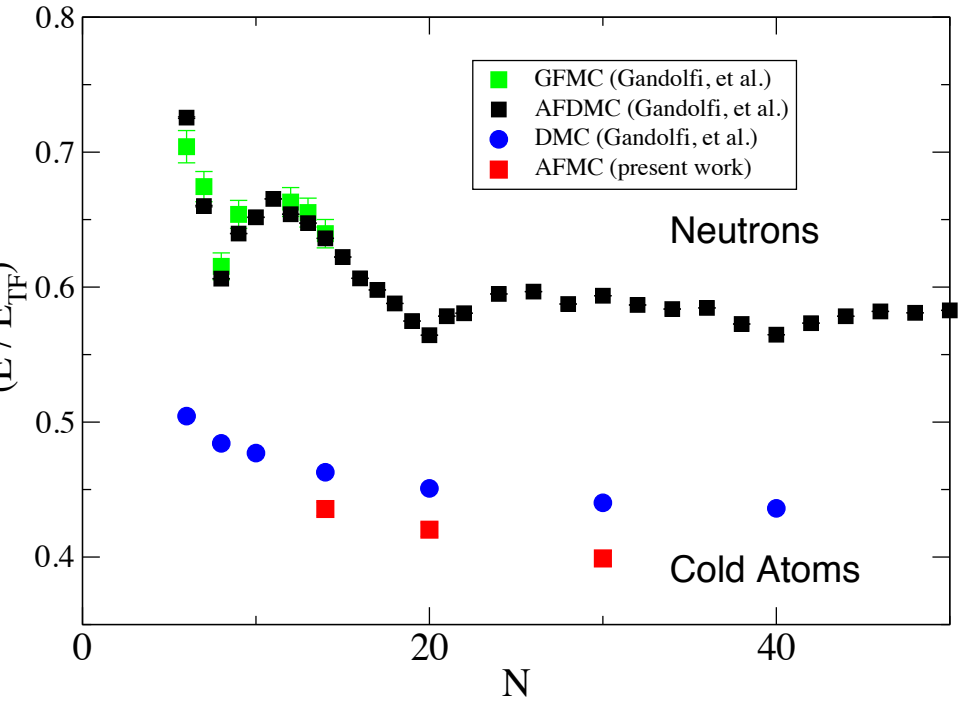
Inhomogeneous Fermi Gas

Low-lying excitations (phonons)
Transitions from 3 dimensions to 2 dimensions
How do finite systems behave - bulk vs. finite
    Density functional
Necessary to understand `exotic' (LOFF,...) phases

Add a spin-independent background potential
Examine the system for:

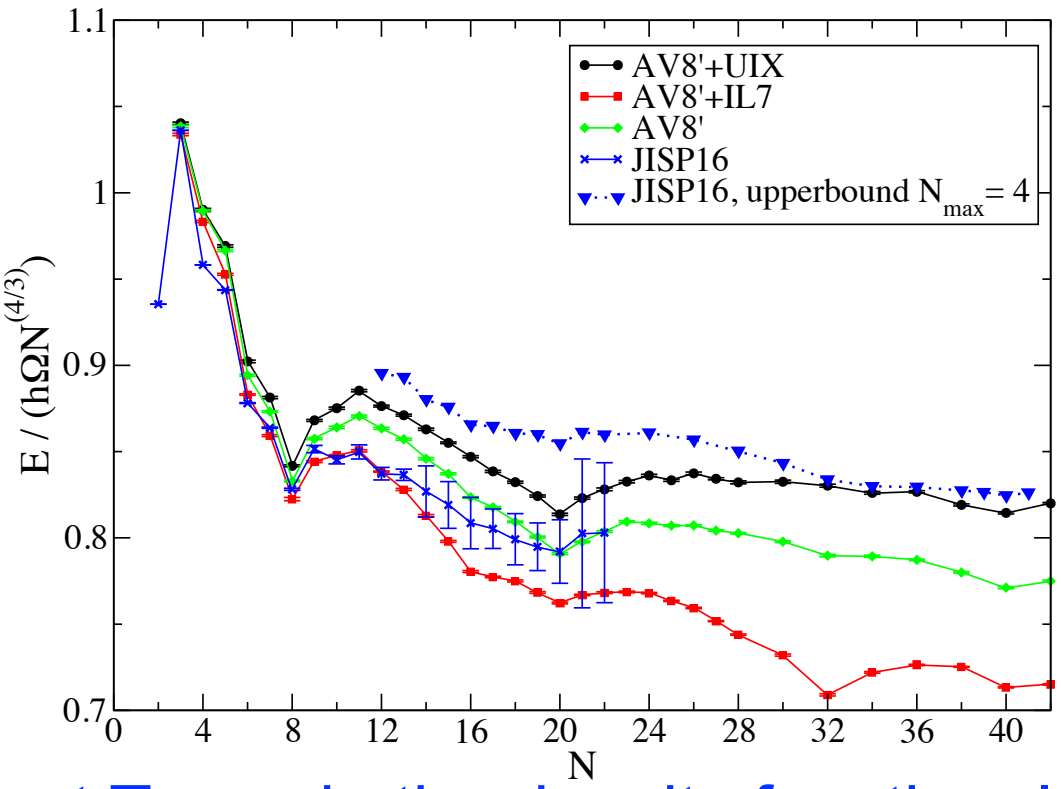
    weak periodic potentials
    Harmonic Oscillator potentials (1d, 2d, 3d,...)

Inhomogeneous Matter: Cold atoms and Neutron Drops



Cold atoms versus neutron drops

Comparison of different Hamiltonians



Constrain Isovector Gradient Terms in the density functional

$$\omega(q) \approx S^1(q)/S^0(q) = q^2/S^0(q)$$

at q/kF = 0.5 $\quad \omega(q) \rightarrow 1/(4 \times 0.629(1)) = 0.397(1)$

Density Response and Sum Rules

$$R(q,\omega) \;=\; \langle 0|\; \rho^{\dagger}(q)\; |f\rangle\langle f|\; \rho(q)\; |0\rangle\; \delta(w-(E_f-E_0))$$

$$\rho(q) = \sum_i \exp\left[i\mathbf{q}\cdot\mathbf{r}_i\right]$$

$$S\;(q) \;=\; \int d\omega\; R(q,\omega) \qquad S\;(q) \xrightarrow{q\to\infty} 1$$

high-q limit determined by contact
Here we are (first) interested in low q

Static Response: Inverse energy weighted sum rule

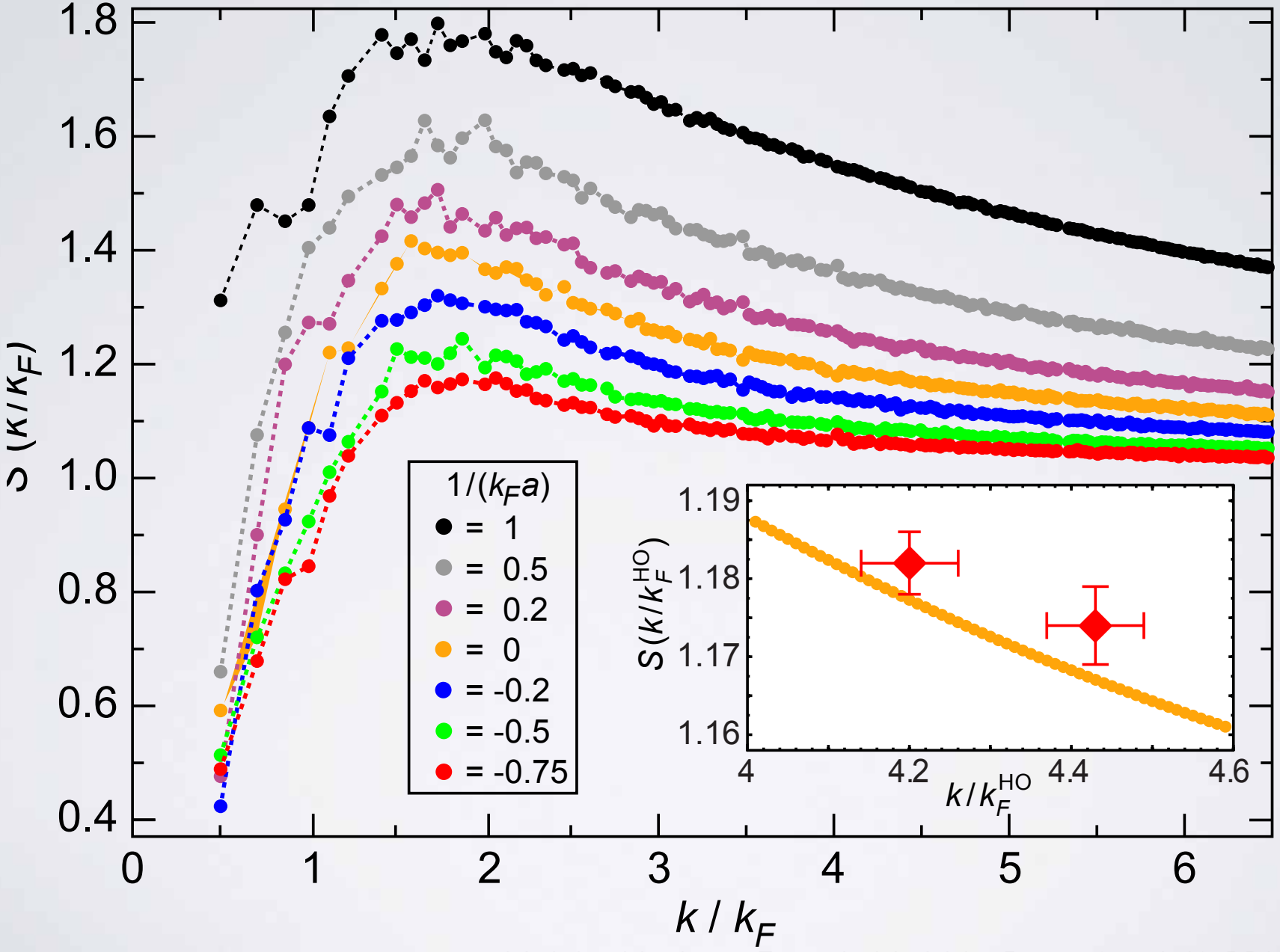
$$R(q,\omega) \;=\; \langle 0|\; \rho^{\dagger}(q)\; |f\rangle\langle f|\; \rho(q)\; |0\rangle\; \delta(w-(E_f-E_0))$$

$$\rho(q) = \sum_i \exp\,[i\mathbf{q}\cdot\mathbf{r}_i]$$

$$S^{-1}\;(q) = \int\; d\omega\; R(q,\omega)/\omega$$

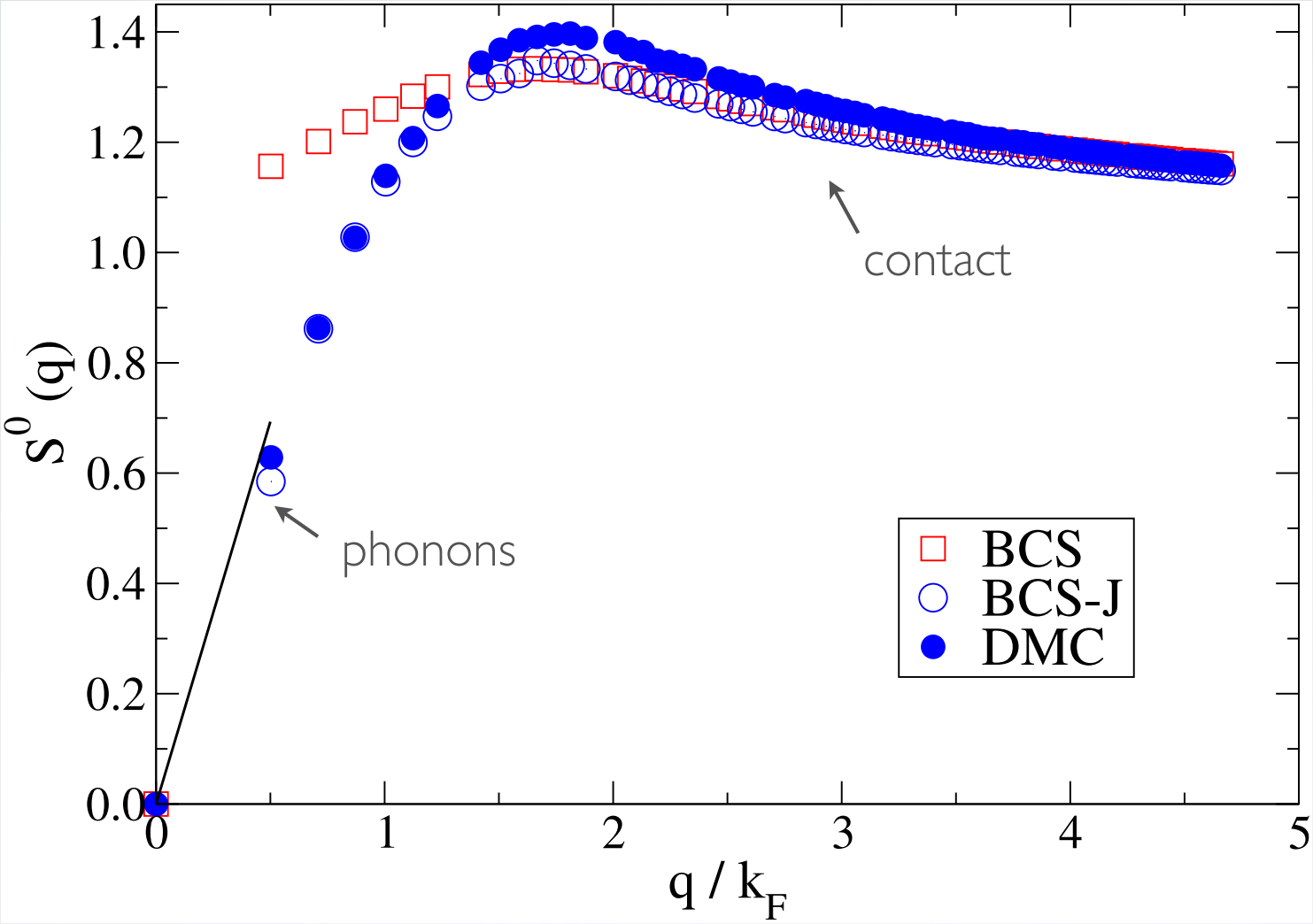
Static Response: response of the system to
a weak static external potential

S(q) for Unitary Fermi Gas: Theory vs.Experiment



Hoinka, Lingham, Fenech, Hu, Vale, Drut, Gandolfi, PRL 2013

S(q) for Unitary Fermi Gas

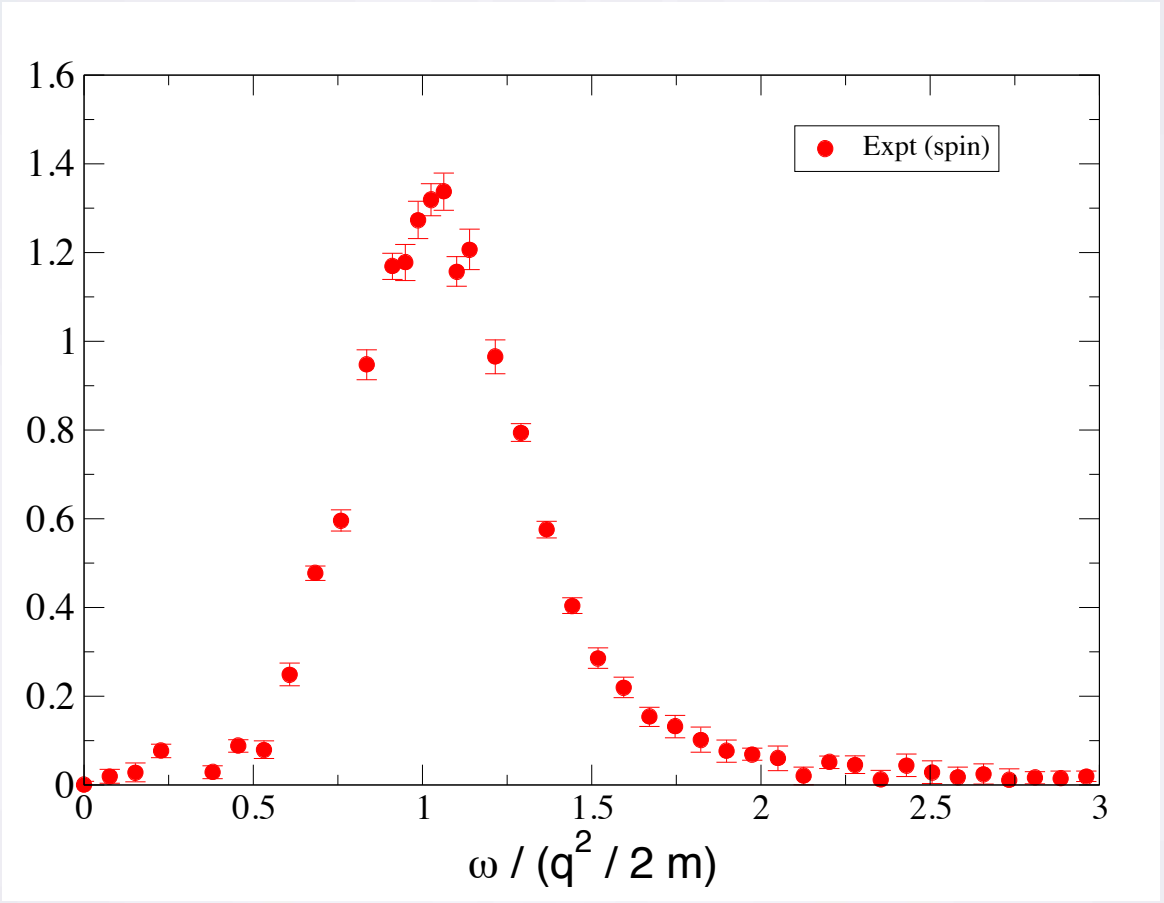


Simple BCS wave function does not describe low-q behavior
added long-range Jastrow to better describe phonons

What about high-energy excitations? Spin Response at high q

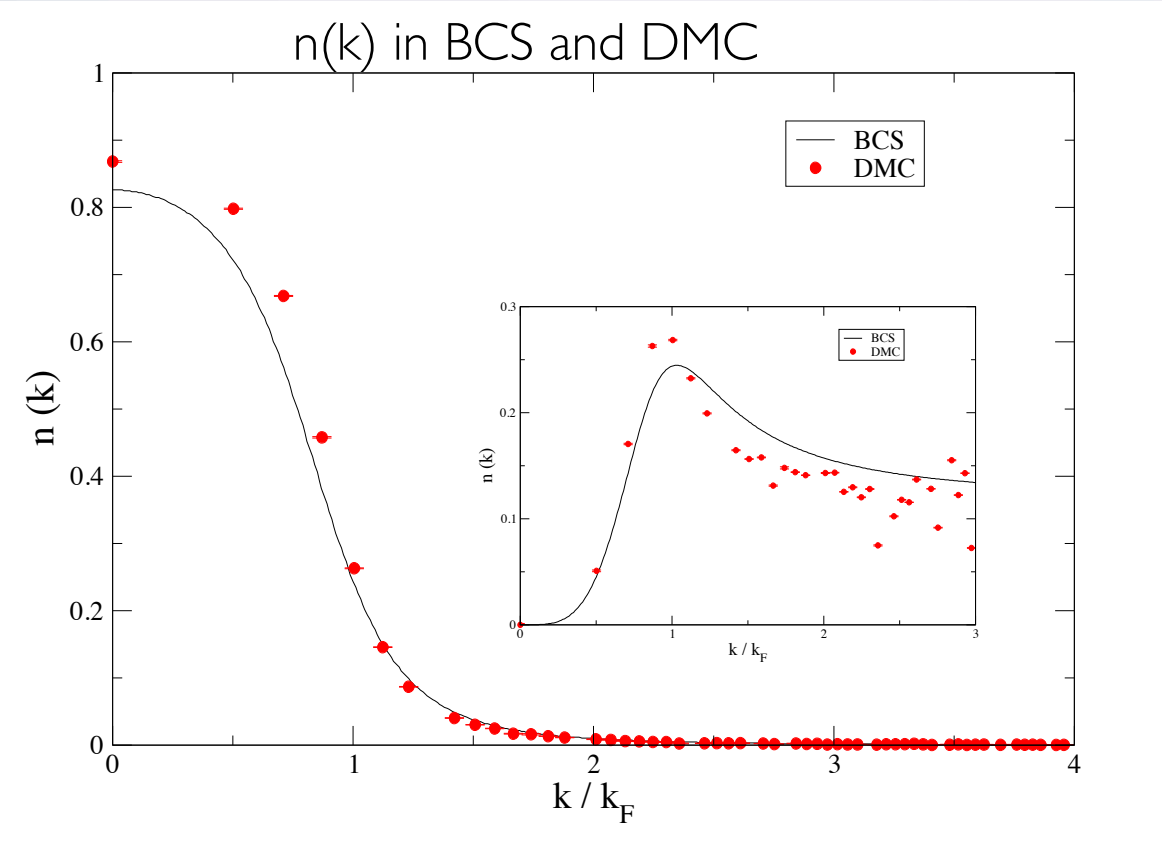
$$R(q,\omega) \;=\; \langle 0|\, \mathbf{j}^{\dagger}(q)\, |f\rangle\langle f|\, \mathbf{j}(q)\, |0\rangle\; \delta(w-(E_f-E_0))$$

$$\mathbf{j}(\mathbf{q}) = \sum_i \sigma_x(i)\;\; \exp[i\mathbf{q}\cdot r_i]$$



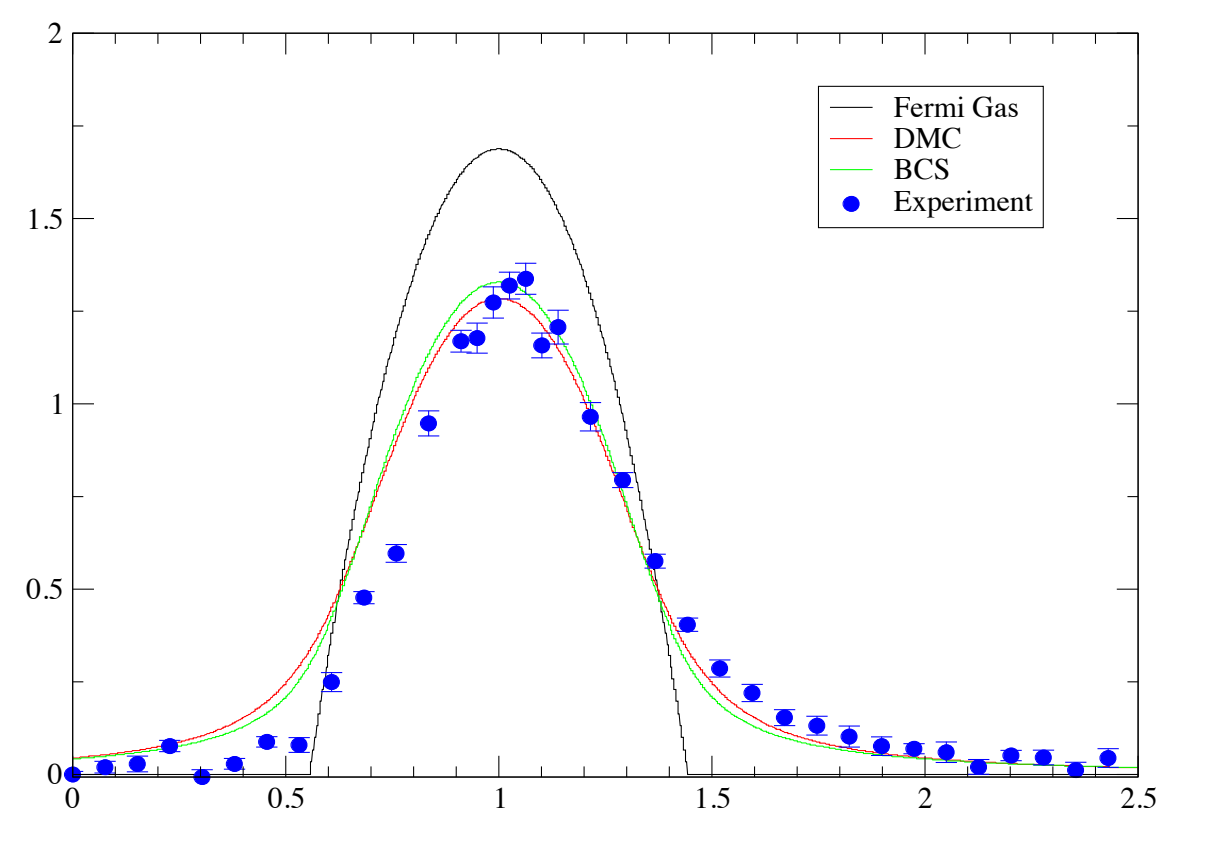
q=4.5 k_F

Looks like nuclear quasi-elastic scattering:
Dominated by single peak at QE kinematics
width of response determined by the momentum distribution



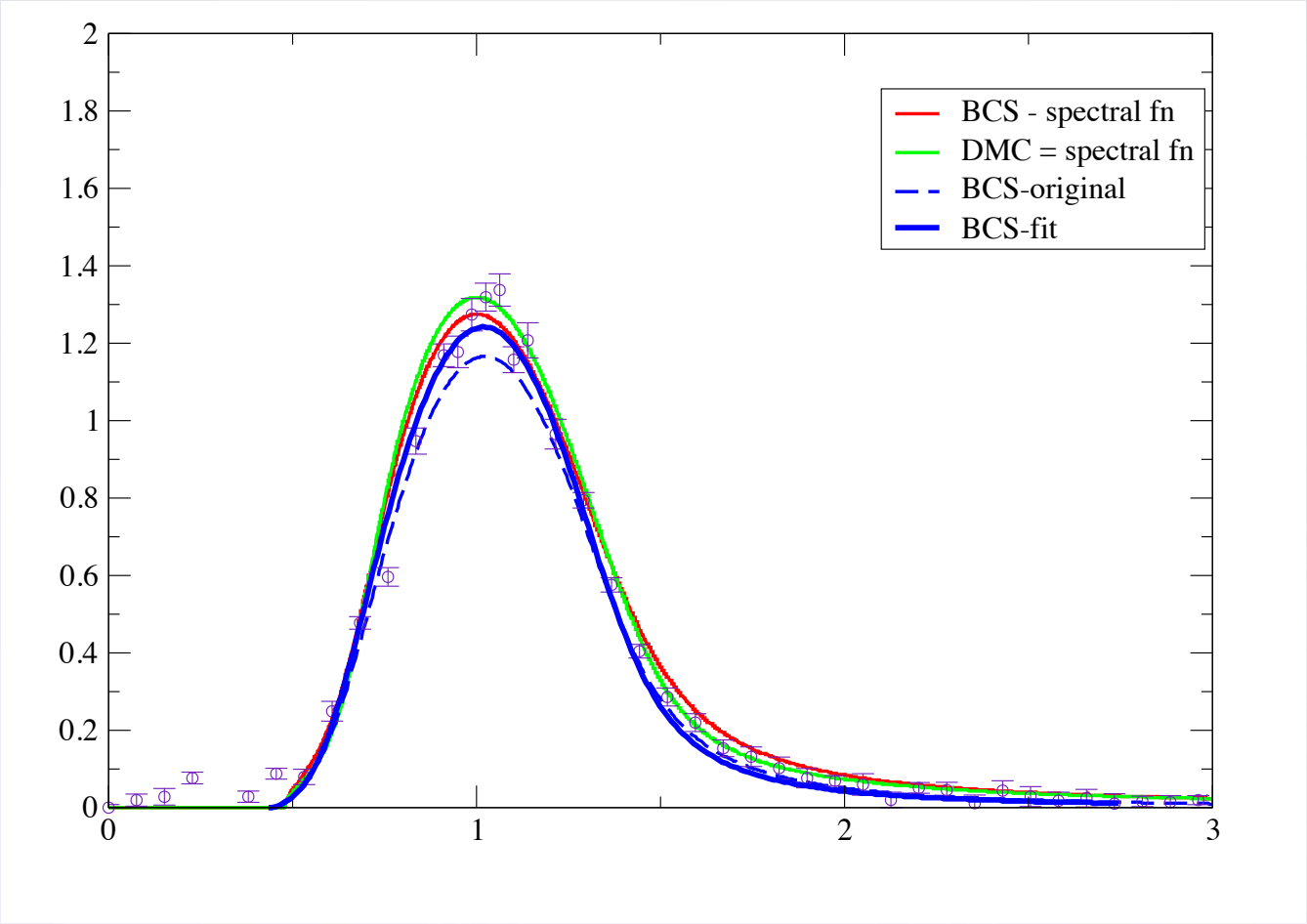
Spin response in PWIA approximation

$$S_{PWIA}(q,\omega) = 2\pi \int k^2 dk \; d\cos(\theta) \; n(k) \; \delta(\omega - q^2 + 2kq\cos(\theta),$$

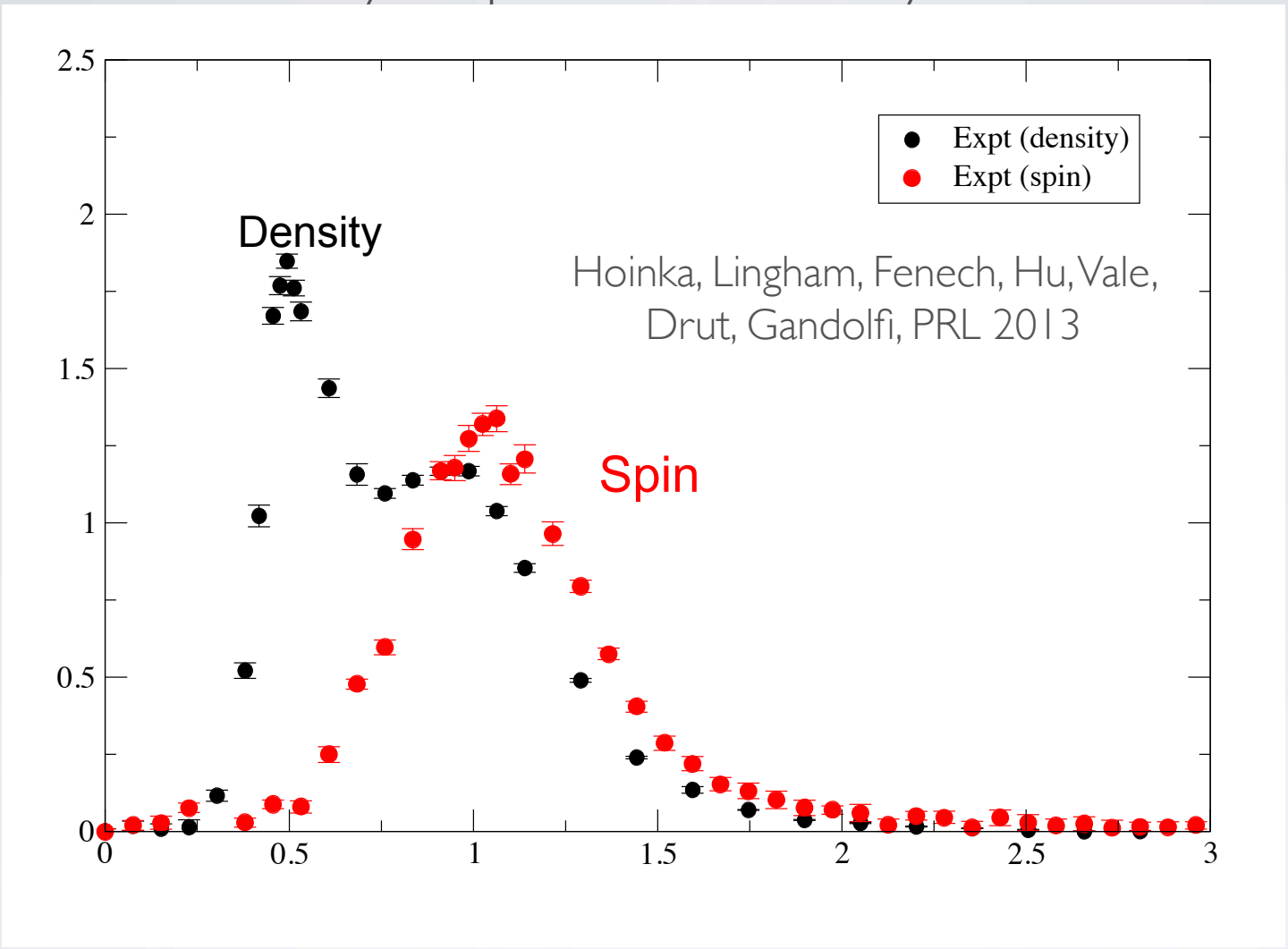


Add spectral function from quasi-particle spectrum

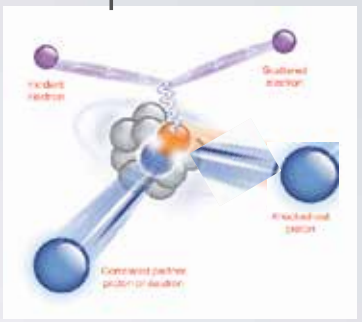
Spin response with spectral function information



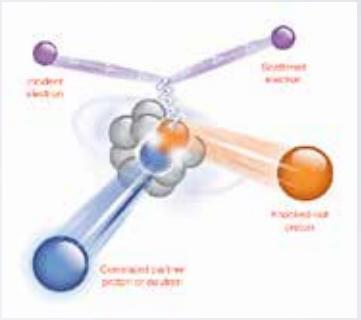
Density response looks very different



Spin



Density

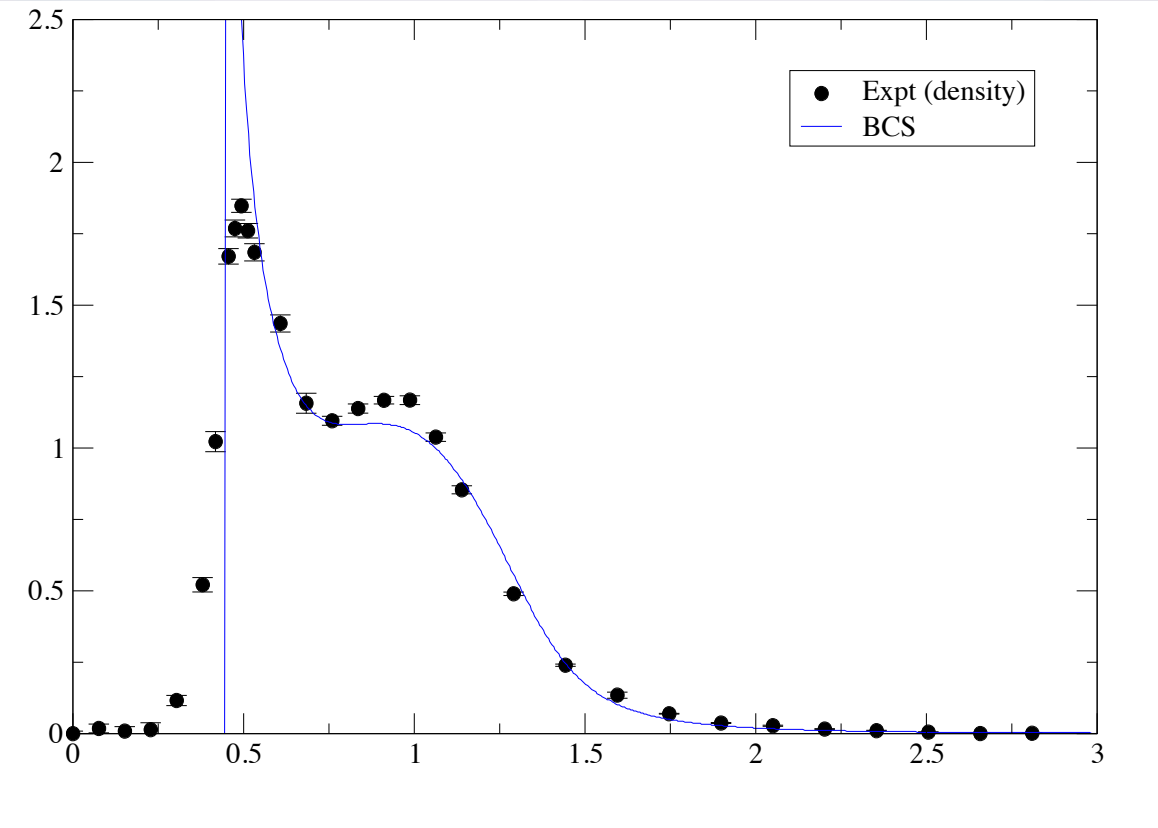


Density response has two peaks: $q^2/(2m)$ for single-particle (also seen in spin response)

$q^2/(4m)$ for pairs

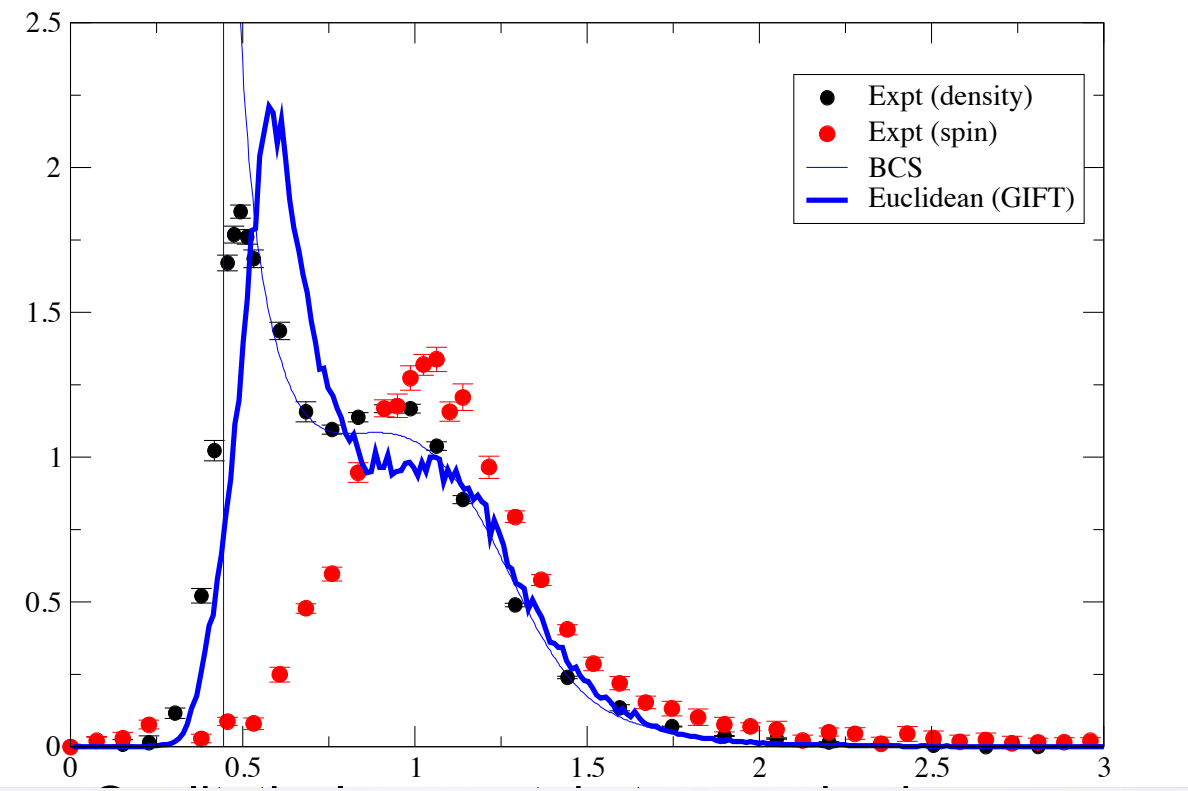
Difference in final state interactions

Density Response: BCS theory



Gives low-energy peak, but too narrow
All pairs at P=0 in BCS

Inversion of QMC Euclidean Response



Qualitatively correct, but more physics input needed