# Density functional theory for fermions in the unitary regime

Thomas Papenbrock
Department of Physics & Astronomy, University of Tennessee
Physics Division, Oak Ridge National Laboratory

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Ref.: cond-mat/0507183 → Phys. Rev. A

Towards a universal density functional for the nucleus, INT Sept. 26-30, 05

# Motivation

- The s-wave scattering length unnaturally large for nucleons.
- Scattering length can be tuned to arbitrary values in ultracold atom gases.
- Bertsch (1998): "What is the energy density of fermions with infinite scattering length and zero range?"
- The only length scale is the two-particle distance (or the Fermi momentum). Energy must be proportional to free Fermi gas:

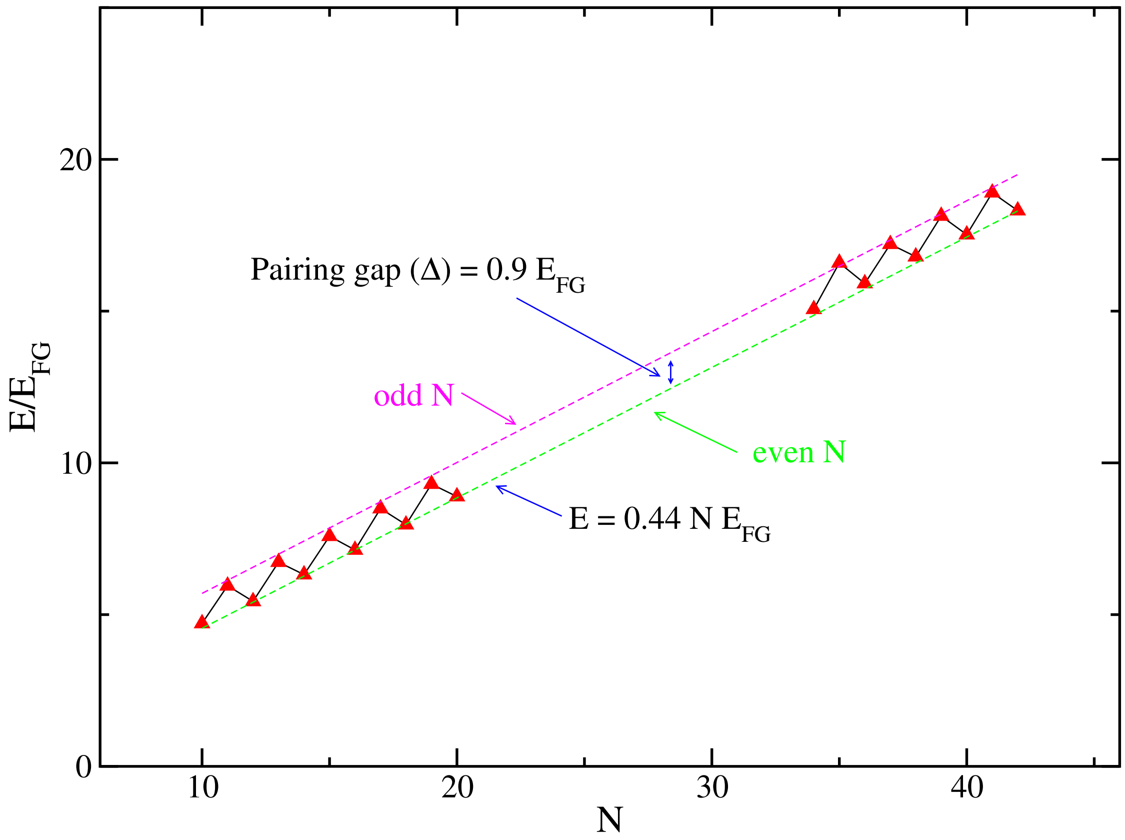
$$E(N) = \xi E_{TF}(N)$$

# What's the value of $\xi$ ?

1. Baker (1999): $\xi$ = 0.326 and $\xi$ =0.568 from Pade approximations to Fermi gas expansion.
2. Heiselberg (2001): $\xi$ =0.33 from ladder resummations (Galitskii eq.).
3. Engelbrecht et al. (1997): $\xi$ =0.59 from BCS theory.
4. Carlson et al (2003): $\xi$ =0.44 +/- 0.01
5. Astrakharchik et al (2004): $\xi$ =0.42 +/- 0.01
6. Lee (2005): $\xi$ < 0.42

# Monte Carlo results by Carlson et al.

PRL 91, 050401 (2003)




- Strong pairing effects
- Absence of shell structure

# Simple approach via DFT (for even N)

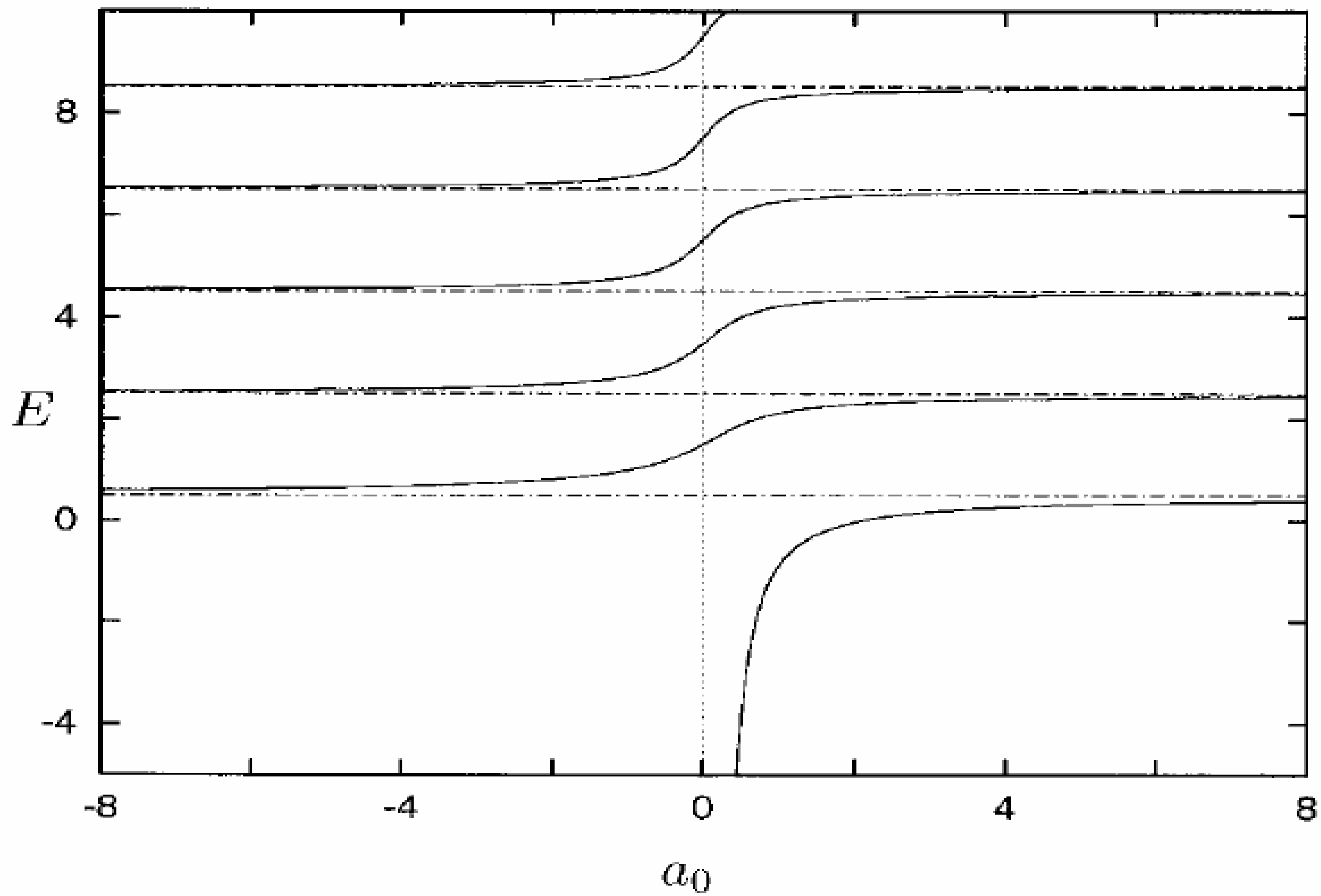
1. Form of density functional constrained.
2. Fit parameters of functional to exact results for two fermions in harmonic trap [Busch et al (1998)].

$$\psi_{\text{rel}}(r) = \frac{1}{\sqrt{2^{3/2}\pi l^3}} \frac{l}{r} \exp\left(-\frac{r^2}{4l^2}\right)$$

$$E = 2\hbar\omega$$

# Spectrum of two-particle system

Busch et al., Found. Phys. 28, 549 (1998)



Warm-up: Thomas-Fermi theory

$$\mathcal{E}_{TF} = \xi\frac{\hbar^2}{m}c\rho^{5/3} + \frac{1}{2}m\omega^2 r^2$$

$$c = \frac{3}{10}(3\pi^2)^{2/3}$$

Energy of N-fermion system

$$E_{TF} = \frac{(3N)^{4/3}}{4}\xi^{1/2}\hbar\omega$$

Matching with exact energy yields $\xi$ =0.56

# $\xi$ from Kohn-Sham DFT

Form of the density functional

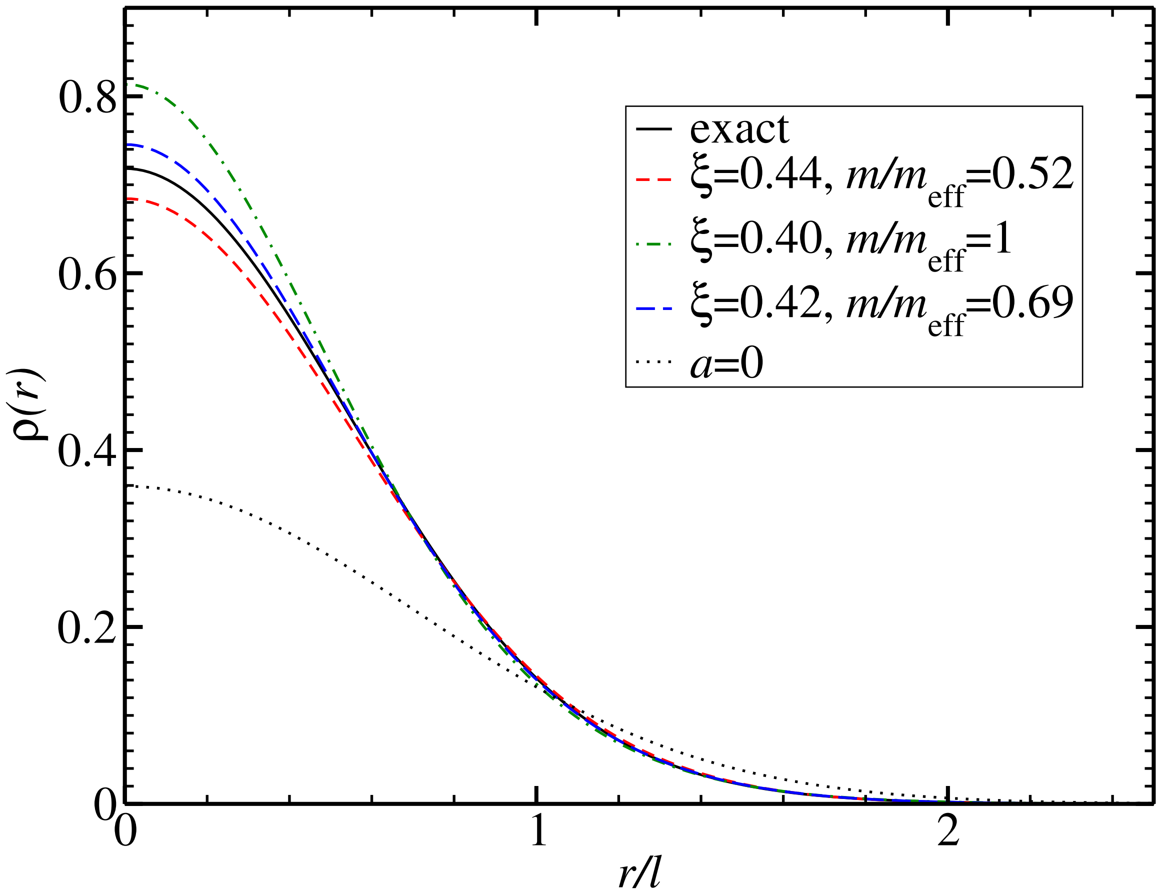
$$\mathcal{E} \;=\; \frac{\hbar^2}{m}\left[\frac{m}{2m_{\text{eff}}}\sum_{J=1}^{N}|\nabla\phi_j(r)|^2+\left(\xi-\frac{m}{m_{\text{eff}}}\right)c\rho^{5/3}\right]$$
$$+\frac{1}{2}m\omega^2r^2\rho$$

Properties:

1. Correct TF-limit

2. Non-localities and gradient terms via effective mass

# Results




$\xi$ = 0.42, $m/m_{eff}$ = 0.69 from best fit

Result for $\xi$ stable w.r.t. changes of $m_{eff}$

# Approximate analytical result

The prefactor of the $\rho^{5/3}$ term is

$$\left|\xi - \frac{m}{m_{\mathsf{eff}}}\right| \approx |0.42 - 0.69| \ll 1$$

→ Neglect $\rho^{5/3}$ term in density functional.
→ Only kinetic term remains.
→ Kohn-Sham Eq. becomes Schroedinger Eq. for harmonic oscillator.
→ Matching of energy yields $\xi$=4/9.

# How good is the density functional ?

Apply to exactly solvable Calogero model

$$
\begin{aligned}
H &= \frac{\hbar^2}{m}\sum_{j=1}^{N}\left(-\frac{1}{2}\frac{\partial^2}{\partial x_j^2}+\sum_{i>j}\frac{\frac{\beta}{2}\left(\frac{\beta}{2}-1\right)}{(x_i-x_j)^2}\right)+\frac{1}{2}m\omega^2\sum_{j=1}^{N}x_j^2 \\
E &= \hbar\omega\left(\frac{N}{2}+\frac{\beta}{4}N(N-1)\right)
\end{aligned}
$$

Interaction is also scale-invariant.

# DFT for Calogero model

Density functional

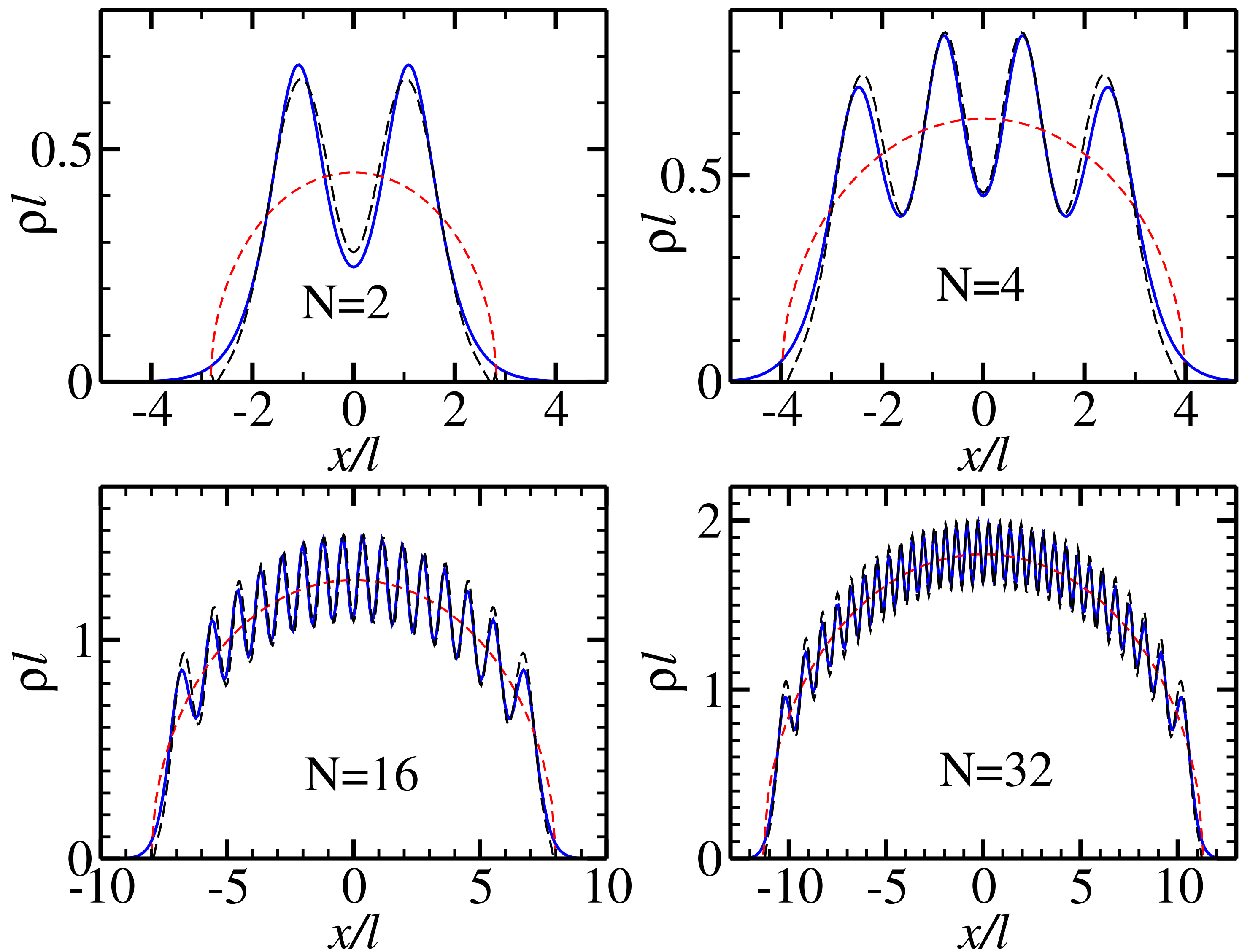
$$\mathcal{E} \;=\; \frac{\hbar^2}{m}\left[\frac{m}{2m_{\text{eff}}}\sum_{J=1}^{N}|\partial_x\phi_j(x)|^2+\frac{\pi^2}{6}\left(\eta^2-\frac{m}{m_{\text{eff}}}\right)\rho^3\right]$$
$$+\frac{1}{2}m\omega^2x^2\rho$$

Parameter $\eta = \beta/2$ from Thomas Fermi theory.

Effective mass from fit to $\beta = 4$ density:

$$\frac{m}{m_{\text{eff}}} \approx 6.3 + \frac{8.0}{N^2}$$

# Results for Calogero model



# Conclusions

- Determination of universal constant $\xi$ = 0.44 from DFT.
- Result stable w.r.t. variations of functional.
- Simple form of density functional tested on Calogero model.

Suggestions for nuclear density functional

(a) include $\rho^{5/3}$ term.

(b) include N-dependent effective mass.