

Finite-temperature lattice methods

Lecture 7.

Joaquín E. Drut

University of North Carolina at Chapel Hill

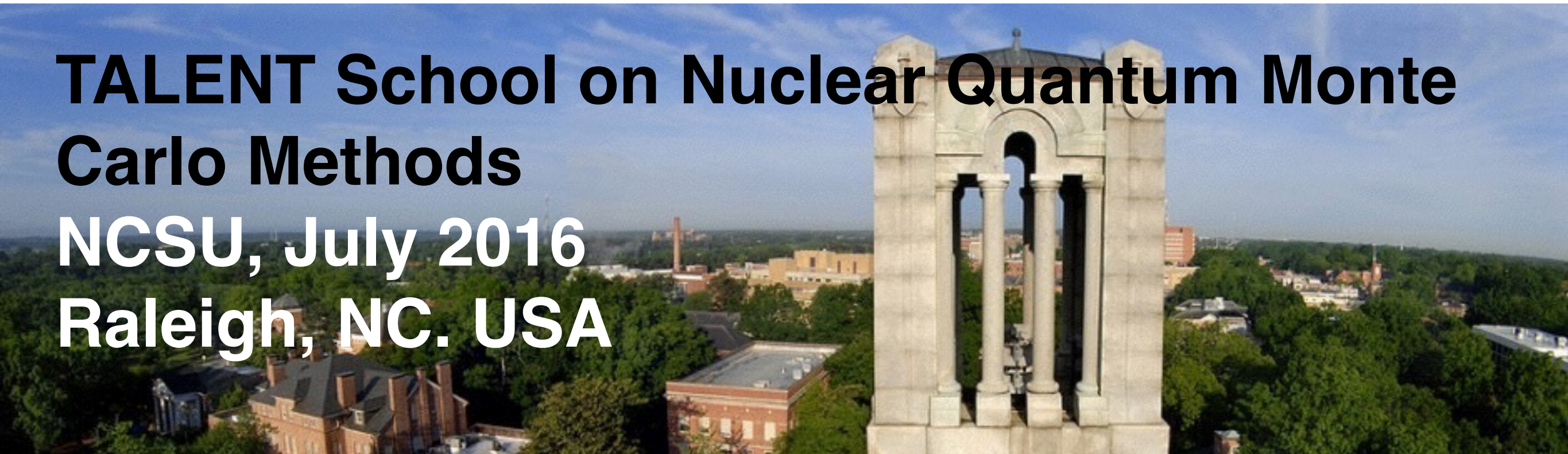


THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL

**TALENT School on Nuclear Quantum Monte
Carlo Methods**

NCSU, July 2016

Raleigh, NC. USA



Goals

- **Lecture 1:**

General motivation. Review of statistical mechanics and thermodynamics. Non-interacting quantum gases at finite temperature.

- **Lecture 2:**

QRL1. Formalism at finite temperature: Trotter-Suzuki decompositions; Hubbard-Stratonovich transformations. From traces to determinants. The sign problem.

- **Lecture 3:**

QRL2. Computing expectation values (finally!). Particle number. Energy. Correlation functions: static and dynamic. Sampling techniques. Signal-to-noise issues and how to overcome them.

Goals

- **Lecture 4:**

Quantum phase transitions and quantum information. Entanglement entropy. Reduced density matrix. Replica trick. Signal-to-noise issues.

- **Lecture 5:**

QRL3. Finite systems and the virial expansion. Signal-to-noise issues. Harmonically trapped systems.

- **Lecture 6:**

QRL5. Perturbation theory on the lattice.

- **Lecture 7:**

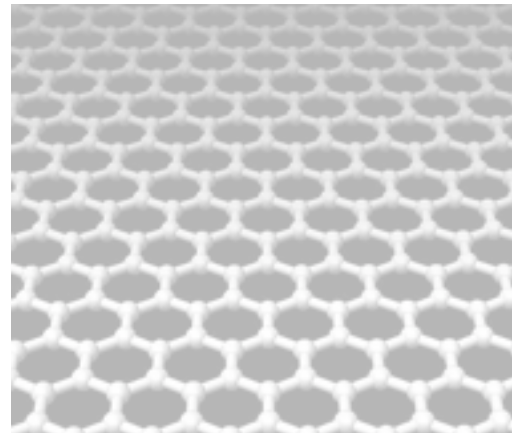
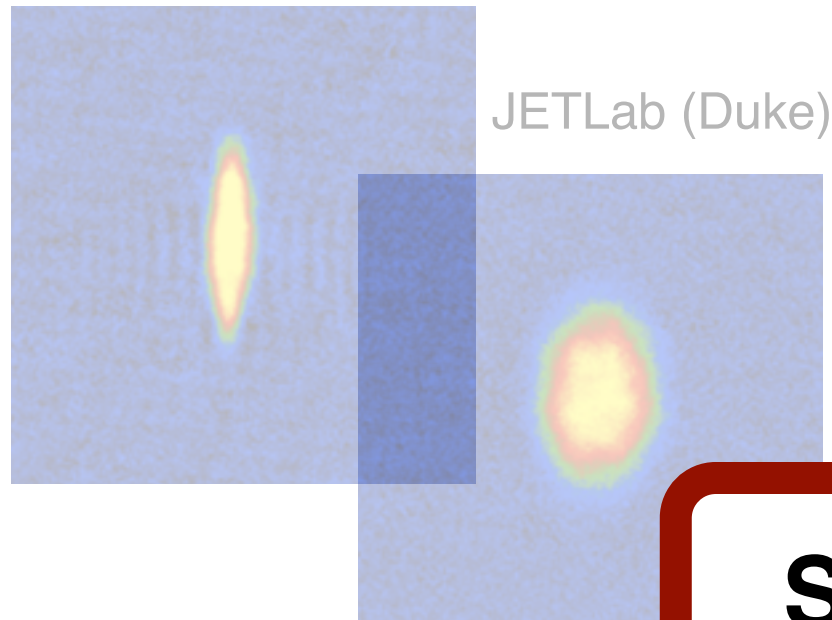
Applications to ultracold atoms in a variety of situations. Beyond equilibrium thermodynamics.

Applications

Ultracold Gases

Condensed Matter Physics

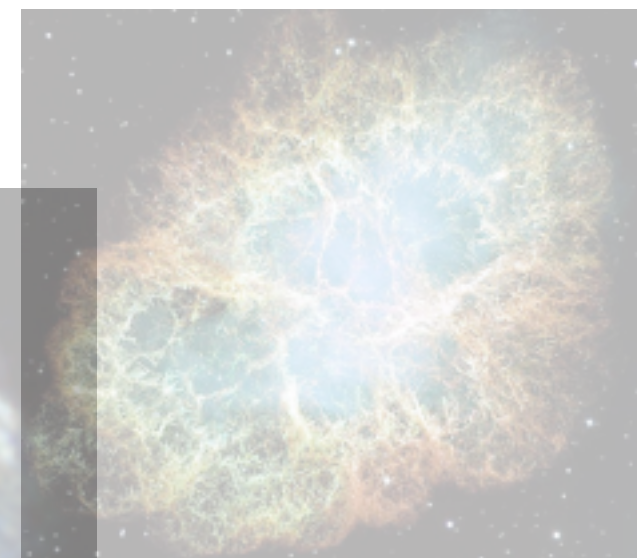
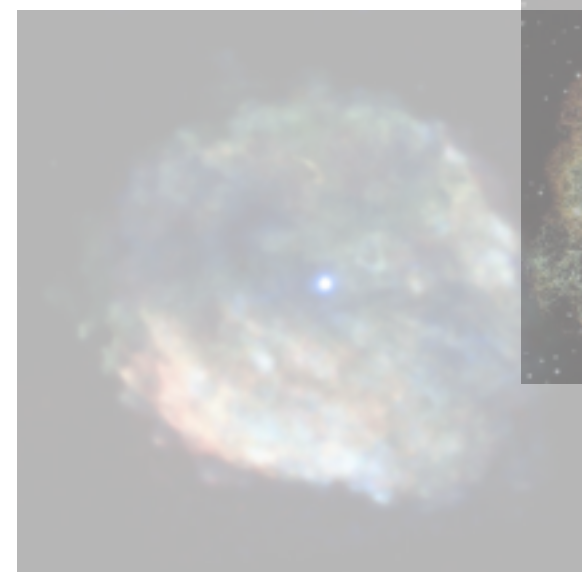
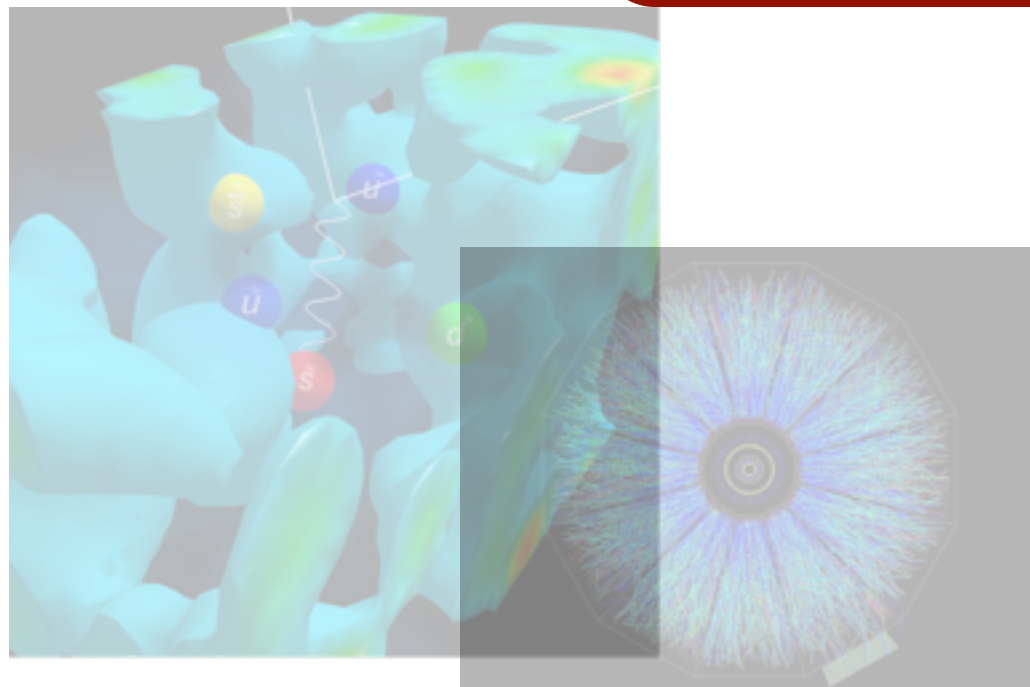
Materials Science



High-Energy Physics
QCD, Low-Energy

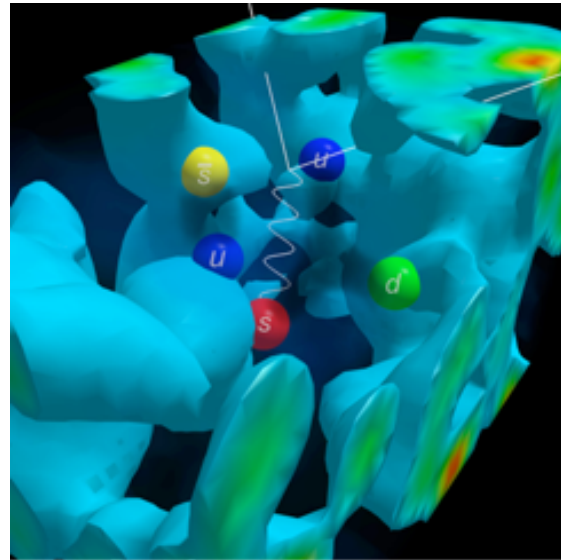
Astrophysics
(e.g., neutron stars)

**Strongly correlated
quantum many-body
systems**



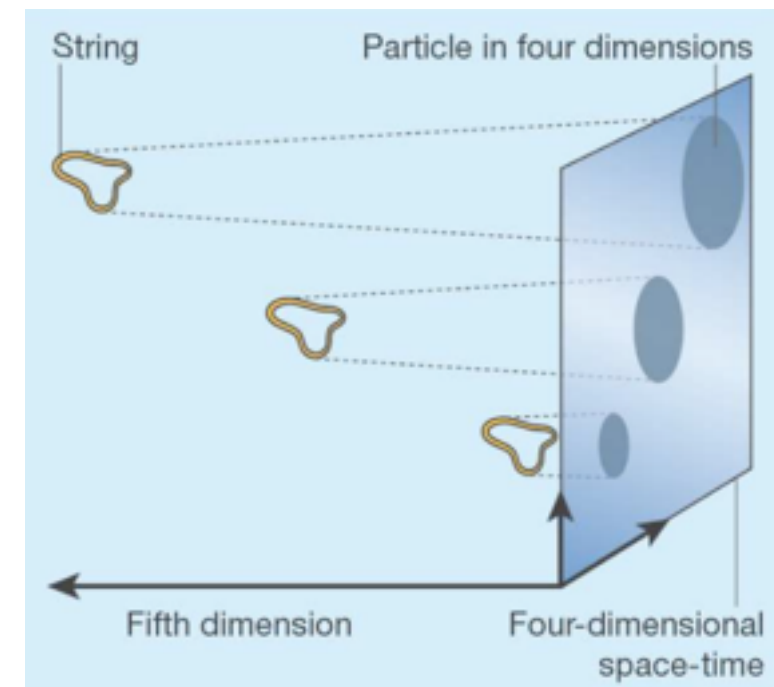
Why ultracold atoms?

- There is a **bigger picture!**



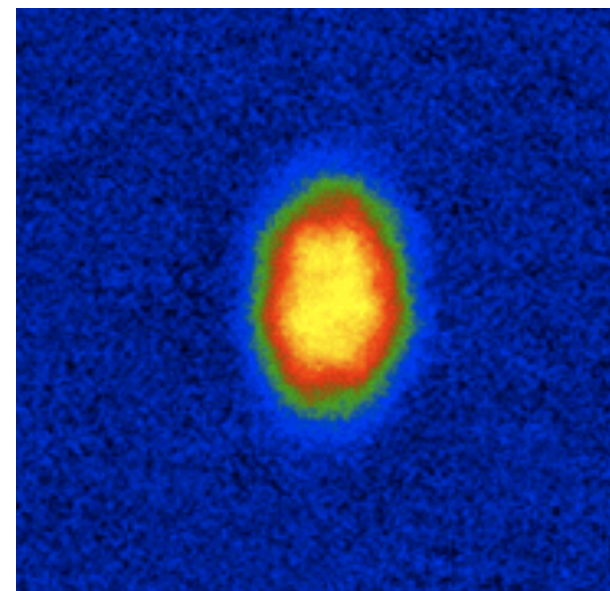
Quantum chromodynamics

Nuclear structure



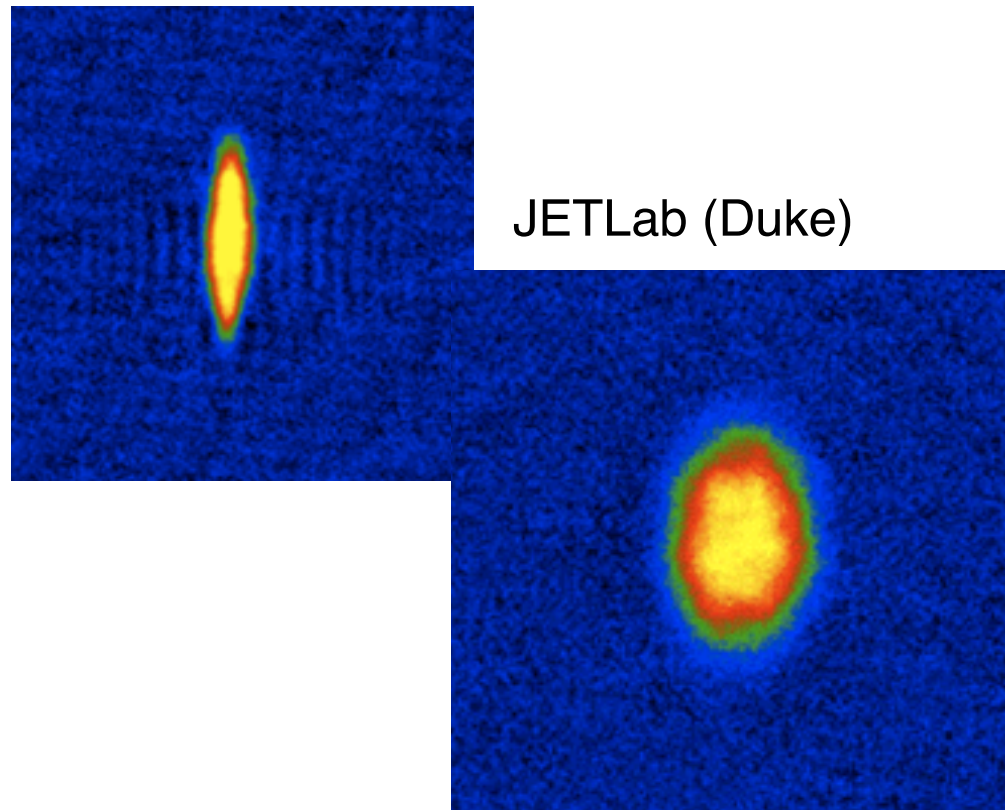
String theory, AdS/CFT

Ultracold atoms



How is this picture even possible?

Fermi gases



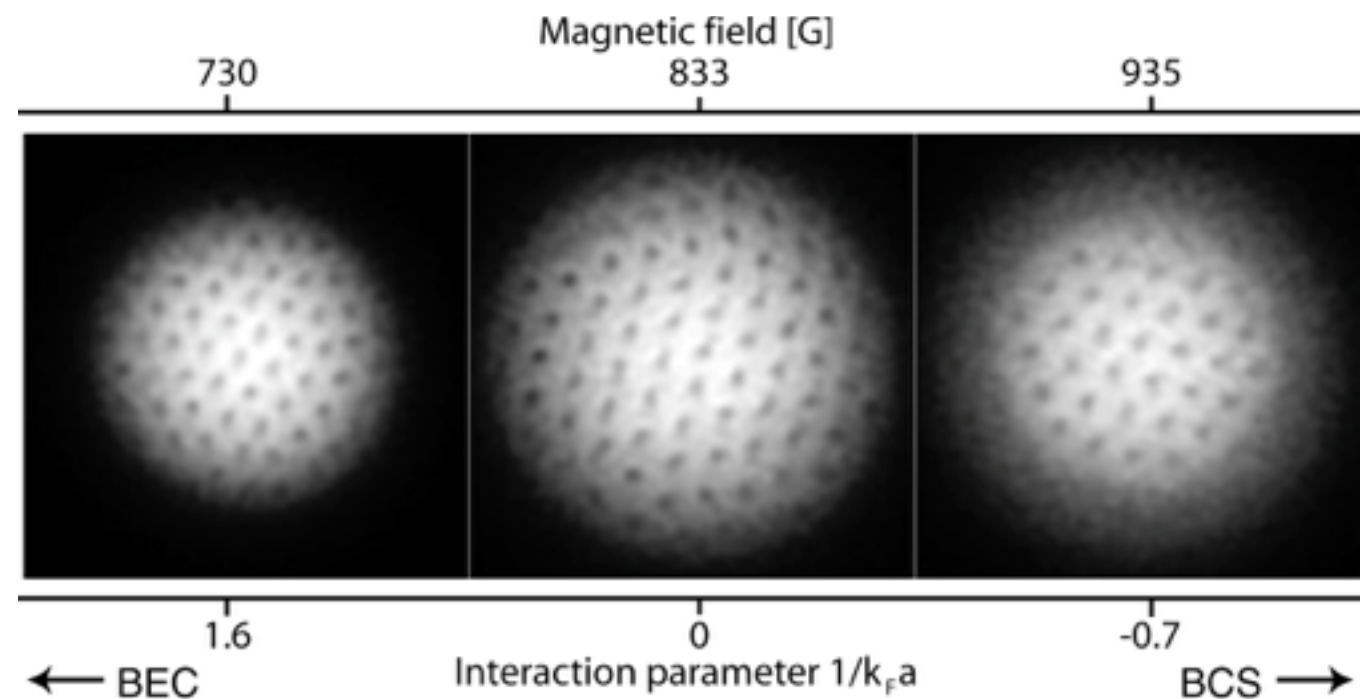
Typically alkali gases

Clean

Interaction is tunable!

Polarization is tunable!

	${}^6\text{Li}$	Neutrons
r_0	20 Bohr	3 fm
a	10^4 Bohr	-19 fm



MIT

Fermi gases

- Spin 1/2 fermions

Let's look at the **two-body** problem, at low momentum

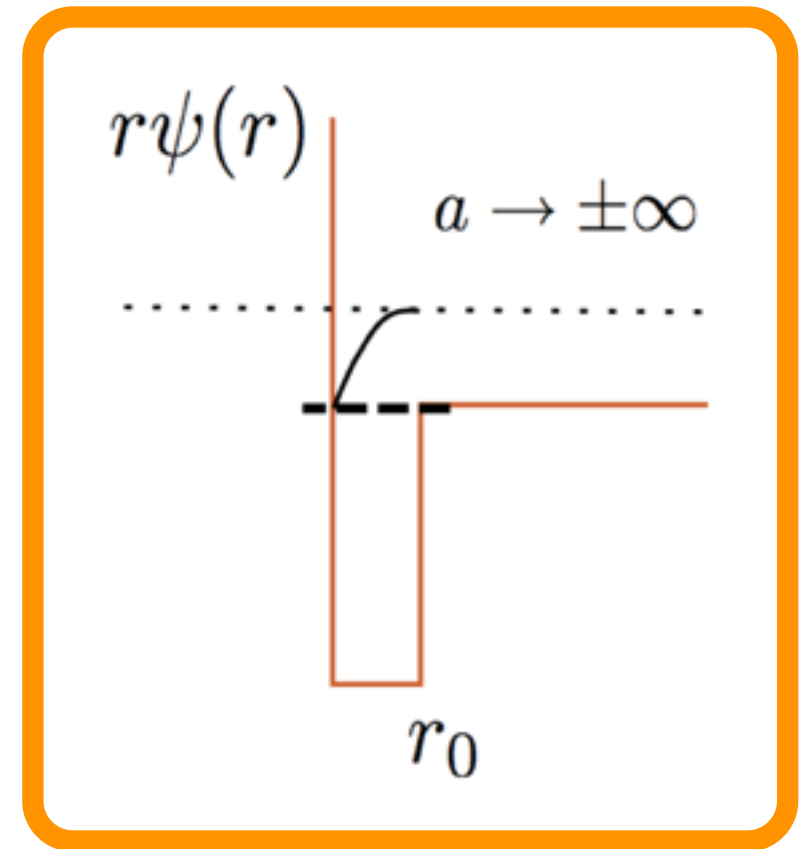
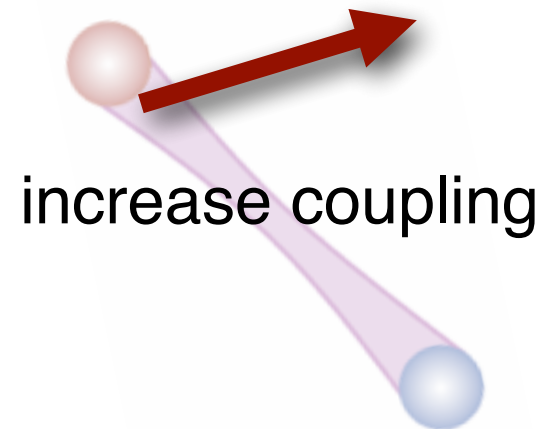
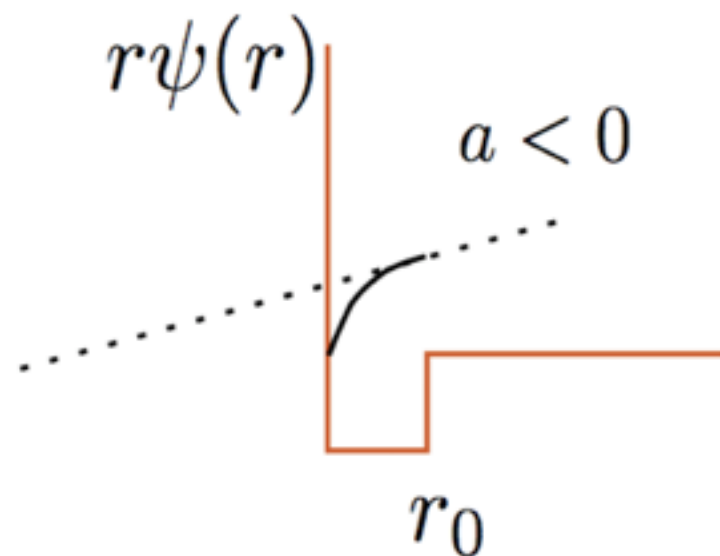


Non-interacting: $\psi(r) \sim \frac{\sin(kr)}{r}$

Fermi gases

- Spin 1/2 fermions, attractive interaction

Let's look at the **two-body** problem, at low momentum



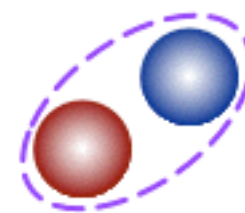
keep increasing coupling

Unitary: $\psi(r) \sim \frac{1}{r}$

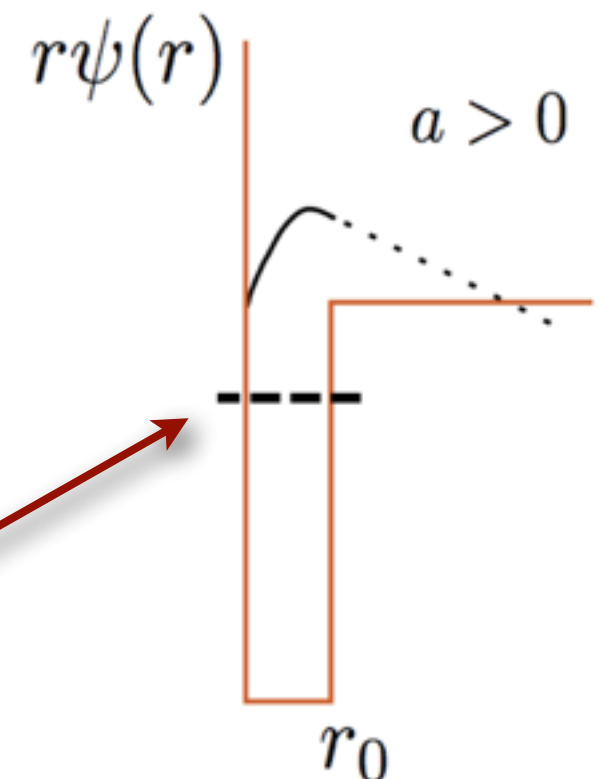
(with $r_0 \rightarrow 0$)

$$k \cot \delta = 0$$

$$\sigma = \frac{4\pi}{k^2}$$



Two-body bound-state!



The unitary limit

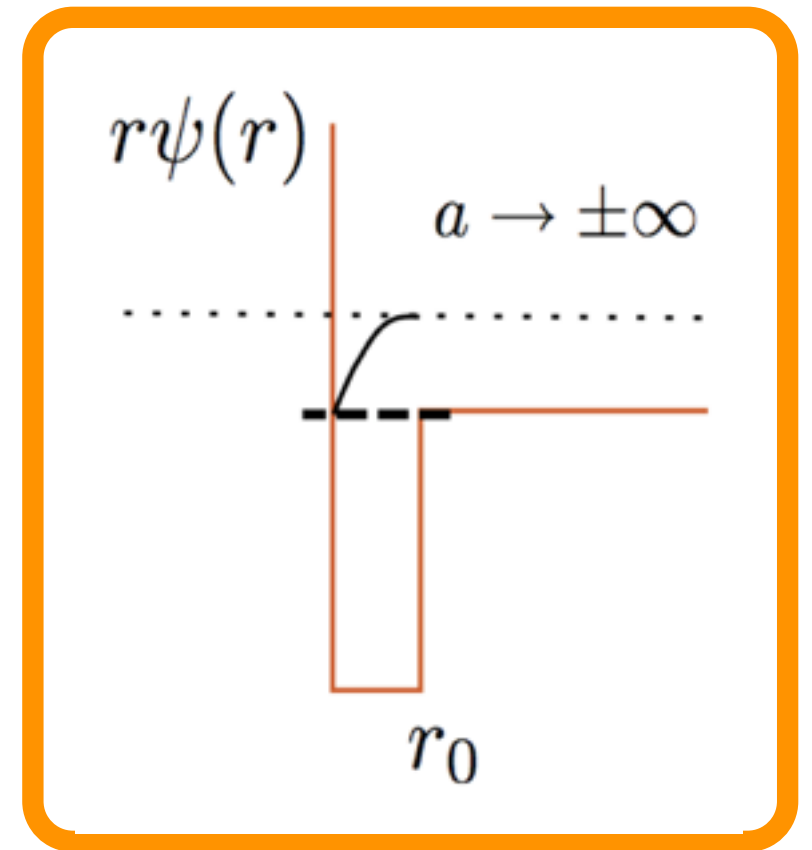
- Spin 1/2 fermions, at unitarity

$$r_0 \rightarrow 0 \ll n^{-1/3} \ll |a| \rightarrow \infty$$

Range of the
interaction

Inter-particle
distance

S-wave
scattering
length



- As many scales as a free gas!

$$k_F = \hbar(3\pi^2 n)^{1/3} \quad \varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

- Qualitatively

Every dimensionful quantity should come as a power of ε_F times a **universal** constant/function.

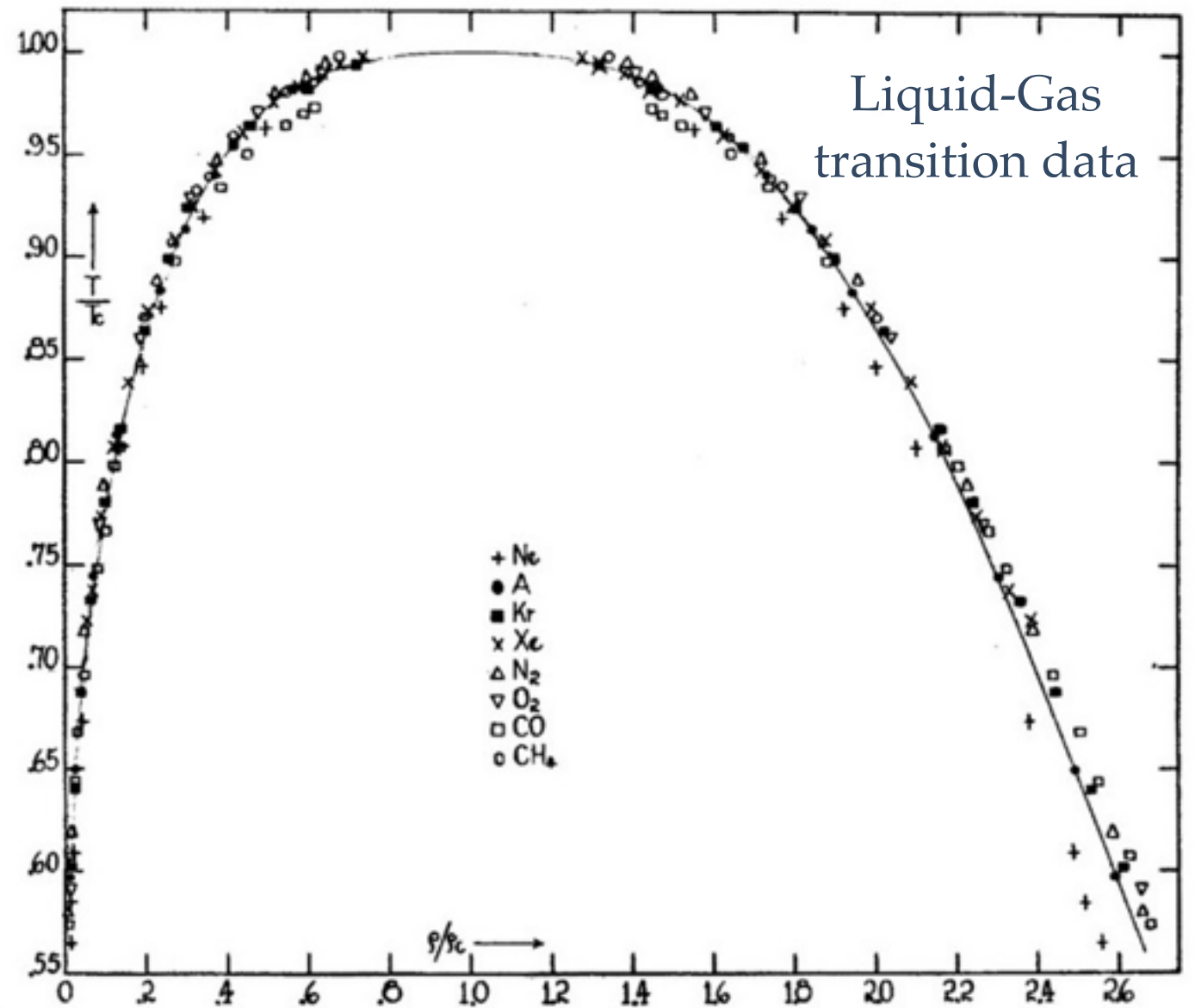
- Quantitatively ?

Universality

● Phase transitions & critical exponents

- Liquid-Gas
- Metal-Insulator
- Superfluid-Normal
- Confined-Deconfined
- ...

Independence from microscopic details, i.e. from the form of the interaction.



E.A. Guggenheim, J. Chem. Phys. **13**, 253 (1945).

Efimov physics

- Bound-state formation beyond 2 bodies (think $N_f > 2$)

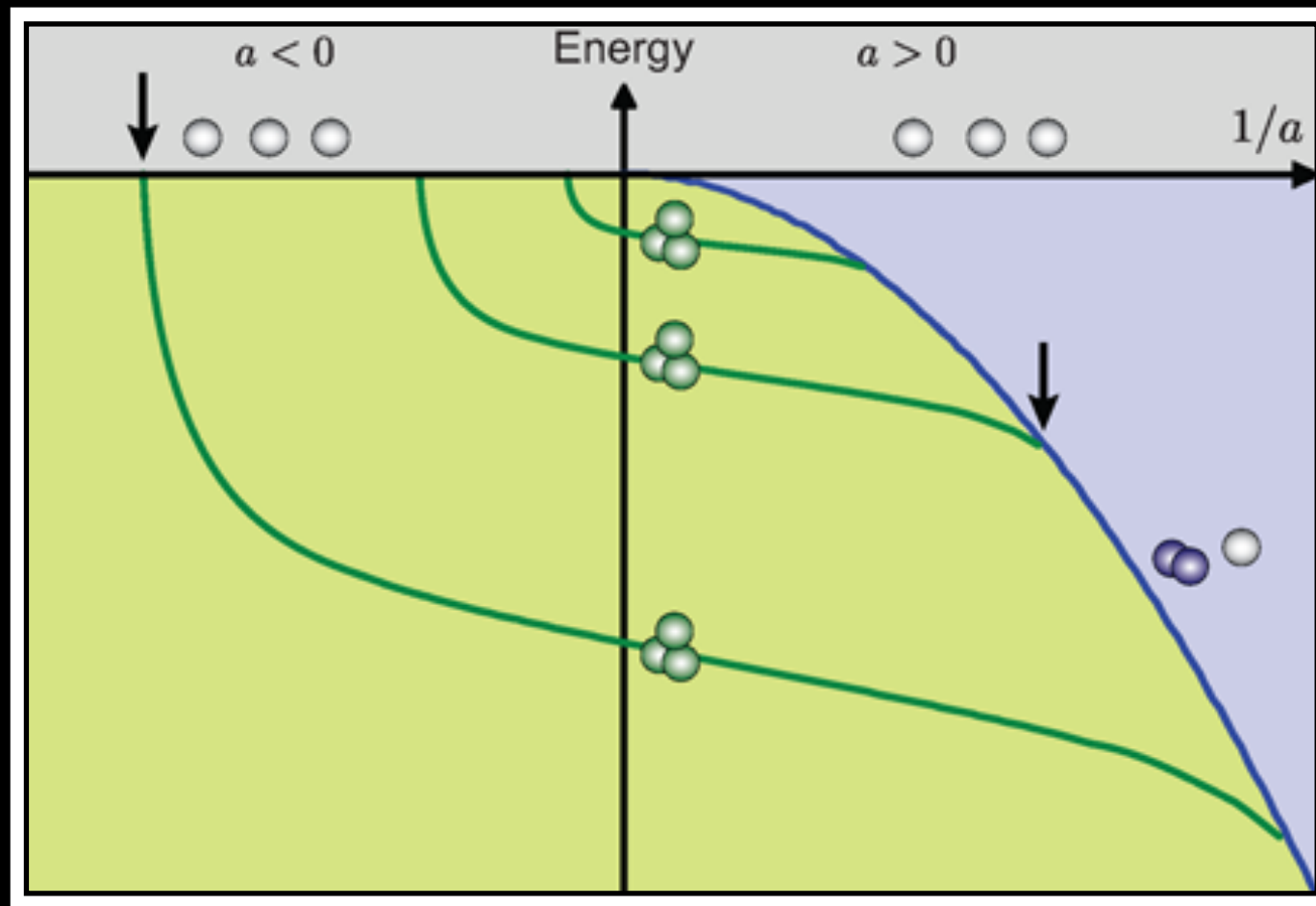
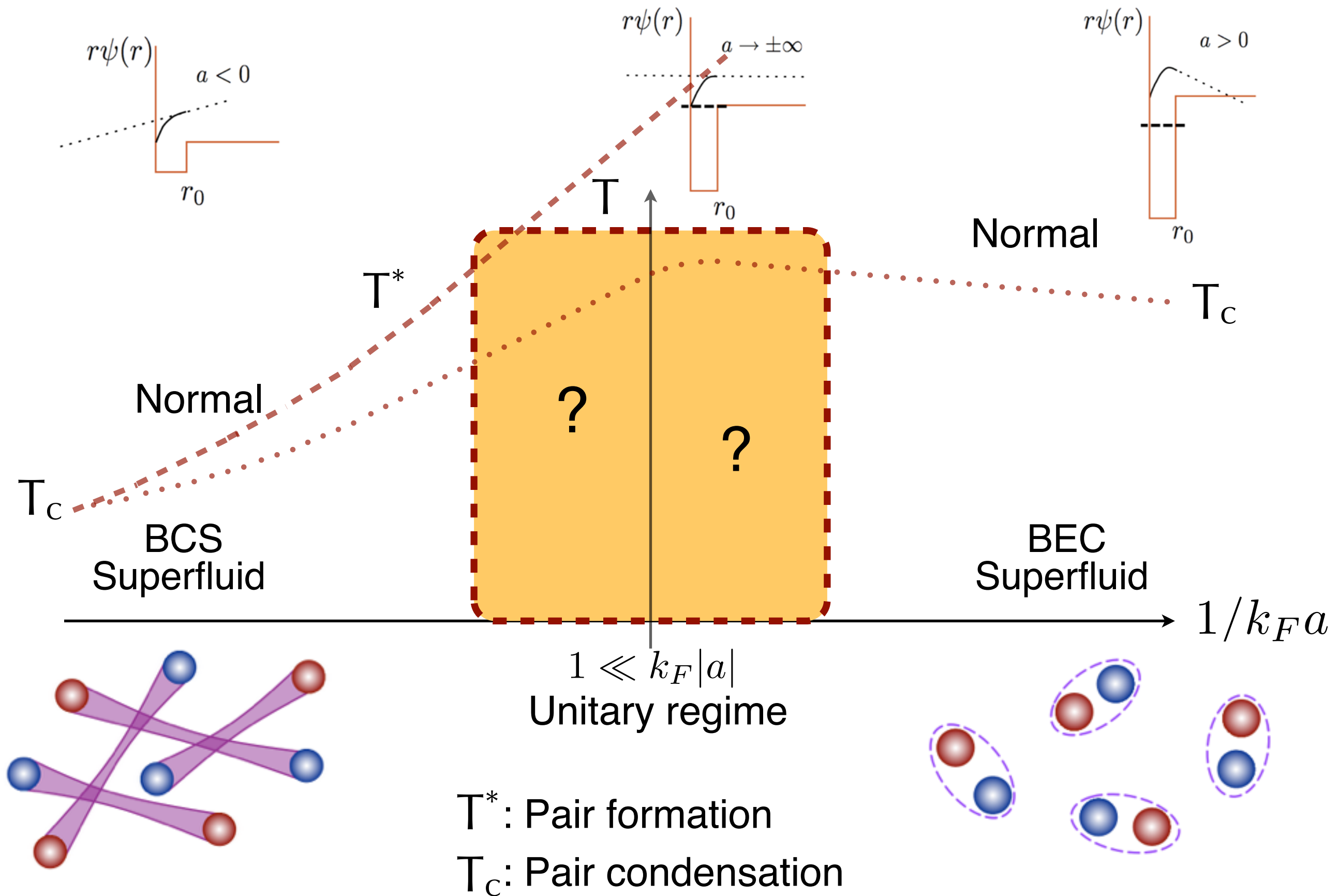


Figure: Ferlino and Grimm. *Physics* **3**, 9 (2010)

Efimov:

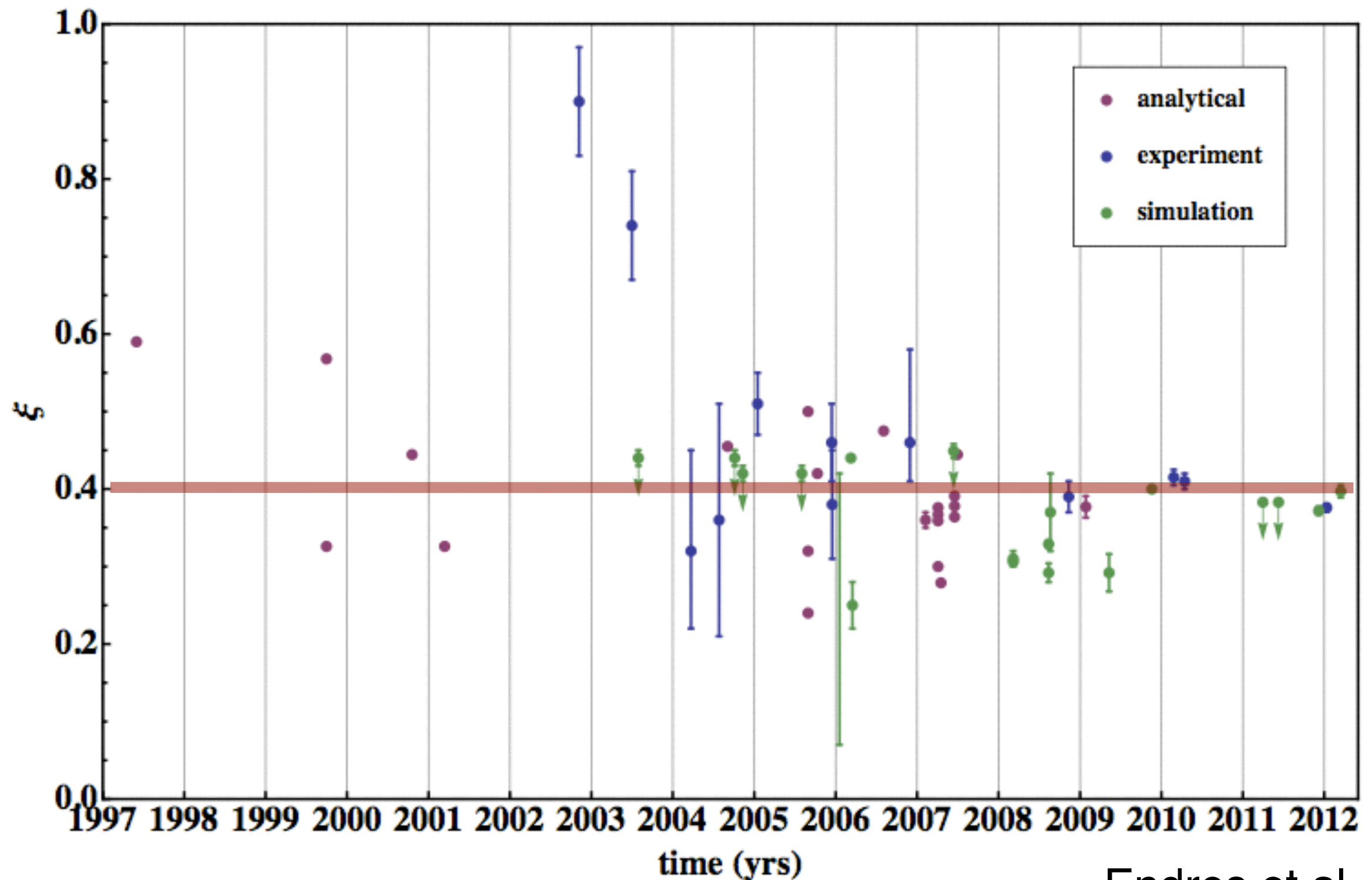
- There is an **infinite number** of 3-body bound states “attached” to the 2-body threshold.
- The binding energies display **discrete scale invariance** (RG limit cycle!)

The BCS-BEC crossover



What do we know?

- Ground state energy per particle



Endres et al.

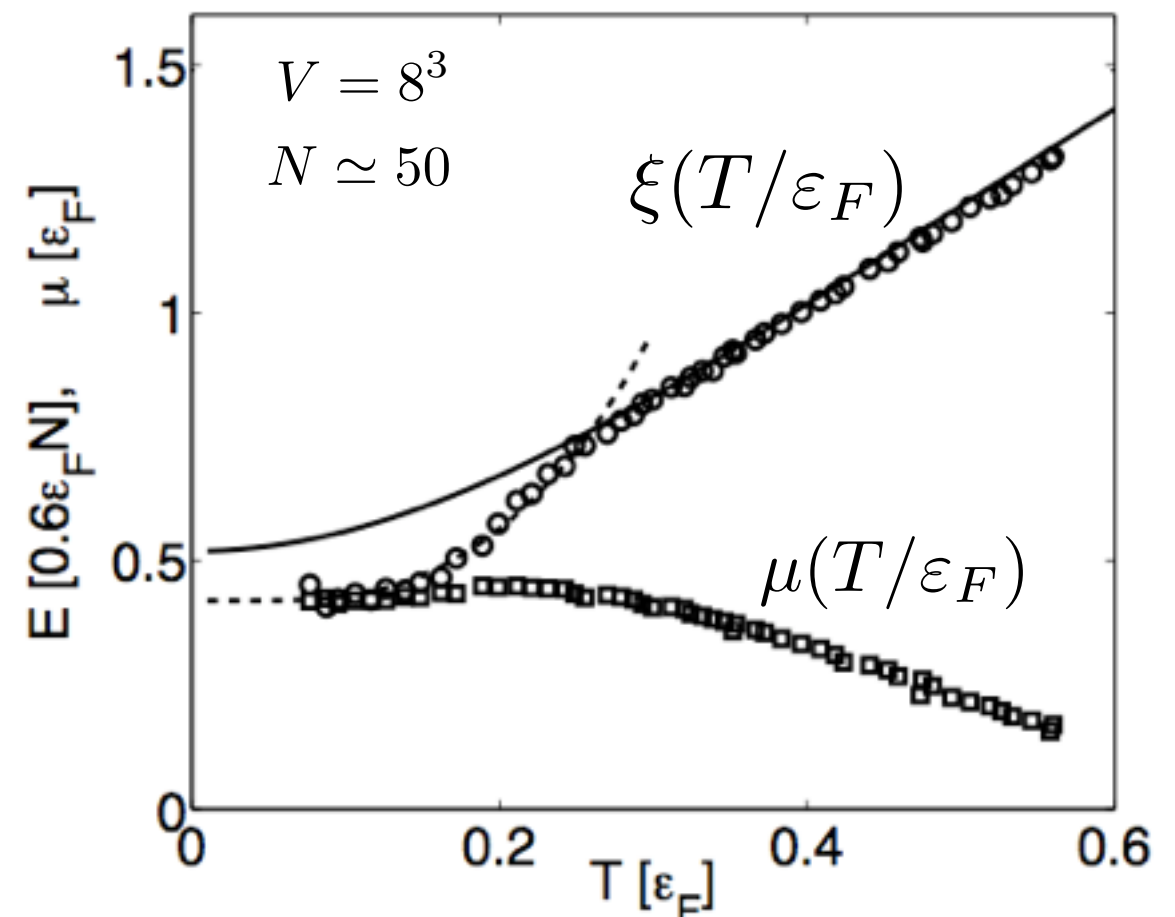
What do we know?

Equation of state

A. Bulgac, J. E. Drut, and P. Magierski,
Phys. Rev. Lett. **96**, 090404 (2006).

$$\xi(T/\varepsilon_F) \quad \mu(T/\varepsilon_F)$$

Auxiliary Field
Determinantal Monte Carlo

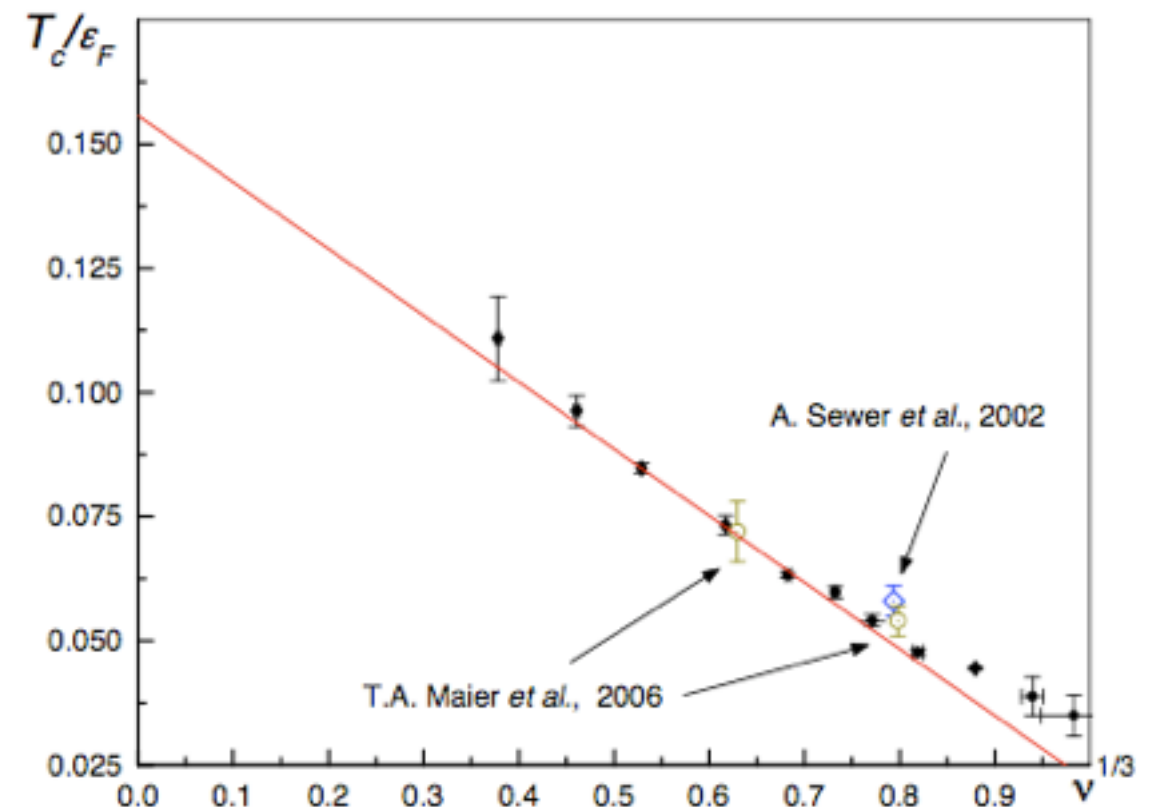


Critical temperature

E. Burovski *et al.*, Phys. Rev. Lett. **96**, 160402 (2006)

$$T_c/\varepsilon_F \simeq 0.15$$

Diagrammatic Monte Carlo



The Tan relations and the “contact”

- Momentum distribution tail

$$n_k \xrightarrow[k \rightarrow \infty]{} C/k^4$$

S. Tan, Annals of Physics **323**, 2952 (2008).

E. Braaten and L. Platter,
Phys. Rev. Lett. **100**, 205301 (2008).

- Energy relation

$$T + U = \sum_{\sigma} \int \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \left(n_{\sigma}(\mathbf{k}) - \frac{C}{k^4} \right) + \frac{\hbar^2}{4\pi m a} C$$

- Short distance density-density correlator

$$\langle n_1(\mathbf{R} + \tfrac{1}{2}\mathbf{r}) n_2(\mathbf{R} - \tfrac{1}{2}\mathbf{r}) \rangle \longrightarrow \frac{1}{16\pi^2} \left(\frac{1}{r^2} - \frac{2}{ar} \right) C(\mathbf{R})$$

- Adiabatic relation

$$C = \frac{4\pi m a^2}{\hbar^2} \frac{d\mathcal{E}}{da}$$

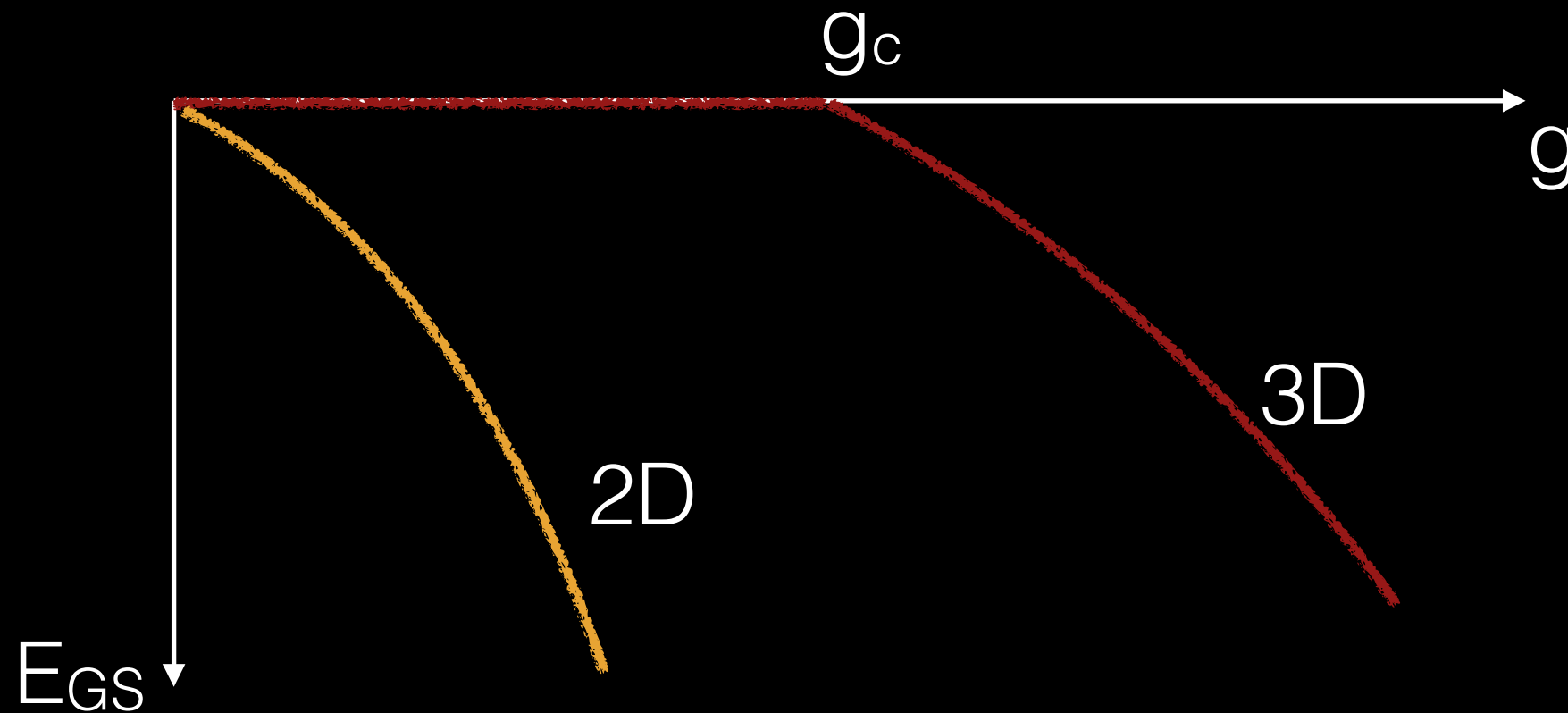
- Pressure relation

$$P = 2\mathcal{E}/3 + C/(12\pi m a)$$

What about 2D?

The two-body problem

(just qualitatively; 2D vs 3D)



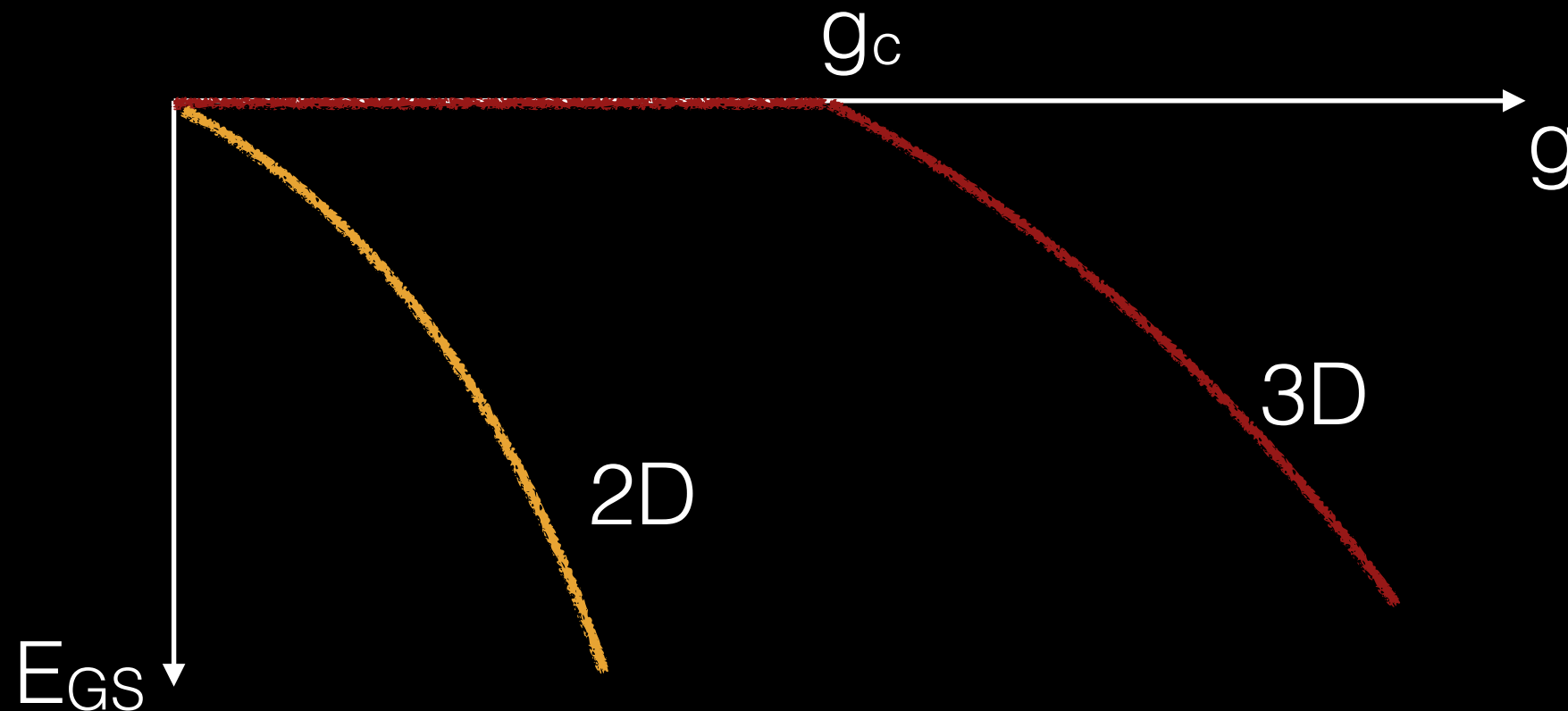
In 3D, there is a **critical coupling** (the “unitary” limit), that displays non-relativistic conformal invariance.

Bare coupling and density determine the **physical coupling**

$$\eta = 1/(k_F a)$$

The two-body problem

(just qualitatively; 2D vs 3D)



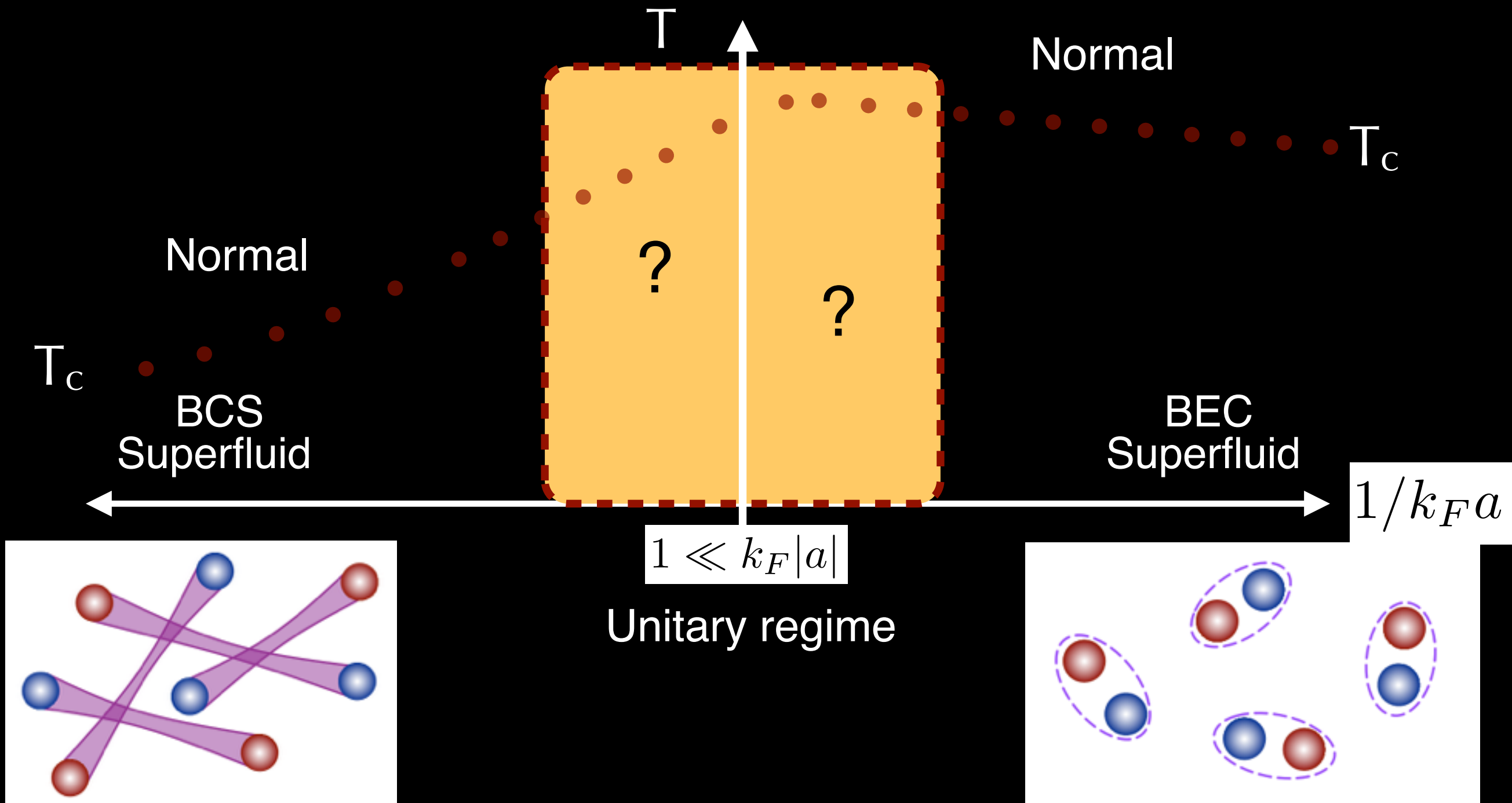
In 2D, “unitarity” **coincides** with the non-interacting limit, but there is still an interesting strongly coupled regime!

Physical coupling

$$\eta = \ln k_F a = \frac{1}{2} \ln(2\varepsilon_F / \varepsilon_B)$$

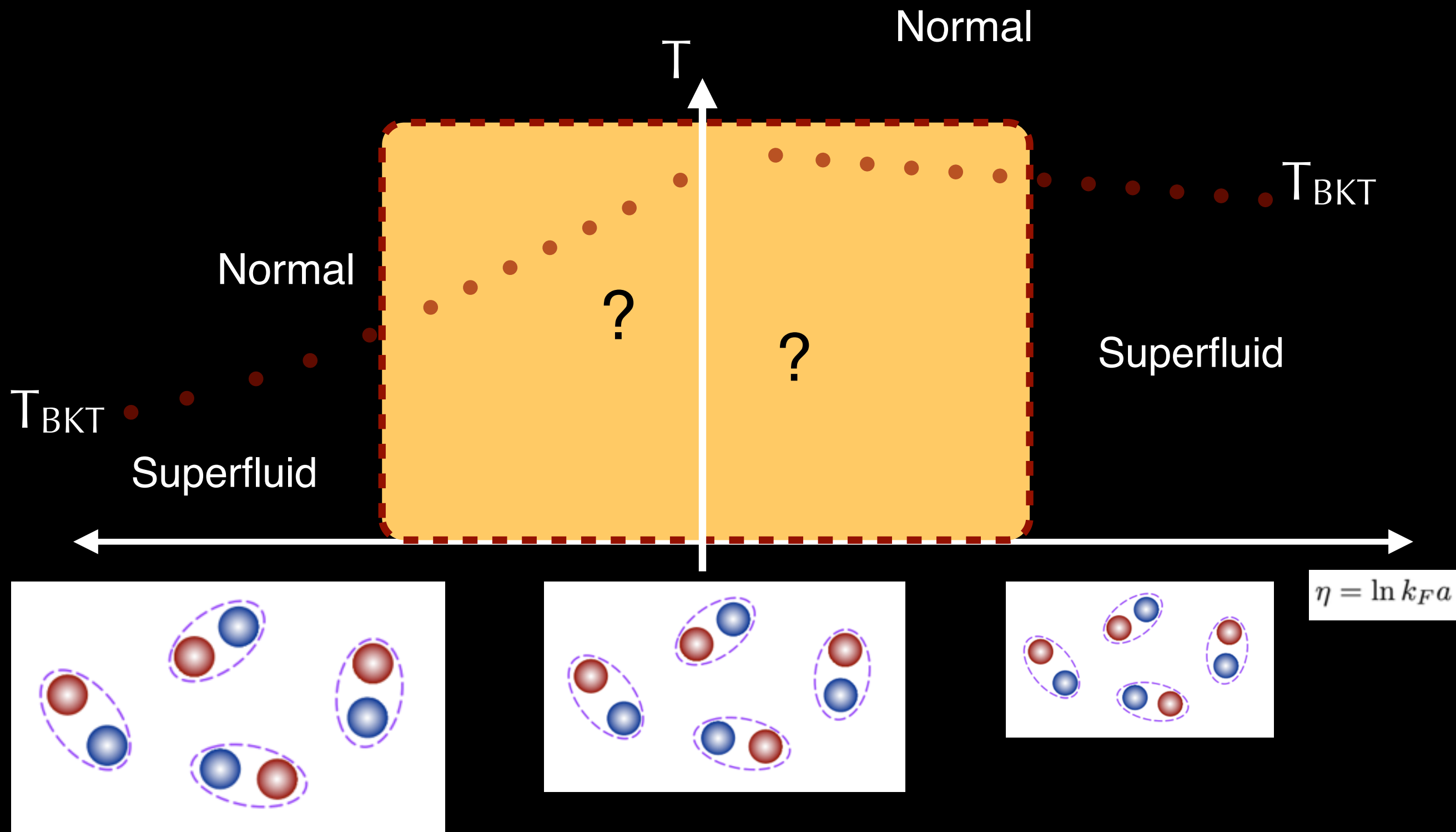
The many-body problem (for spin 1/2)

3D BCS-BEC crossover



The many-body problem (for spin 1/2)

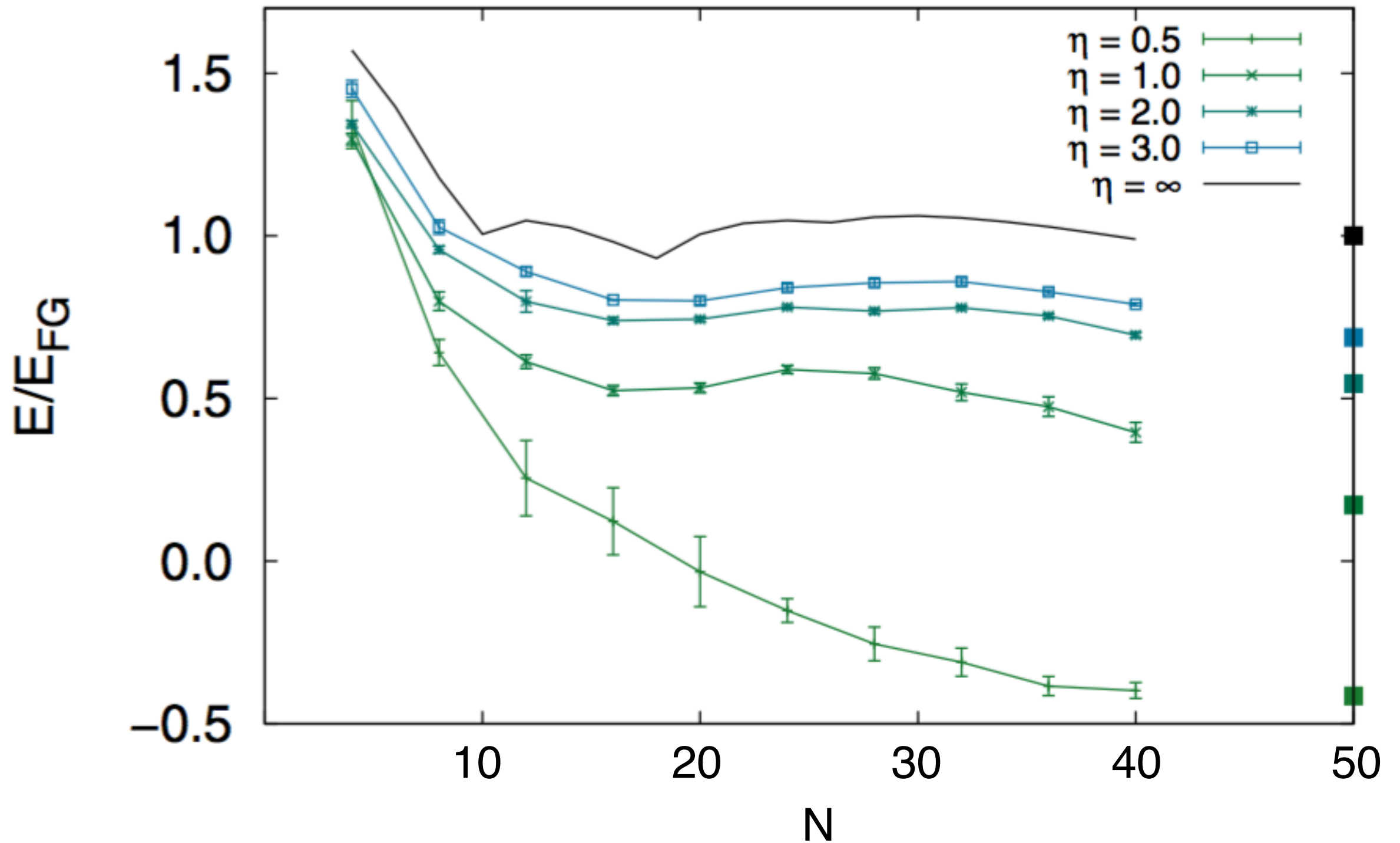
2D BCS-BEC crossover



Why 2D?

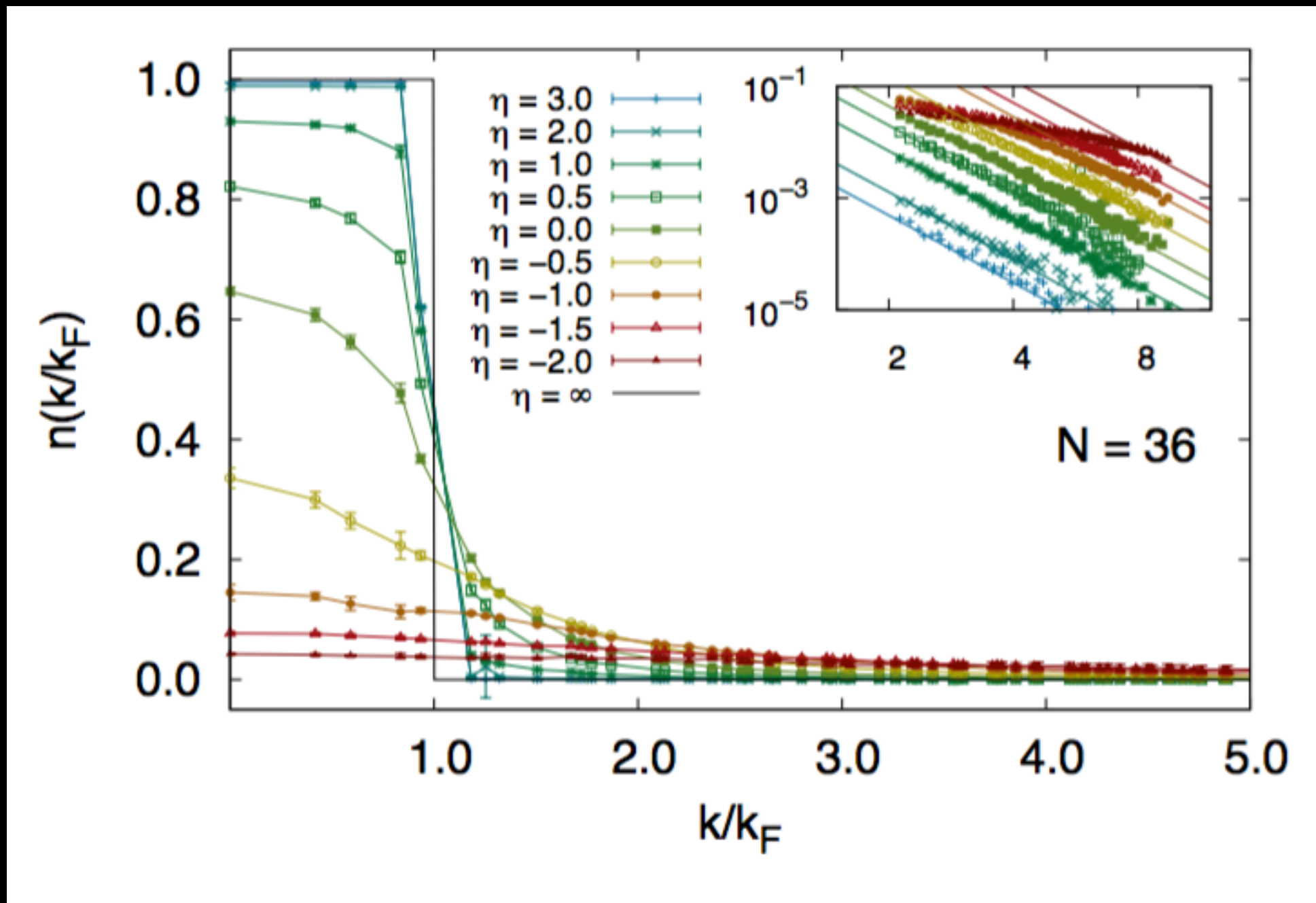
- Phase transitions are expected to be of the **BKT type** (i.e. no spontaneous symmetry breaking)
- Correlations are more important in 2D than in 3D (i.e. we do not expect mean field to be reliable at all)
- Scale invariance is an **anomalous** symmetry (as in $SU(N)$ gauge theories in 4d, i.e. a scale emerges from quantum fluctuations)

Results: Energetics

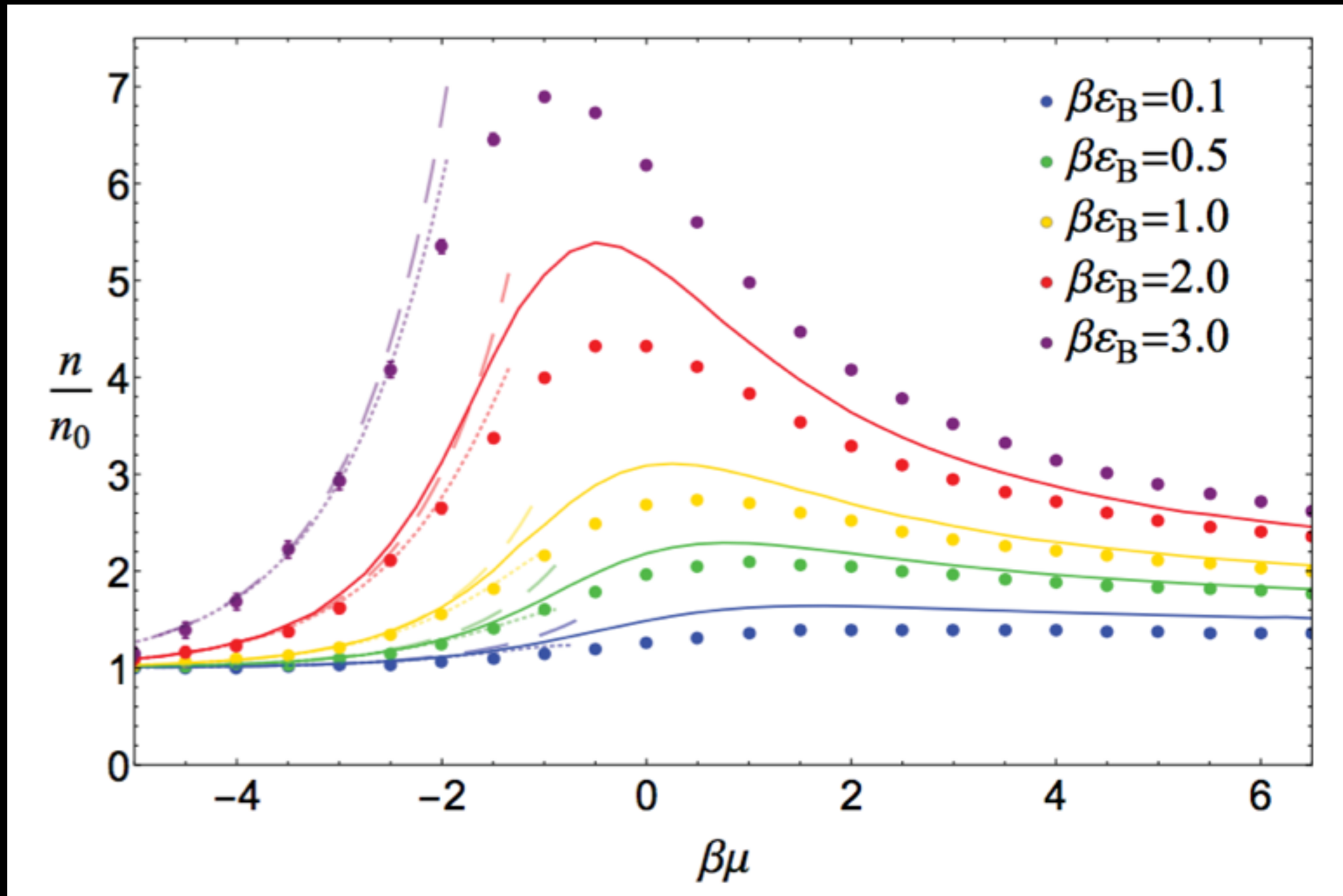


L. Rammelmüller, W. J. Porter, J. E. Drut
Phys. Rev. A **93**, 033639 (2016).

Results: Momentum distribution

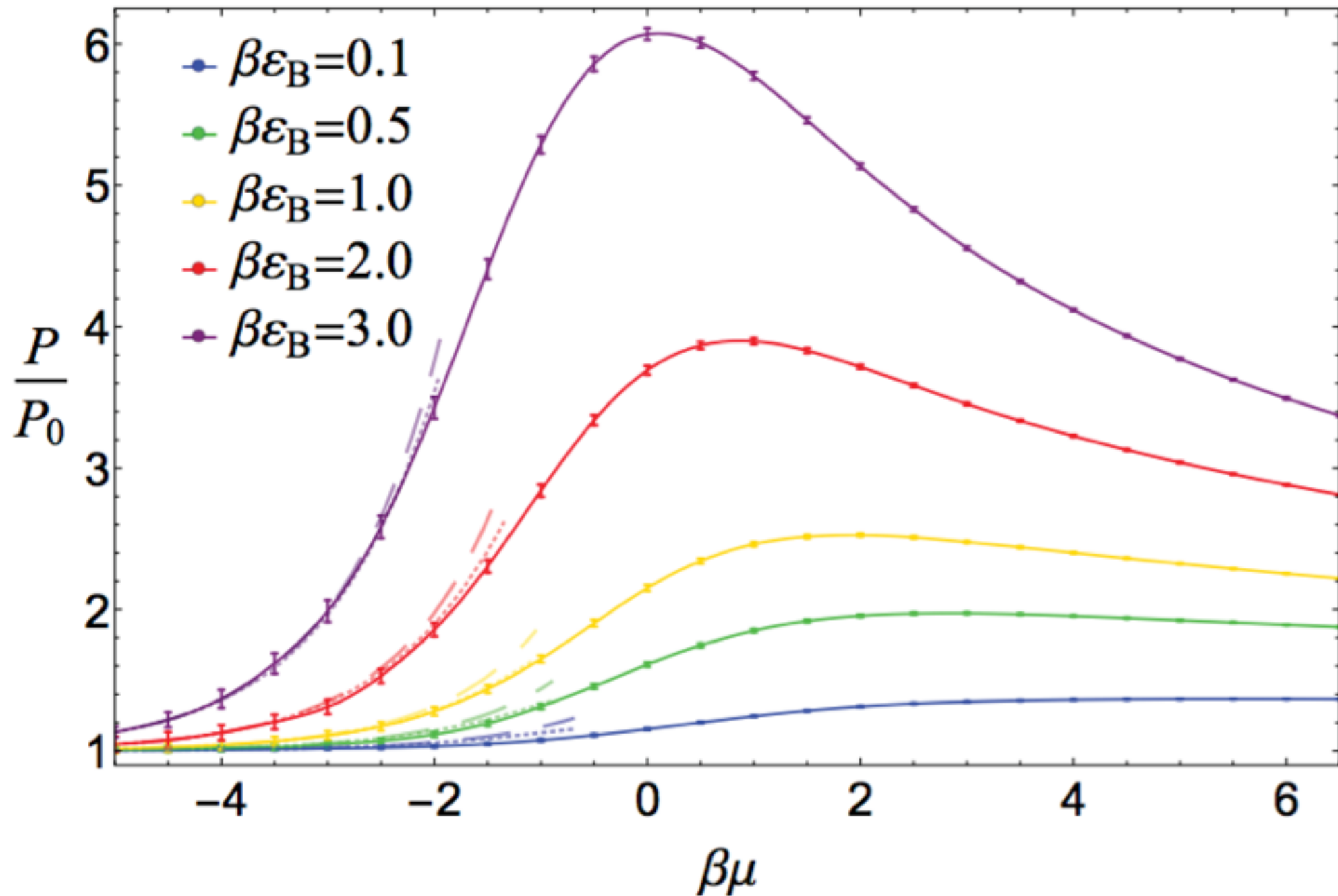


Results: Density EoS



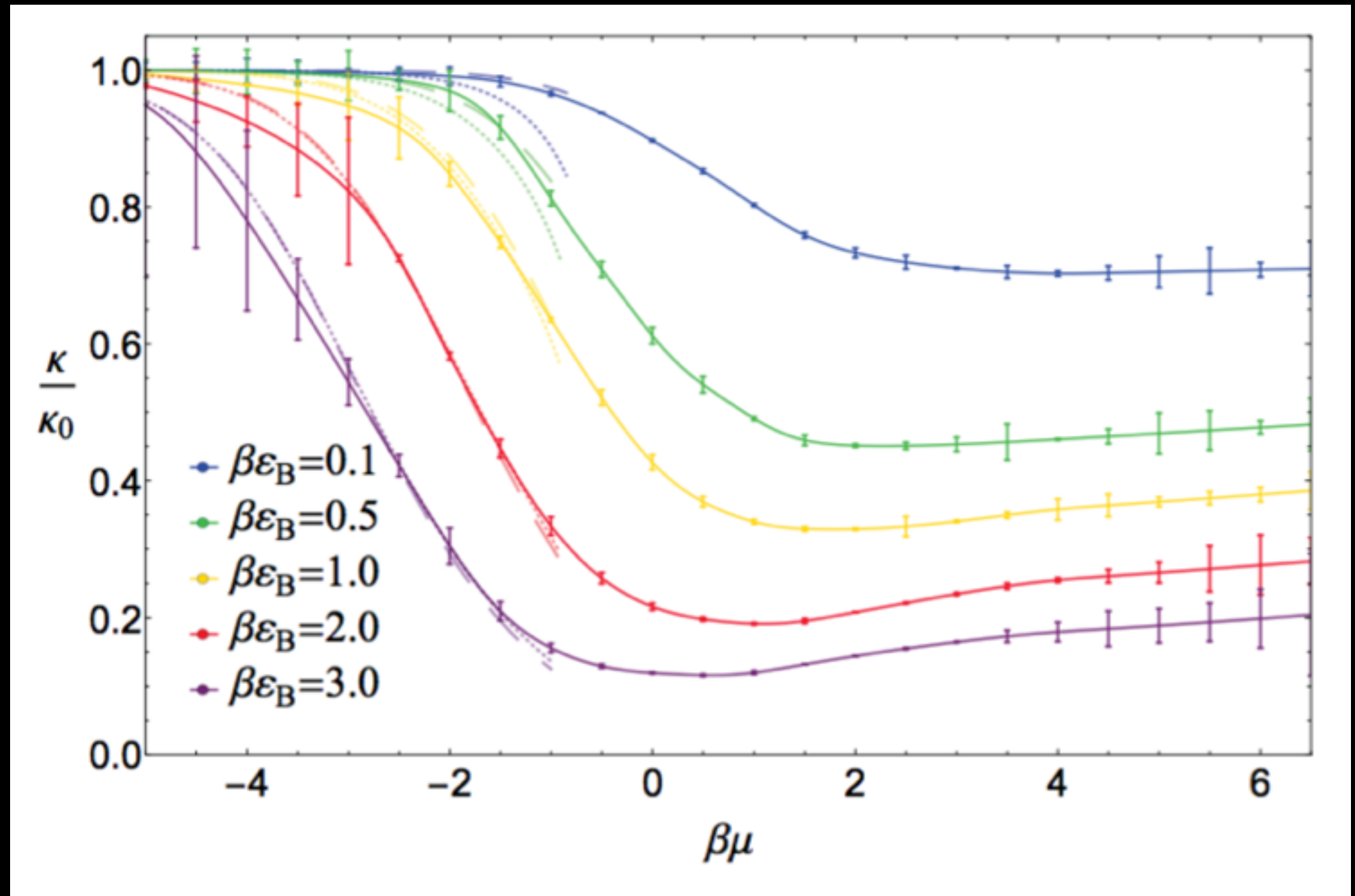
E. R. Anderson, J. E. Drut
Phys. Rev. Lett. **115**, 115301 (2015)

Results: Pressure EoS



E. R. Anderson, J. E. Drut
Phys. Rev. Lett. **115**, 115301 (2015)

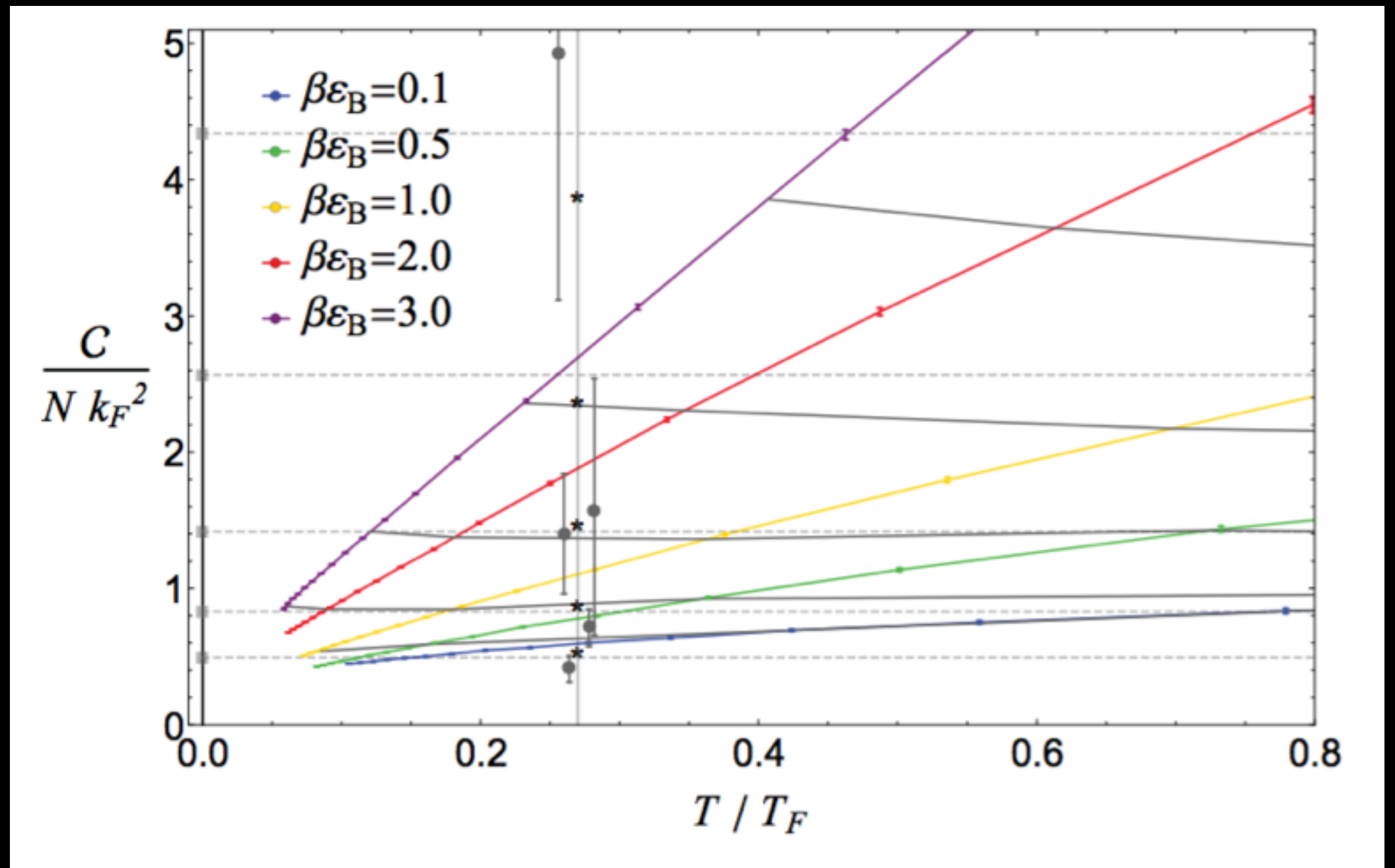
Results: Compressibility



$$\kappa = \frac{\beta}{n^2} \left. \frac{\partial n}{\partial(\beta\mu)} \right|_{\beta}$$

E. R. Anderson, J. E. Drut
Phys. Rev. Lett. **115**, 115301 (2015)

Results: Tan's contact



$$C \equiv \frac{2\pi}{\beta} \left. \frac{\partial(\beta\Omega)}{\partial \ln(a_{2D}/\lambda_T)} \right|_{T,\mu}$$

E. R. Anderson, J. E. Drut
Phys. Rev. Lett. **115**, 115301 (2015)

Summary

- Resonant Fermi gases are at the interface of several fields, most notably condensed matter, atomic, and nuclear physics, but also string theory.
- They are defined as the limit of large scattering length and short interaction range. They have no intrinsic scales.
- They are realized in ultracold atom experiments and approximately in the crust of neutron stars.
- Precise quantitative answers require numerical calculations (largely Monte Carlo, with few exceptions).
- However, there are exact analytic results (most notably the Tan relations).