Thermodynamics of the polarized unitary Fermi gas from complex Langevin

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Acknowledgements

Organizers

Group at UNC-CH (esp. Andrew Loheac)

UW & INT

TECHNISCHE UNIVERSITÄT DARMSTADT

J. Braun, L. Rammelmueller

+ Disclaimer

A sequence of papers

Thermal equation of state of polarized fermions in one dimension via complex chemical potentials
A. C. Loheac, J. Braun, J. E. Drut, D. Roscher
Phys. Rev. A **92**, 063609 (2015)

Third-order perturbative lattice and complex Langevin analyses of the finite-temperature equation of state of non-relativistic fermions in one dimension
A. C. Loheac, J. E. Drut
Phys. Rev. D **95**, 094502 (2017)

Surmounting the sign problem in non-relativistic calculations: a case study with mass-imbalanced fermions
L. Rammelmueller, W. J. Porter, J. E. Drut, J. Braun
Phys. Rev. D **96**, 094506 (2017)

Polarized fermions in one dimension: density and polarization from complex Langevin calculations, perturbation theory, and the virial expansion
A. C. Loheac, J. Braun, J. E. Drut
arXiv:1804.10257

Finite-temperature equation of state of polarized fermions at unitarity
L. Rammelmueller, A. C. Loheac, J. E. Drut, J. Braun
arXiv:1807.04664

Come to Andrew's talk! Tomorrow at 3:15pm

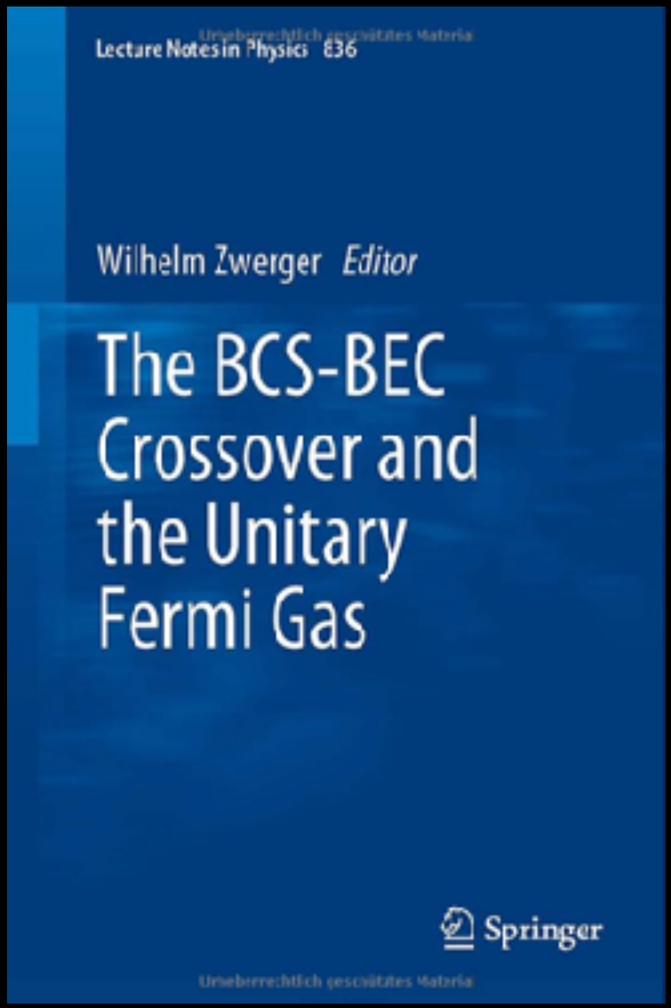
Outline

Definition, motivation, and “some” history of the UFG

Formalism and technique: Path integrals and CL

Results: Equations of state

Summary & Conclusions



Definition: Hamiltonian & scales

Two species of fermions with a contact two-body force

$$\hat{H} = \int d^3x \left[\sum_{s=\uparrow,\downarrow} \hat{\psi}_s^\dagger(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}_s(\mathbf{x}) - g \hat{n}_\uparrow(\mathbf{x}) \hat{n}_\downarrow(\mathbf{x}) \right]$$

Coupling is dimensionful $[g] = L$

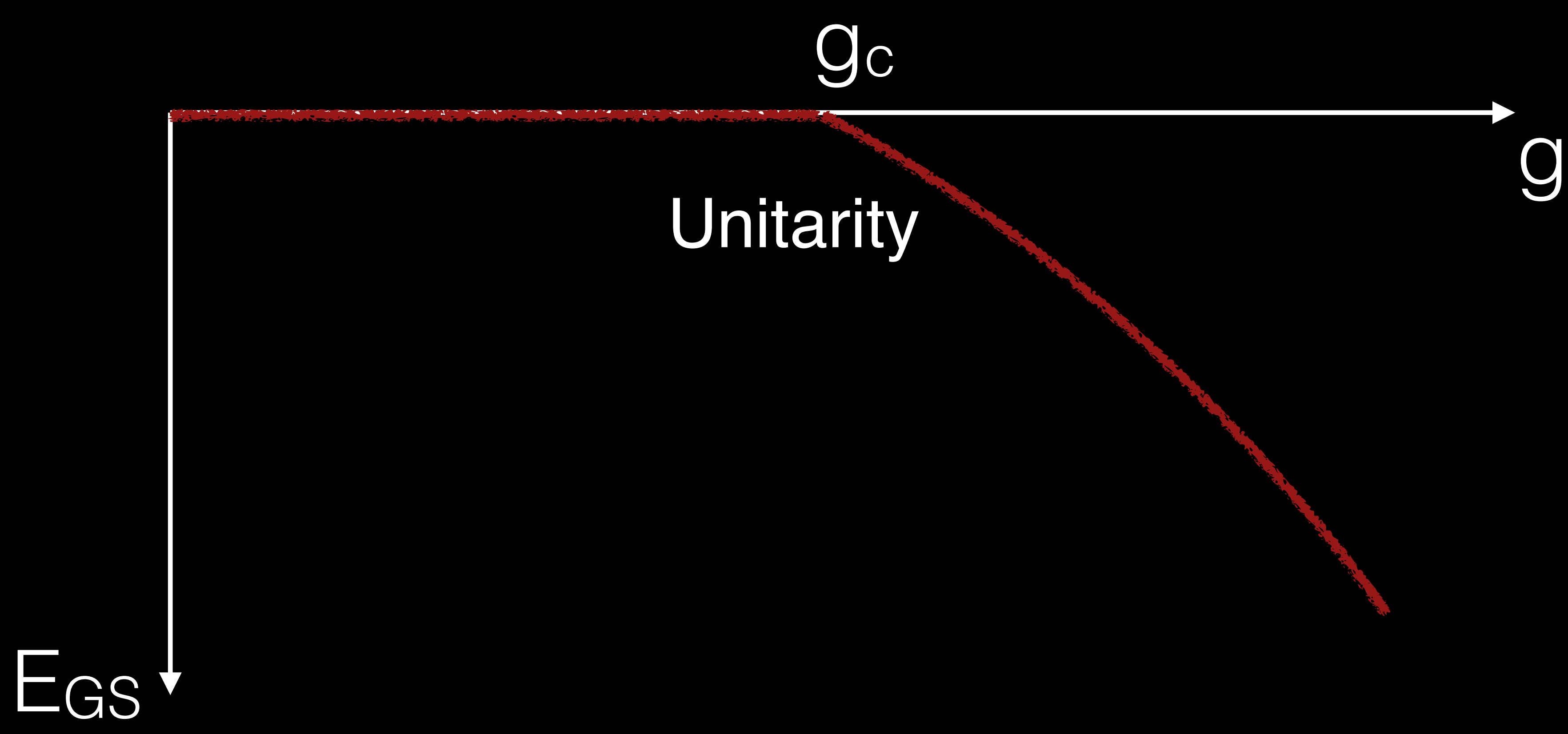
Renormalize by solving the two-body problem and relating bare coupling to scattering length

$$\frac{1}{g} = \frac{1}{L^3} \sum_k \frac{1}{2\epsilon_k - E}$$

$$p \cot \delta(p) = -\frac{1}{a} + \frac{1}{2} r_{\text{eff}} k^2 + \ldots$$

Two-body problem

Bound state appears at a critical attractive coupling



Scattering length and density determine the **physical dimensionless coupling** for the many-body problem

$$\boxed{1/(k_F a)}$$

$$k_F = (3\pi^2 n)^{1/3}$$

Scale invariance & universality

Lack of scales other than the density

$$0 \leftarrow r_0 \ll k_F^{-1} \ll a \rightarrow \infty$$

Dimensionful observables must get their units from powers of k_F

E.g. the ground-state energy

$$E = \xi E_{\mathrm{FG}}$$

$$E_{\mathrm{FG}} = \frac{3}{5} N \epsilon_F \qquad \epsilon_F = \frac{k_F^2}{2}$$

Bertsch parameter

Beyond: Tan's contact, epsilon expansion,
NR conformal invariance, sum rules, viscosities,
Efimov effect,…

Motivation: Nuclear physics

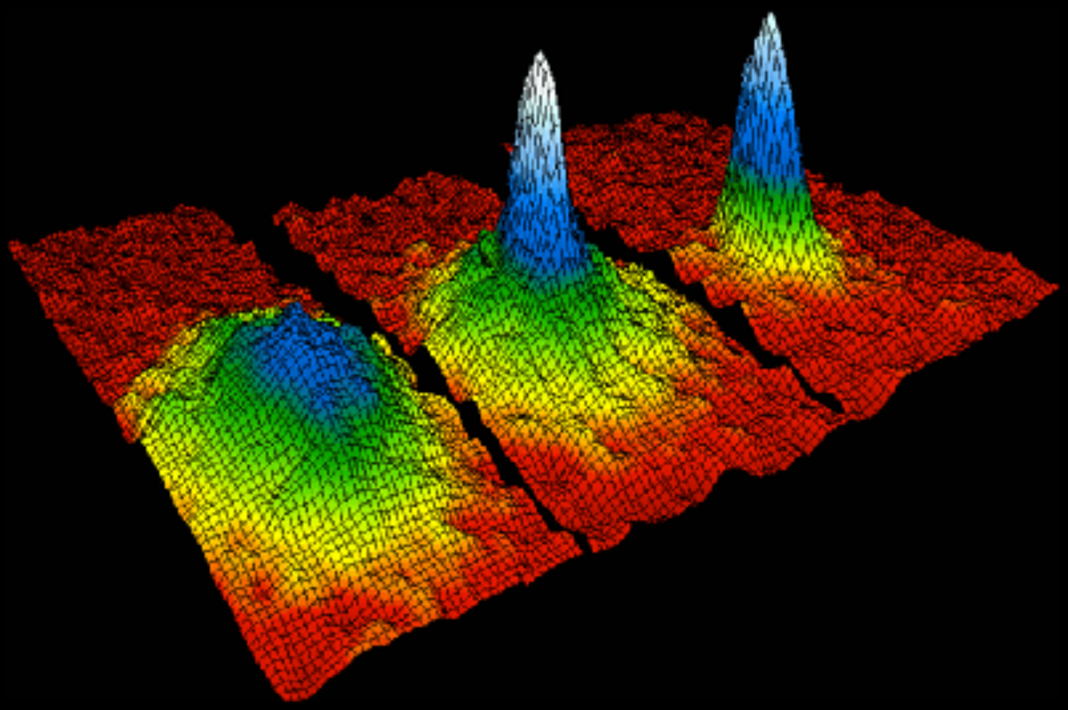
Dilute neutron matter

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

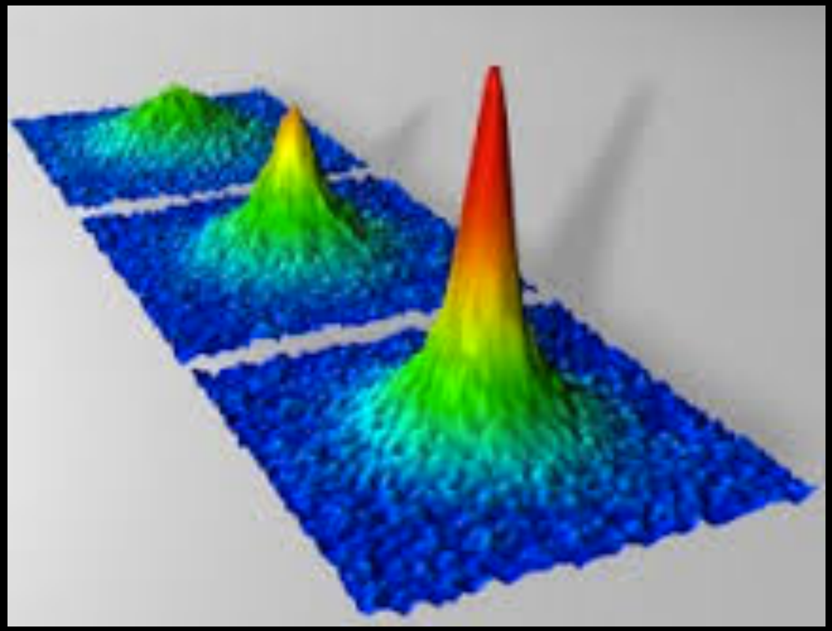
Bertsch Many-body X Challenge

Is the unitary limit stable? If so, what is the ground-state energy?

Motivation: Ultracold atoms



Bose-Einstein condensates (1995)



Fermionic condensates (2004)

Motivation: Ultracold atoms

Astonishing degree of control…

- **Temperature** (Superfluid transitions)
- Polarization (LOFF-type phases, polarons)
- **Coupling** (BEC-BCS crossover)
- Shape of external trapping potential
- Mass imbalance (different isotopes)
- **Dimension** (highly anisotropic traps & lattices)
- Bosons, fermions, mixtures: Li, K, Sr, Yb, Dy, Er,…

… and astonishing degree of measurement/detection…

- Thermodynamics
- Phase transitions
- Collective modes
- Spin response
- Hydrodynamic response
- Entanglement
- Time-dependent dynamics
- …

A bit of history…

First thermodynamic measurements

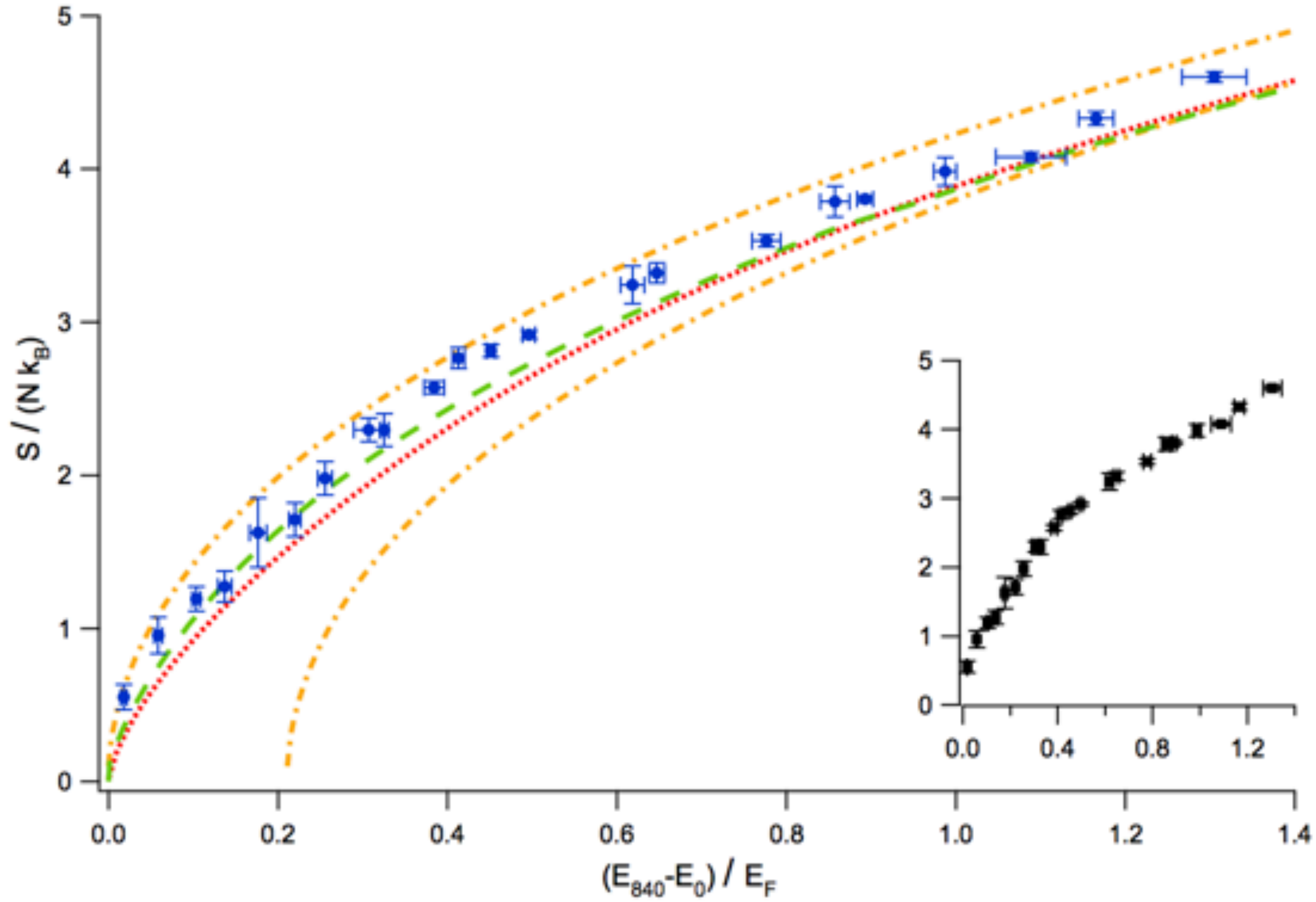


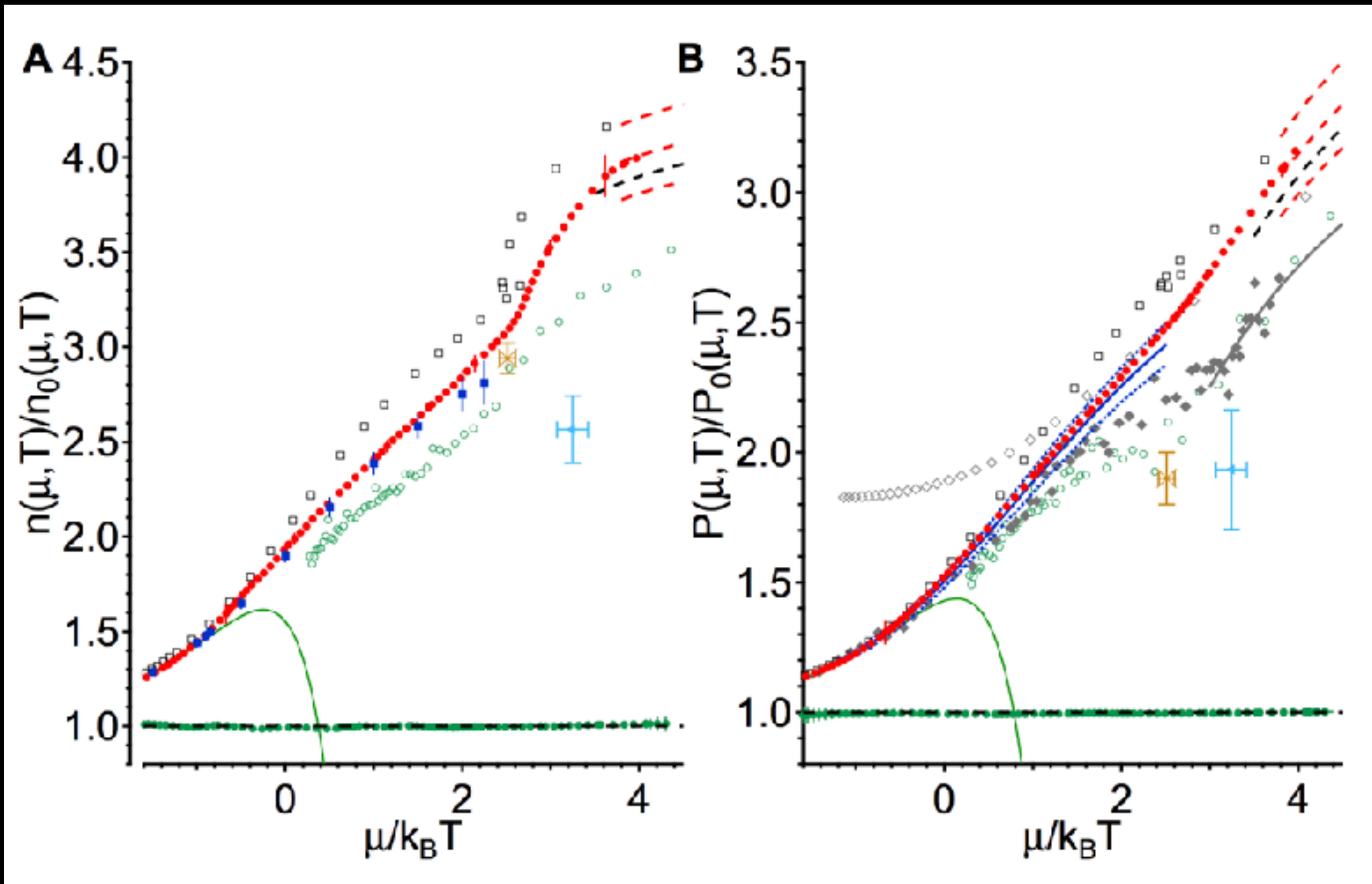
Figure 2: Measured entropy of a strongly interacting Fermi gas at 840 G versus its total energy (blue dots). The entropy is estimated from the measured cloud size at 1200 G after an adiabatic sweep of the magnetic field from 840 G. Lower orange dot-dashed curve– ideal gas entropy; Upper orange dot-dashed curve– ideal gas entropy with the ground state energy shifted to E_0; Red dots– pseudogap theory (*25*); Green dashes– quantum Monte Carlo prediction (*32*). Inset– entropy versus energy data showing knee at $E_c - E_0 = 0.41\, E_F$.

L. Luo et al
PRL **98**, 080402 (2007)

A bit of history…

“Best” experiments

M. Ku et al
Science **335**, 563 (2012)



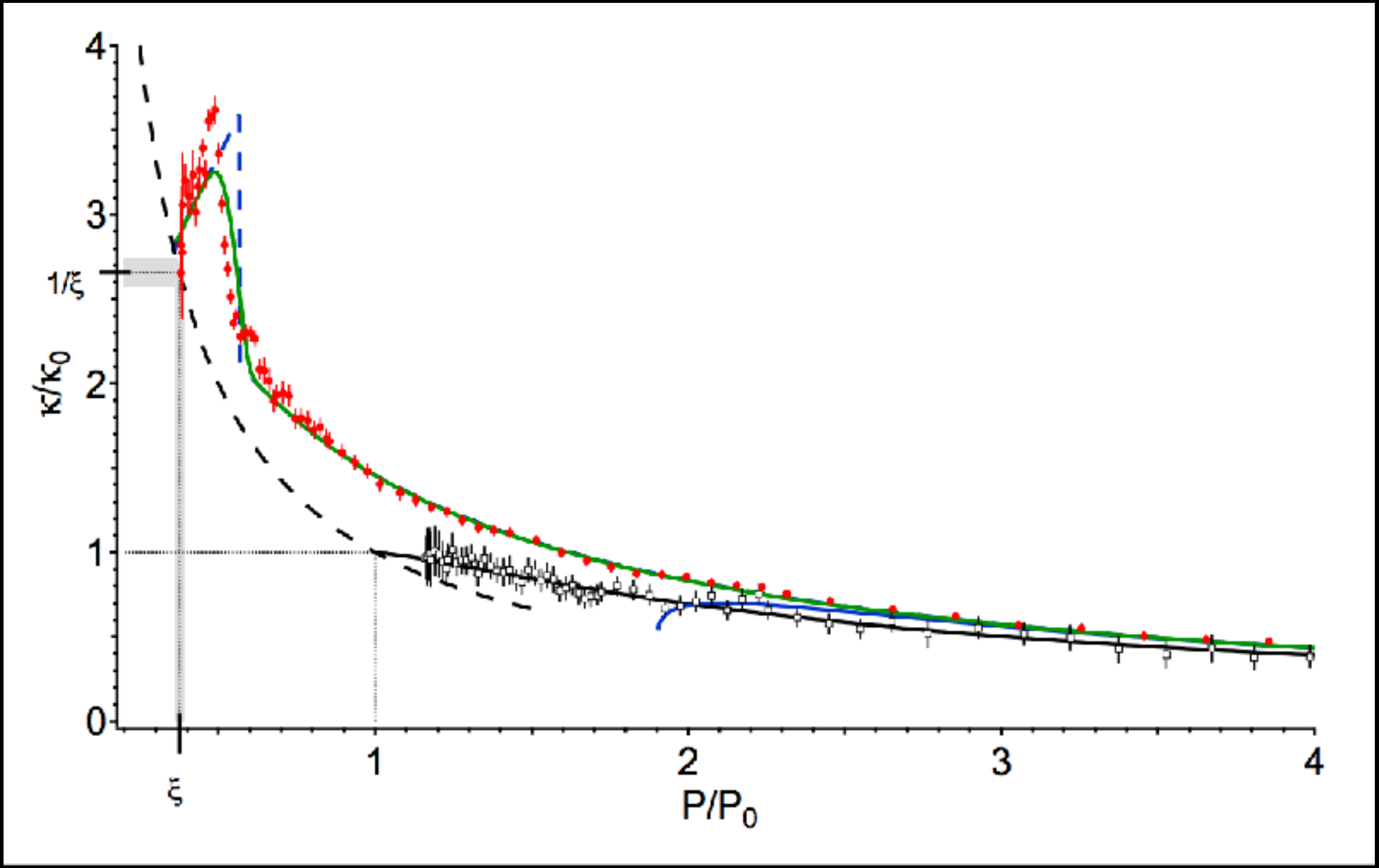
Density EoS

Pressure EoS

A bit of history…

"Best" experiments

M. Ku et al
Science **335**, 563 (2012)

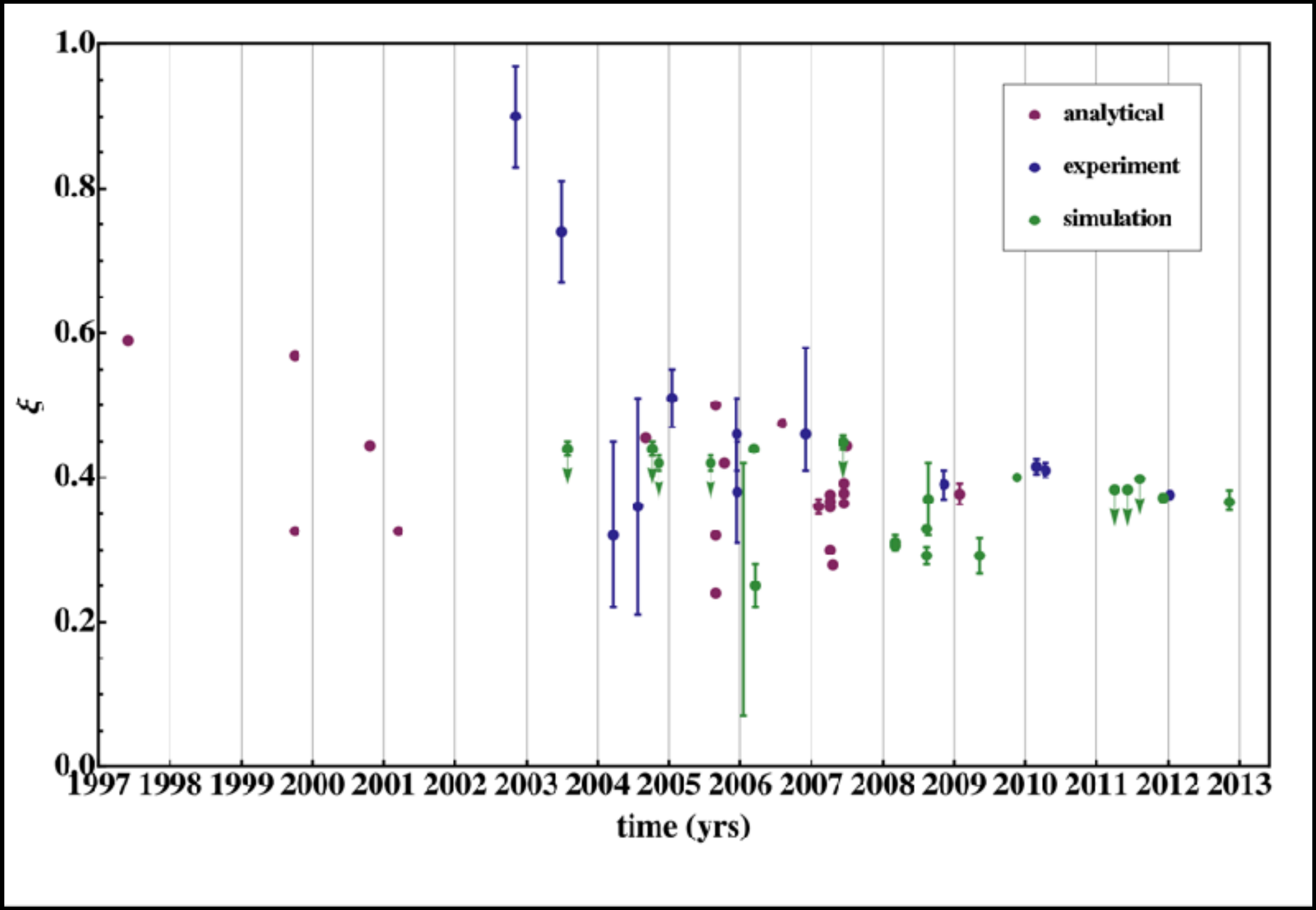


Pressure-Compressibility plot

A bit of history…

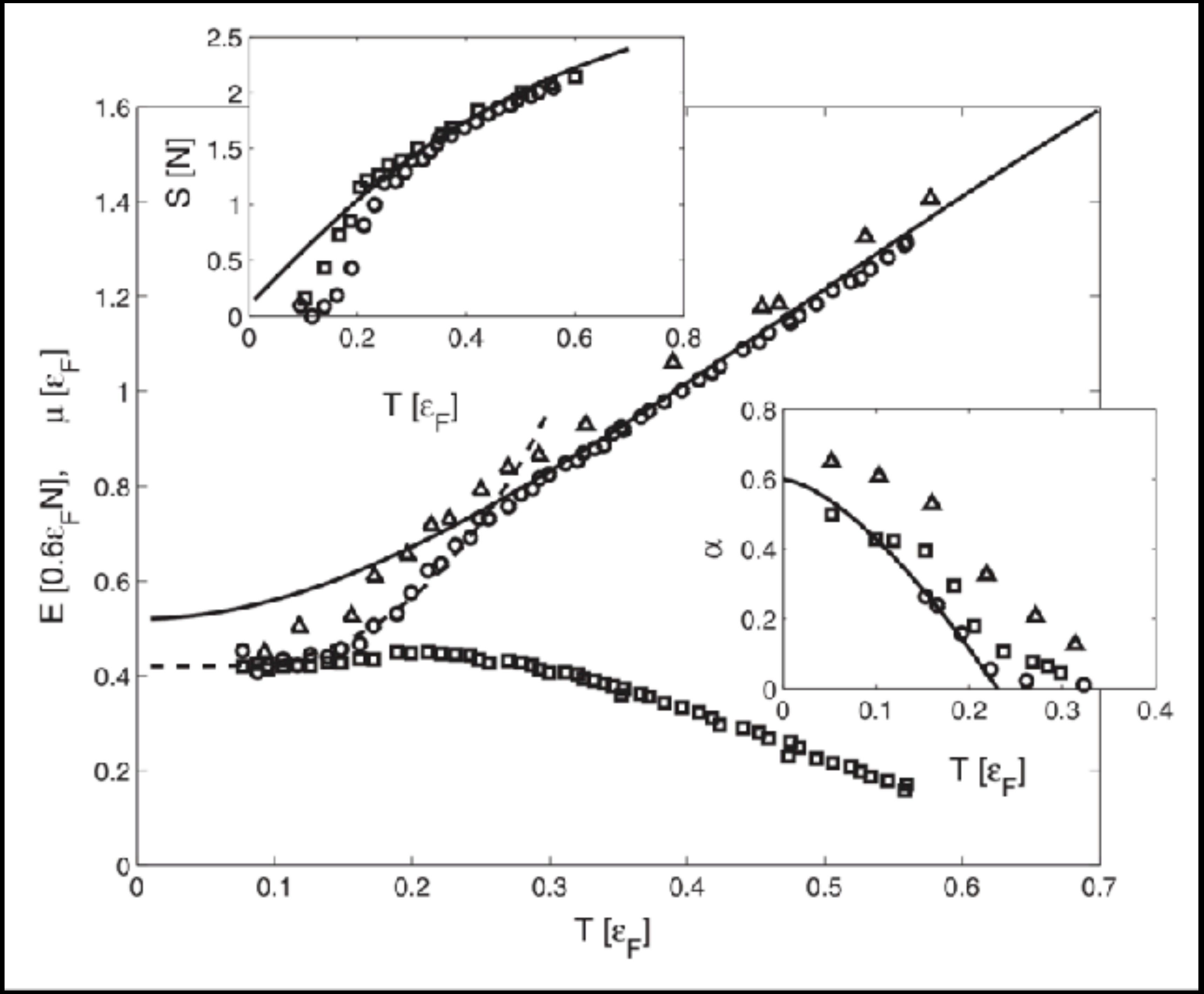
On the theory side: ground-state energy
The Bertsch parameter as a function of time

Endres et al
PRA **87**, 023615 (2013)



A bit of history…

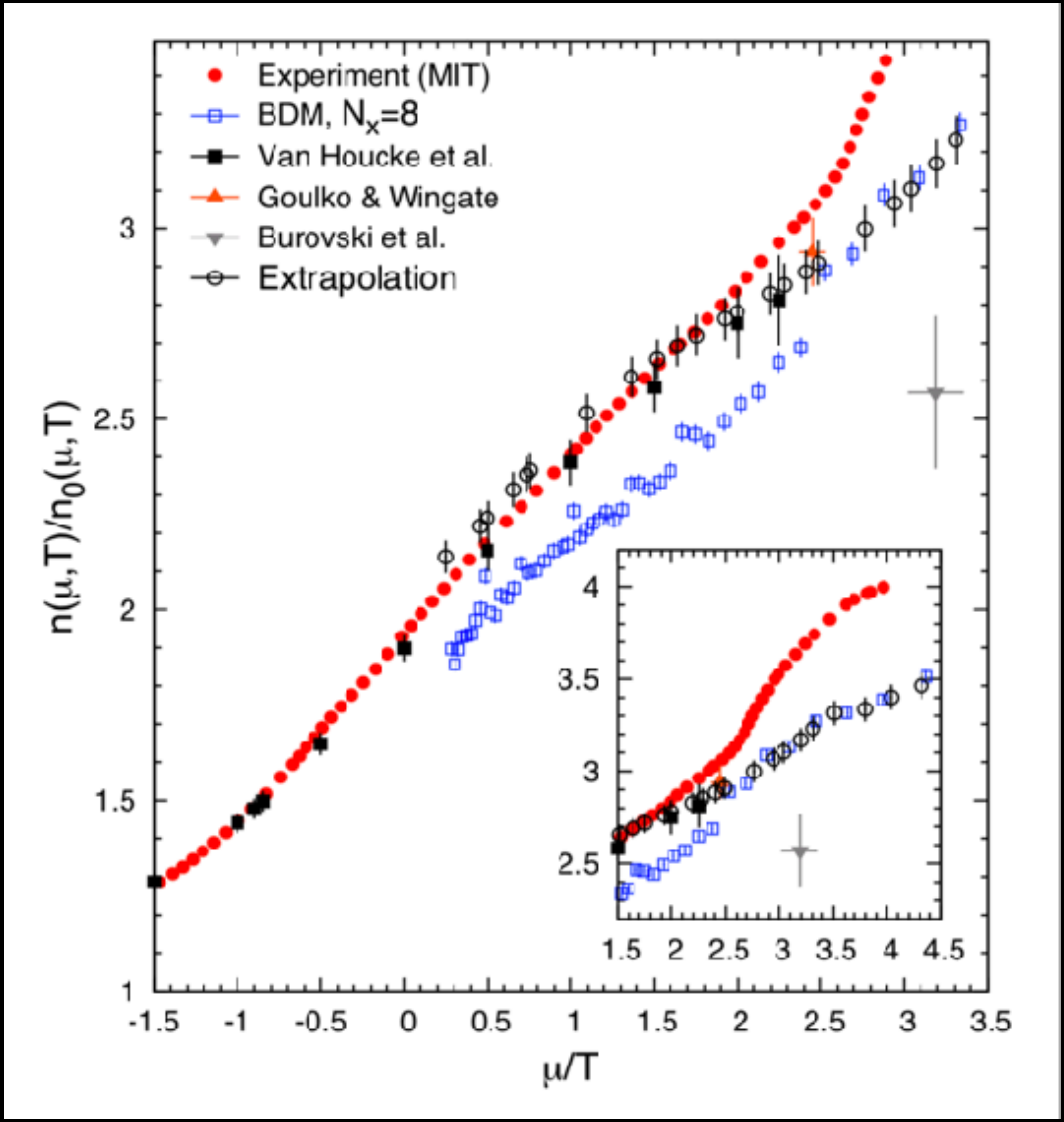
More on the theory side: finite temperature EoS



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

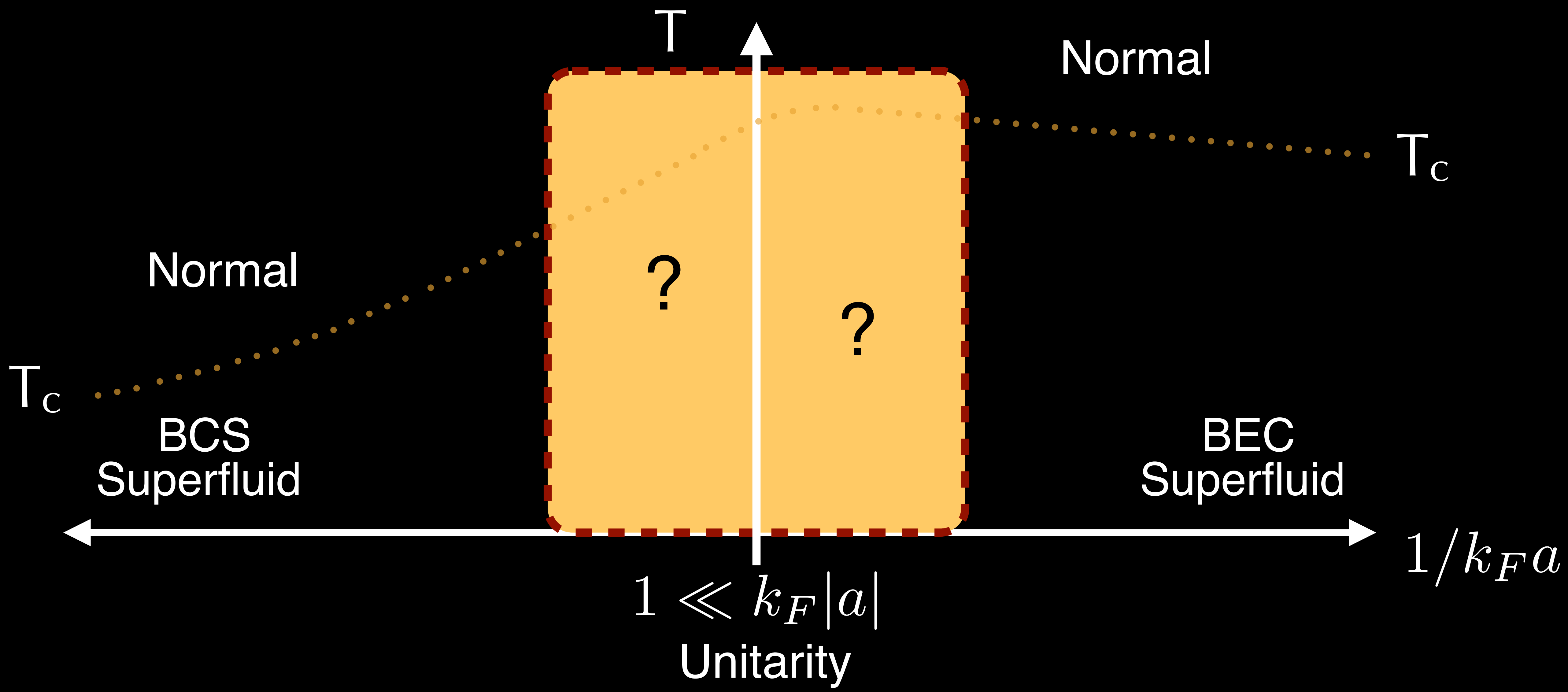
A bit of history…

…and an update



Drut, Lähde, Wlazłowski, Magierski
PRA **85**, 051601(R) (2012)

The 3D BCS-BEC crossover



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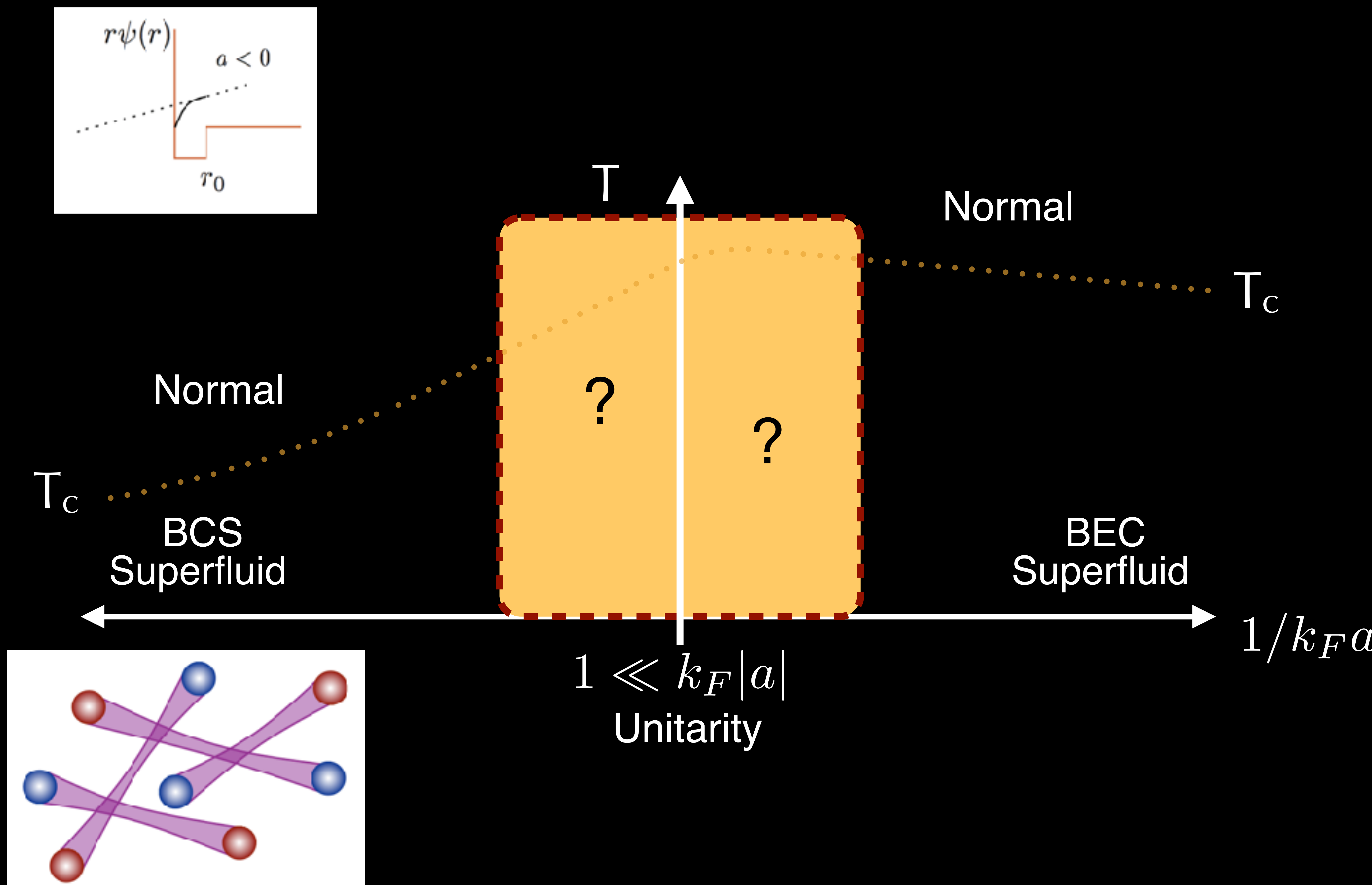

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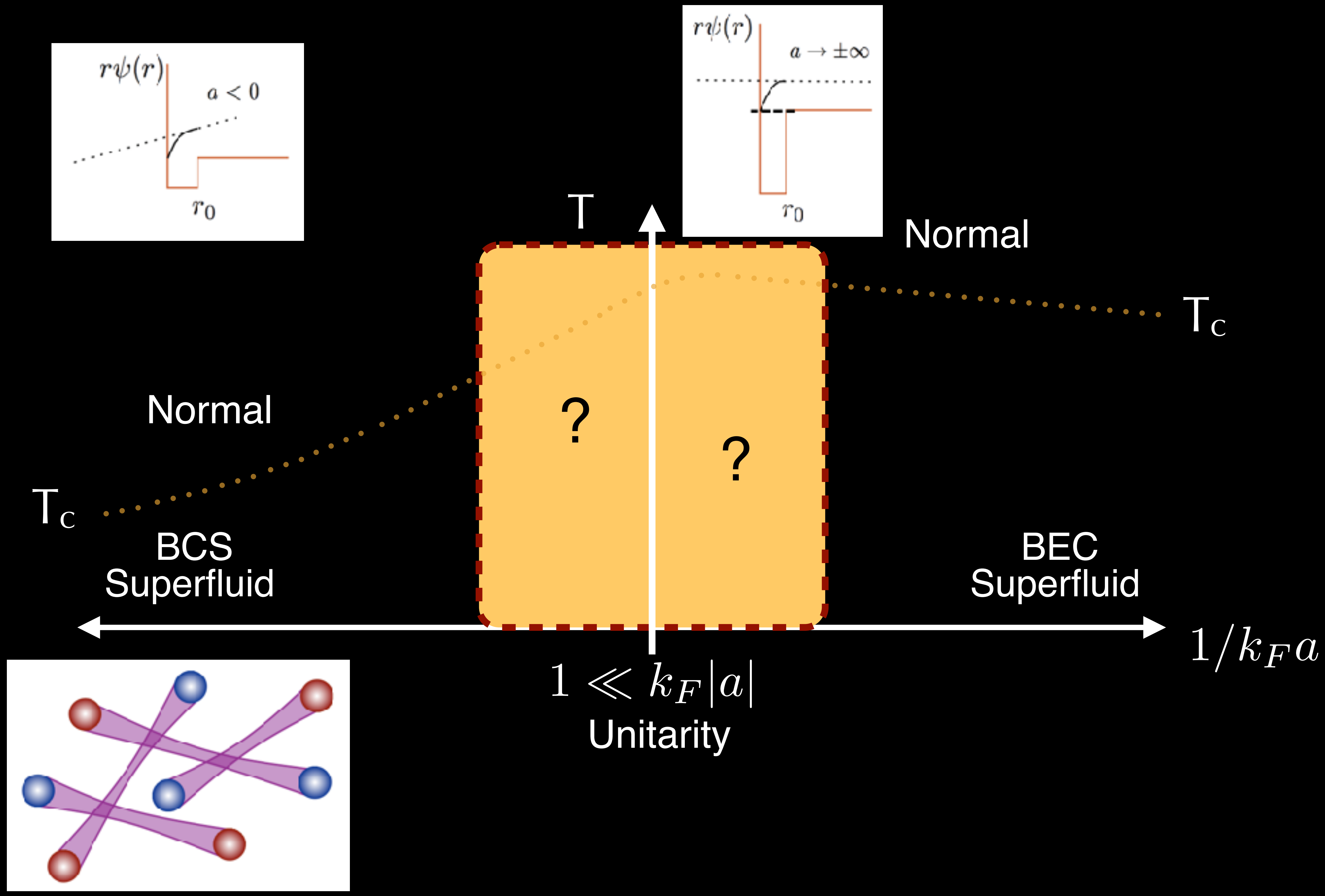
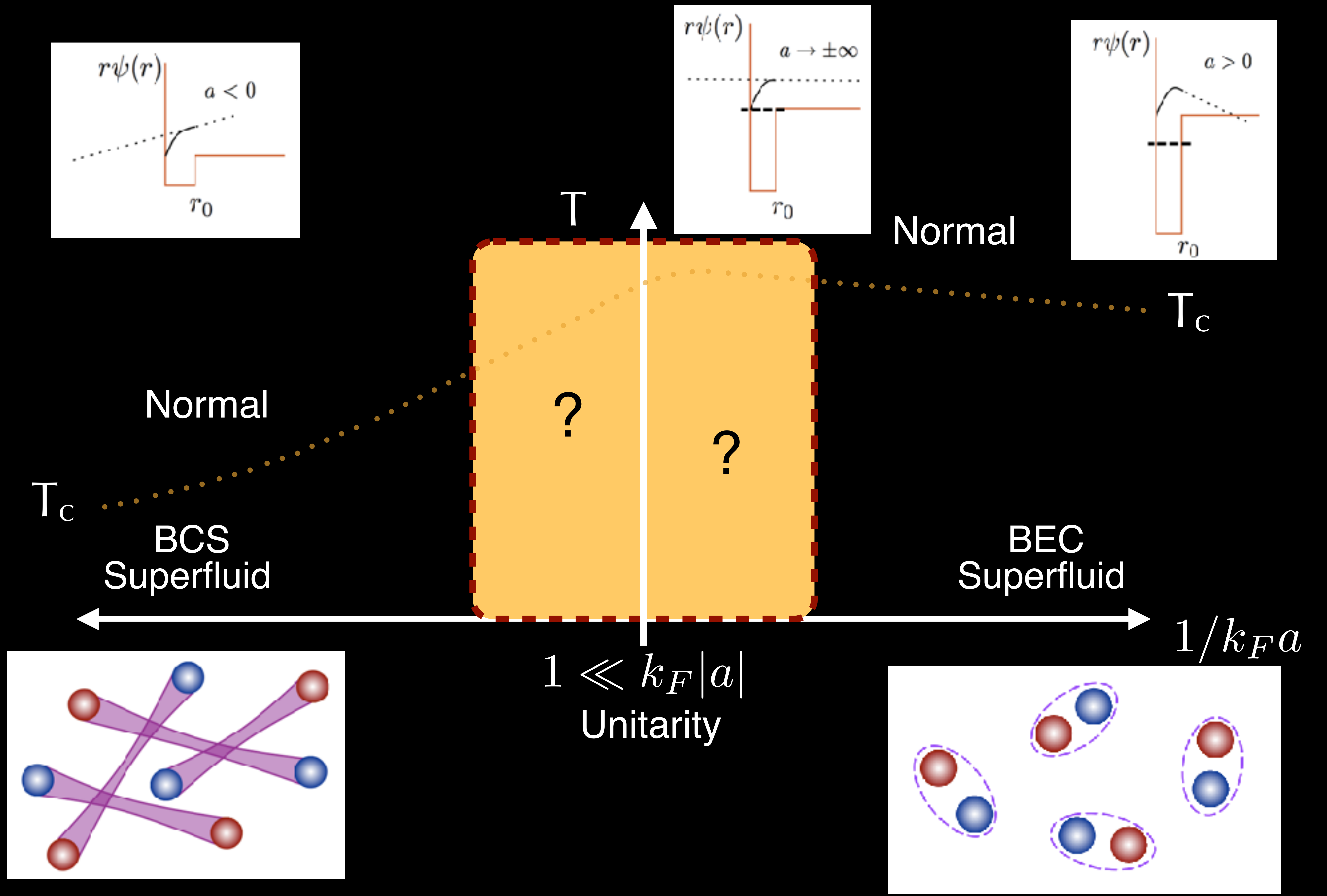
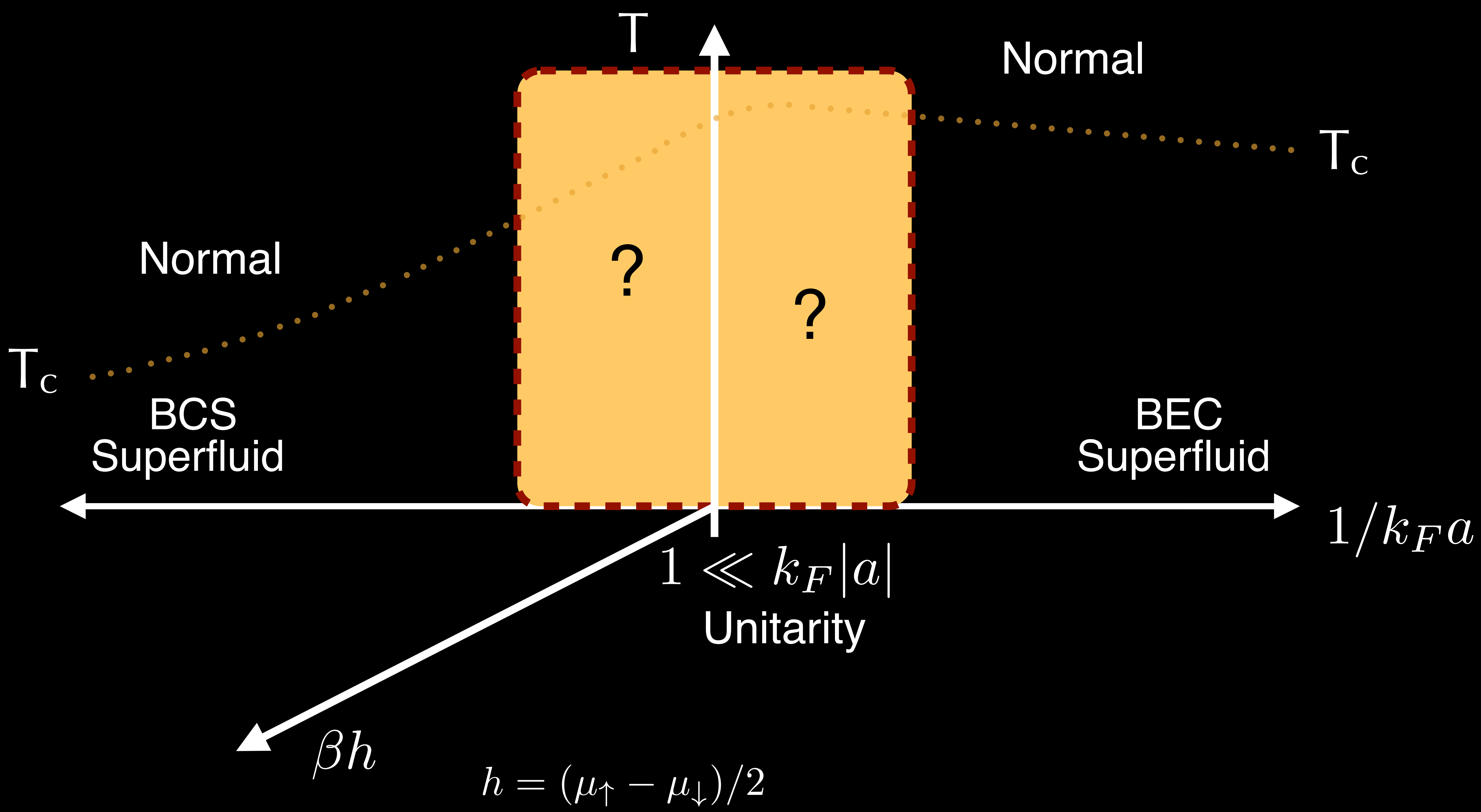


The 3D BCS-BEC crossover

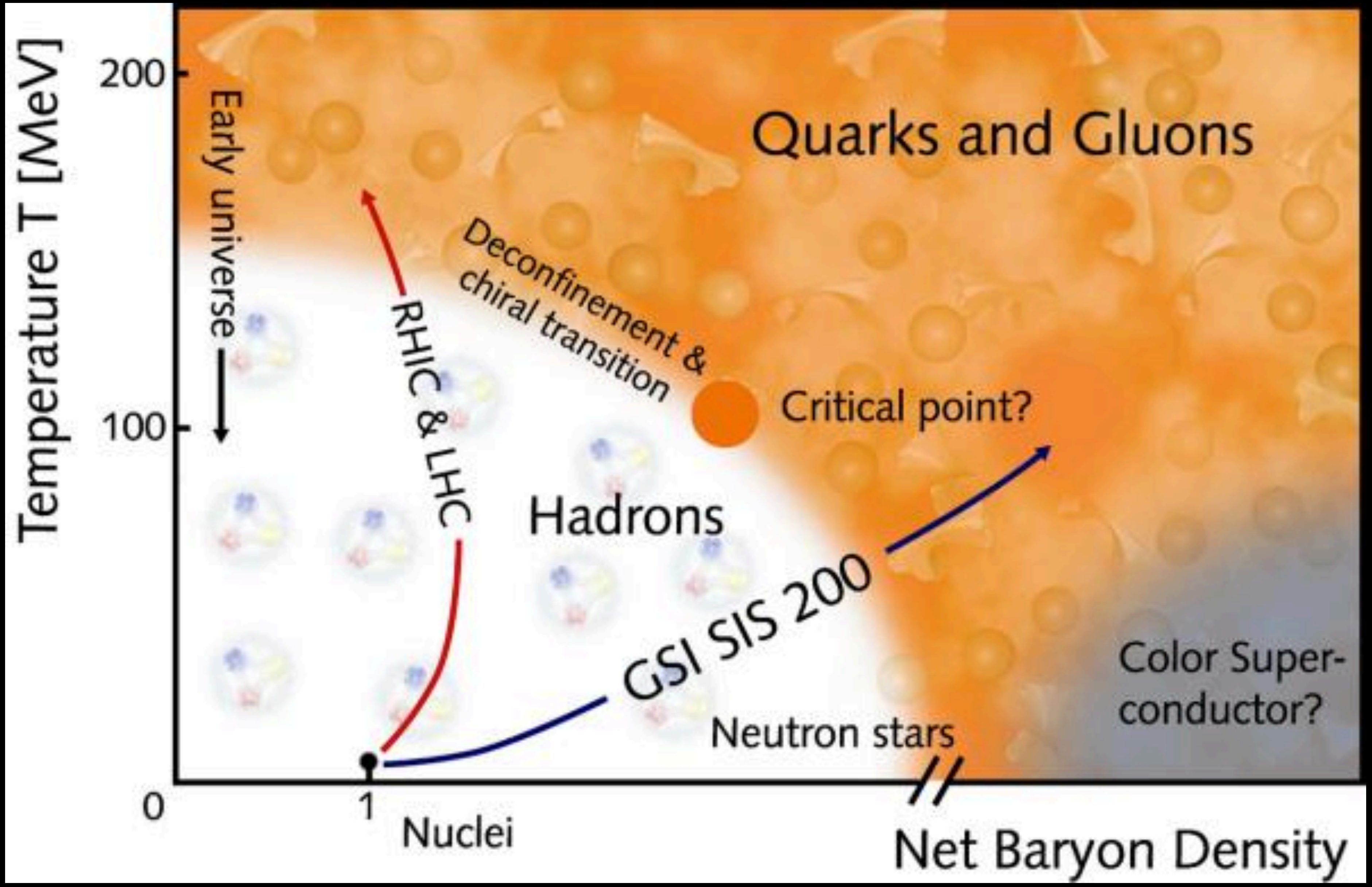


Objective

Explore the thermodynamics and phase transitions of the unitary Fermi gas at finite polarization.



Btw: also interesting for QCD



Many-body formalism

Path integral formulation

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu_\uparrow \hat{N}_\uparrow - \mu_\downarrow \hat{N}_\downarrow)}\right]$$

Many-body formalism

Path integral formulation

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Suzuki-Trotter
Hubbard-Stratonovich

$$\mathcal{Z} = \int \mathcal{D}\sigma \; \det M_\uparrow[\sigma] \det M_\downarrow[\sigma] \; \exp\left(-S[\sigma]\right)$$

Many-body formalism

Path integral formulation

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Suzuki-Trotter
Hubbard-Stratonovich

$$\mathcal{Z} = \int \mathcal{D}\sigma \; \det M_\uparrow[\sigma] \det M_\downarrow[\sigma] \; \exp\left(-S[\sigma]\right)$$

Big problem:
Conventional QMC approaches require a constant-sign integrand

Methods: Stochastic quantization

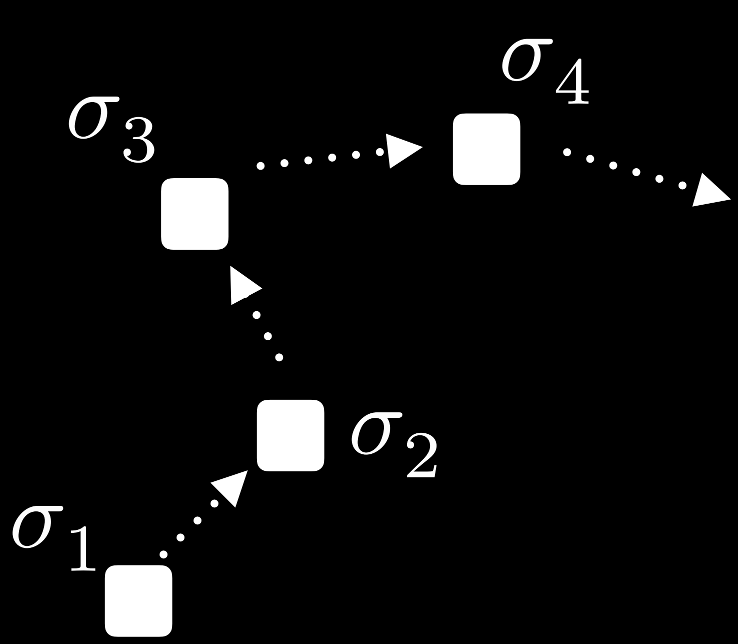
Langevin approach: use random force field to explore configuration space

$$\dot{\sigma} = -\frac{\delta S}{\delta \sigma} + \eta$$

$$S[\sigma] = -\ln P[\sigma]$$

$$P[\sigma] = \det M[\sigma] e^{-S_g[\sigma]}$$

Computational sampling



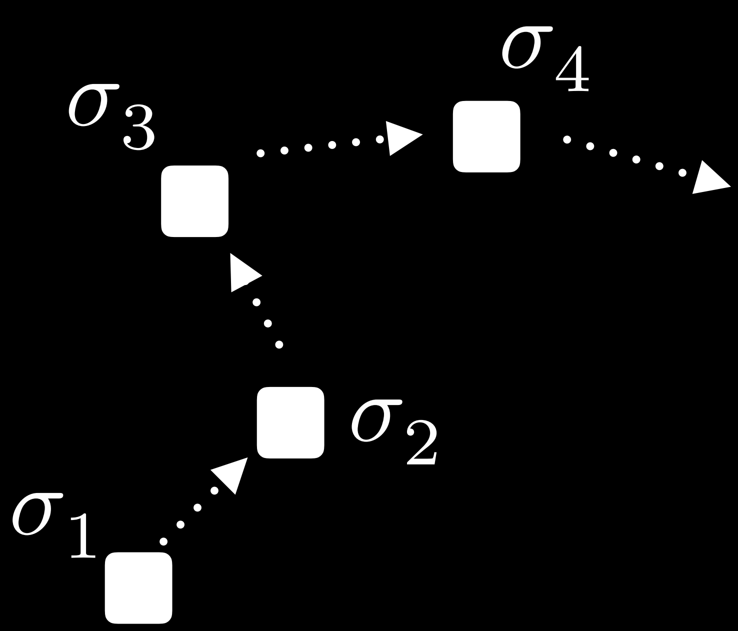
Langevin algorithm:
Sample configuration space using random noise (closely related to hybrid Monte Carlo)

Methods: Complex Langevin

Stochastic quantization gone complex

$$\dot{\sigma} = -\frac{\delta S}{\delta \sigma} + \eta \quad \Rightarrow \quad \left[\begin{array}{l} \dot{\sigma}_R = -\mathrm{Re}\left[\frac{\delta S}{\delta \sigma}\right] + \eta \\ \dot{\sigma}_I = -\mathrm{Im}\left[\frac{\delta S}{\delta \sigma}\right] \end{array} \right.$$

Computational sampling



Complex Langevin algorithm:
Make your field complex
Sample configuration space using random noise

Methods: Complex Langevin

Problems

Numerical instabilities

Uncontrolled excursions into the complex plane

Singular drift

Complex Langevin method: When can it be trusted?

Gert Aarts, Erhard Seiler, and Ion-Olimpiu Stamatescu
Phys. Rev. D **81**, 054508 – Published 22 March 2010

Results

First, a few definitions:

$$h = (\mu_\uparrow - \mu_\downarrow)/2$$

$$\mu = (\mu_\uparrow + \mu_\downarrow)/2$$

n_0 : noninteracting, unpolarized density

Lattice parameters:

$$N_x = 7, 9, 11$$

$$N_\tau = 160$$

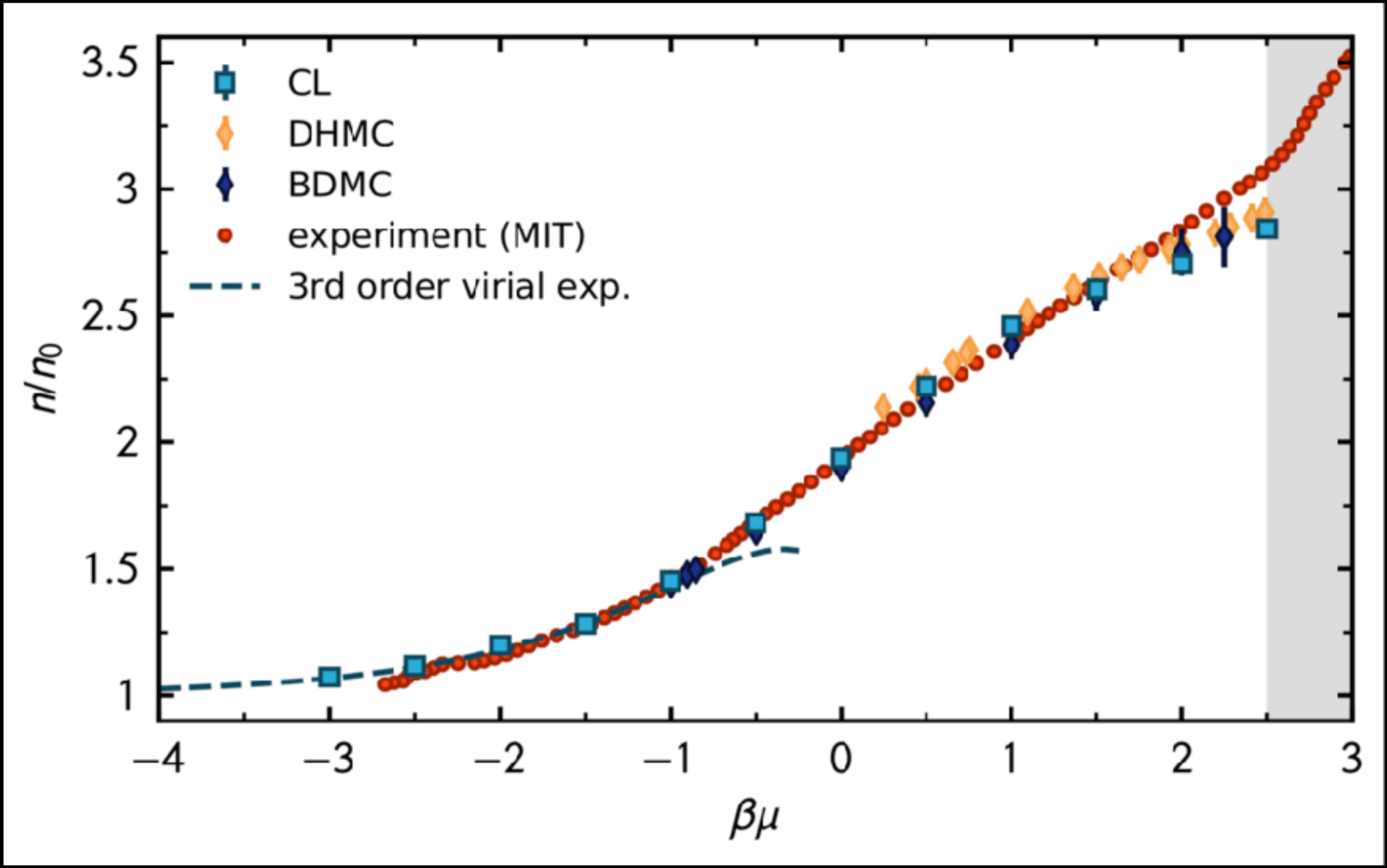
Continuum limit

$$1 = \ell \ll \lambda_T, \lambda_F \ll L = N_x \ell$$

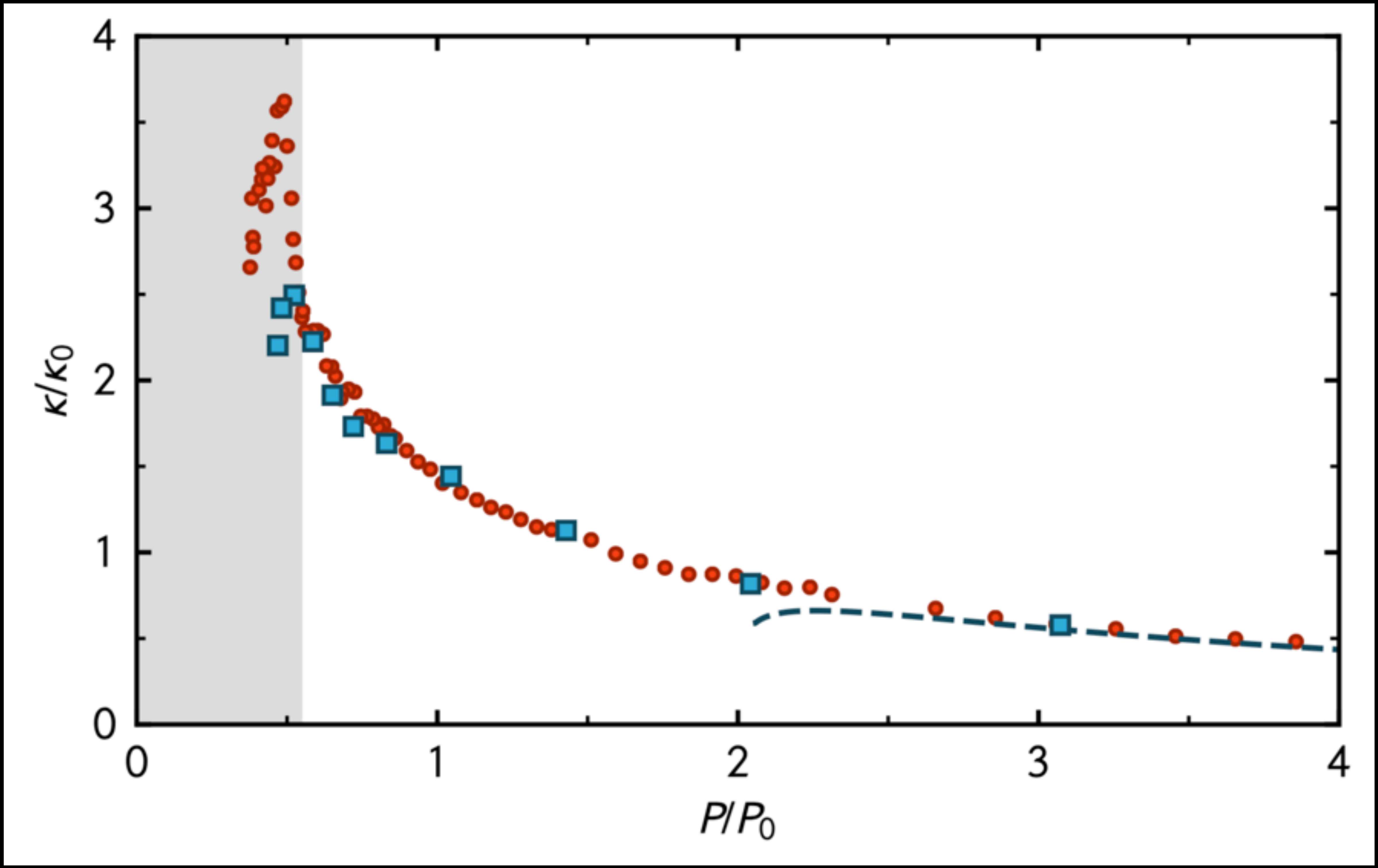
$$\lambda_T \simeq 7$$

$$\lambda_F \simeq 3$$

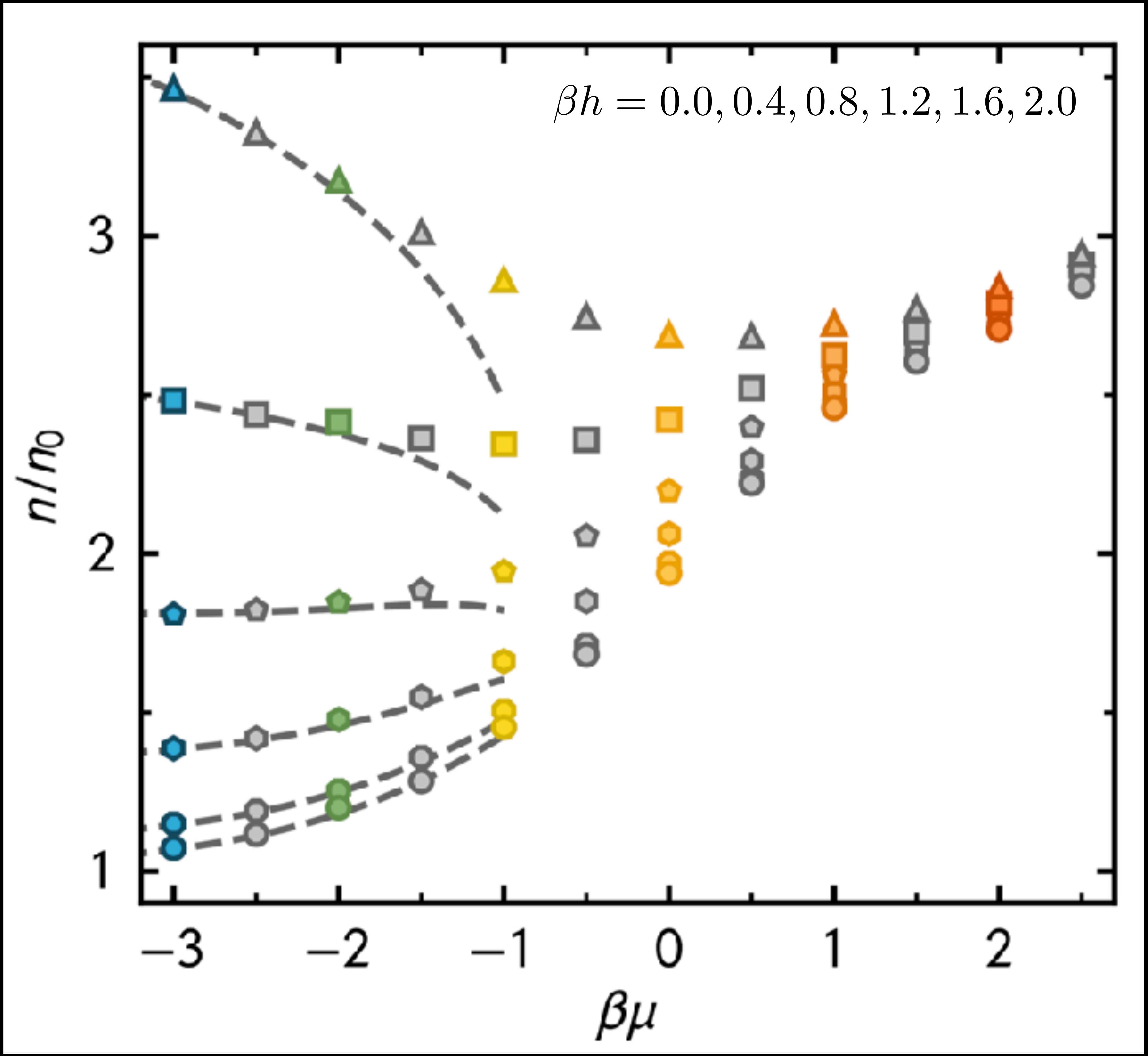
Results: Density EoS (check)



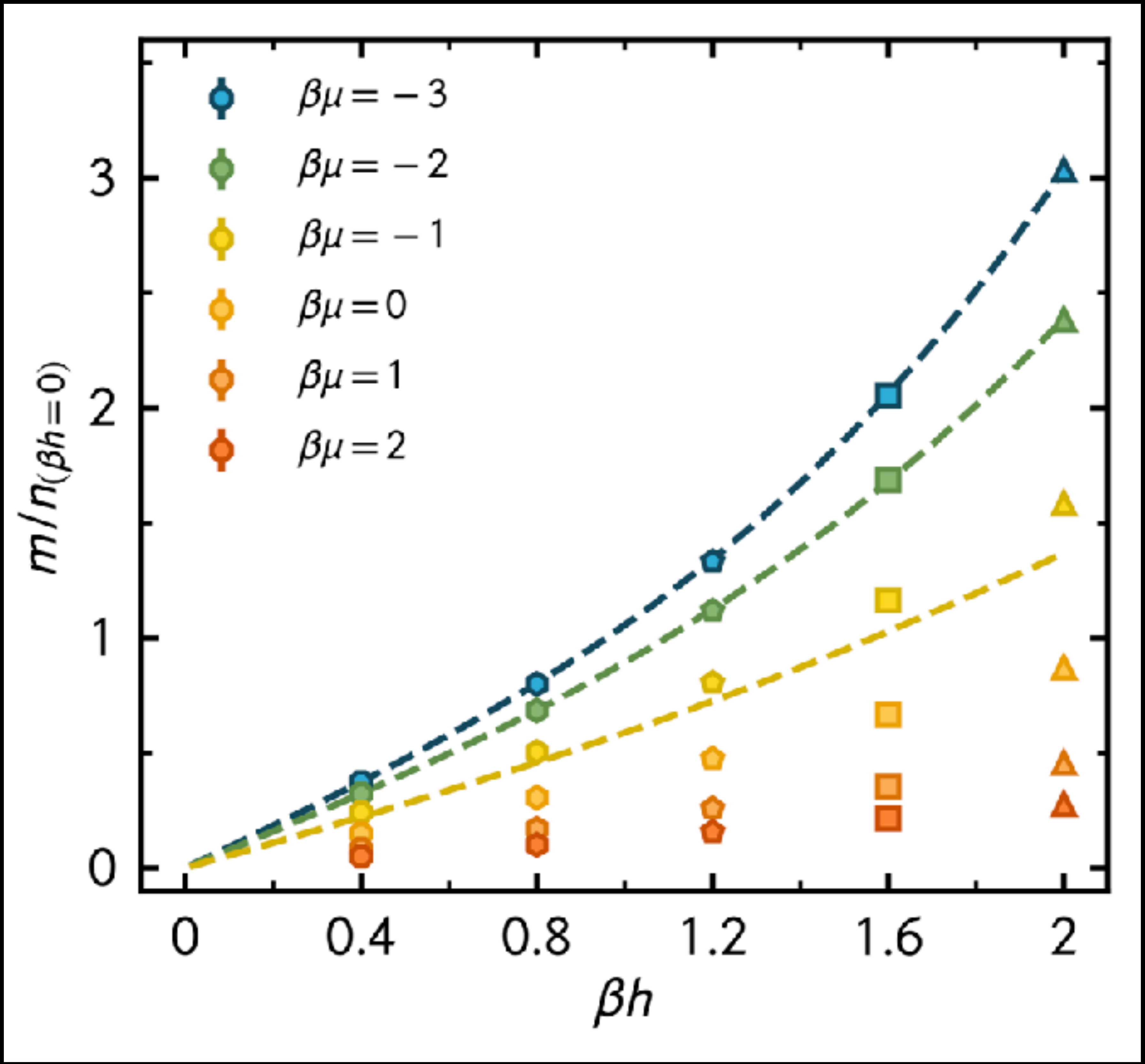
Results: Compressibility



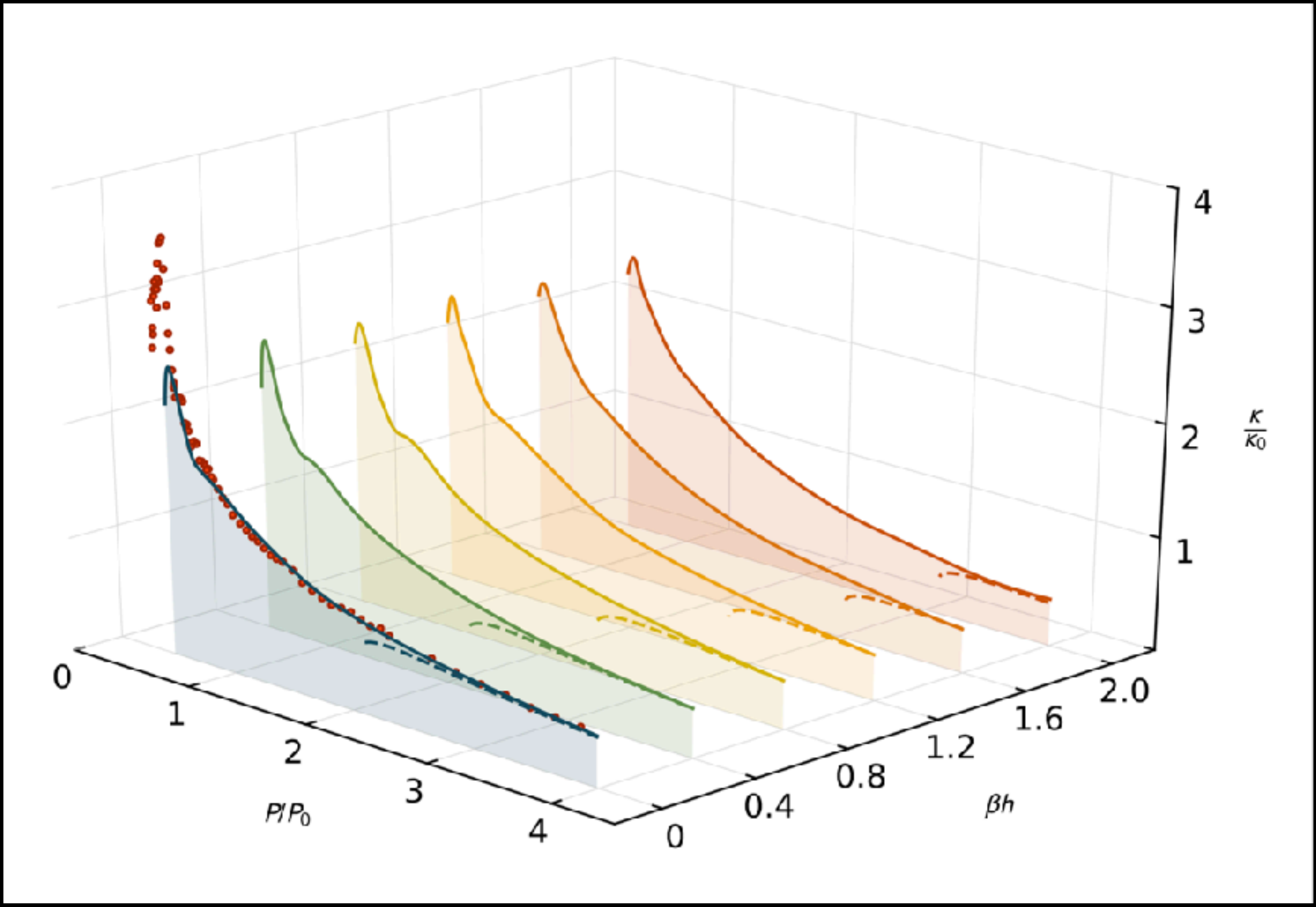
Results: Density EoS



Results: Magnetization EoS



Results: Susceptibility



Summary & conclusions

Polarized nonrelativistic matter, in particular the unitary Fermi gas (UFG), will typically have a sign problem.

Complex stochastic quantization (CL) provides a way to carry out nonperturbative calculations with complex actions. However, its mathematical underpinnings remain uncertain.

We have carried out multiple explorations of polarized matter at finite temperature in 1D, 2D, 3D (UFG), and other situations that have a sign problem when using AFQMC.

Our calculations for the UFG heal to known answers (virial, mid/low-T) in the range explored ($T > h/2$). We see little or no variation in the location of the superfluid critical point, but much more needs to be done to reach that regime.

Thank you!