Toward high-order virial coefficients via automated algebra

Joaquín E. Drut
Associate Professor & Melchor Fellow
University of North Carolina at Chapel Hill

THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL

ECT* Workshop:
Nuclear Physics meets Condensed Matter: symmetry, topology, and gauge
July 2021

RPMBT-XXI at UNC Chapel Hill, NC. Fall ~~2021~~

Recent Progress in Many-Body Theories

2022 (hopefully)

THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

Duke UNIVERSITY

NC STATE UNIVERSITY

OAK RIDGE National Laboratory

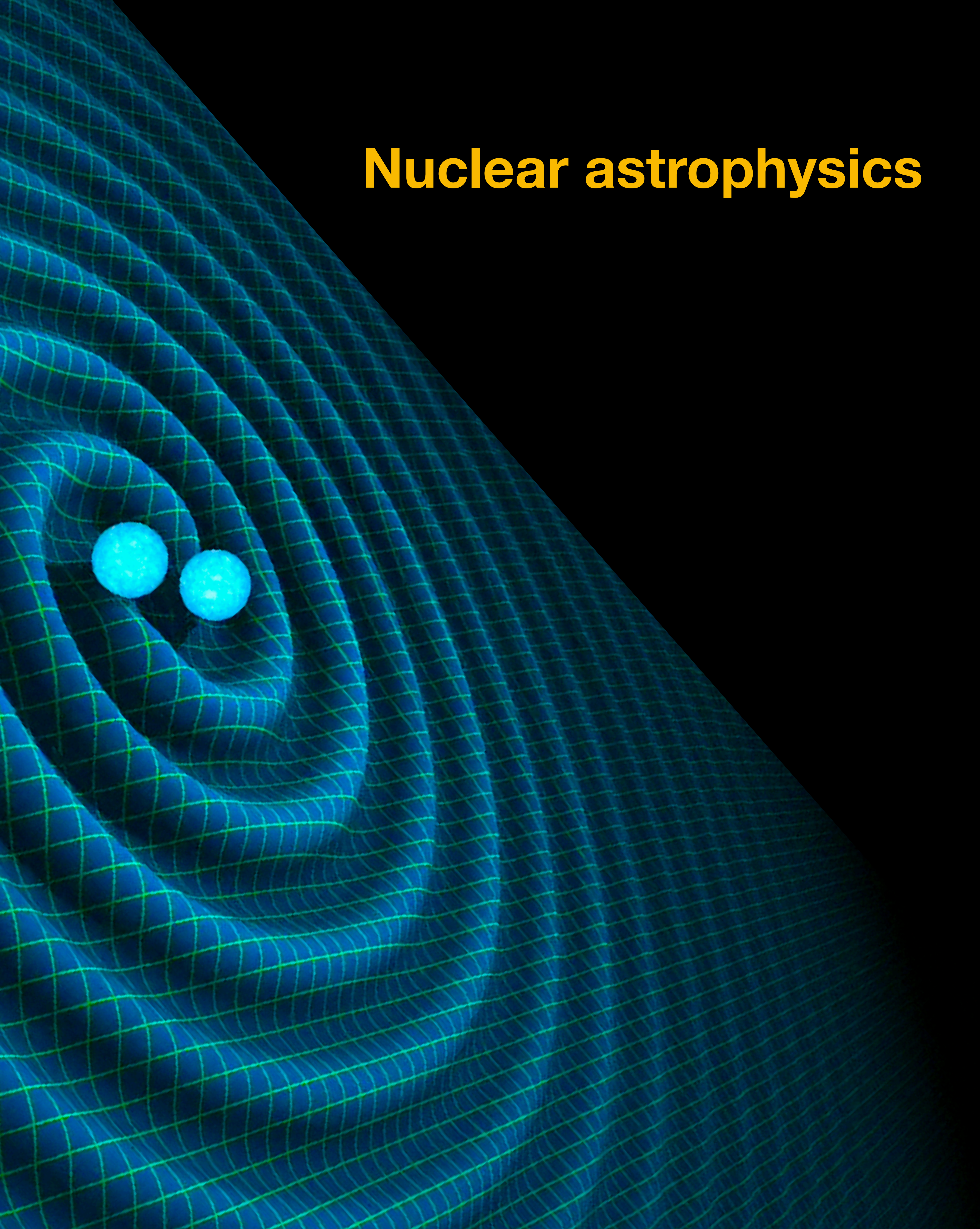
Claim of this talk

There is huge untapped potential in algebra automation for quantum many-body theory, in particular at finite temperature.

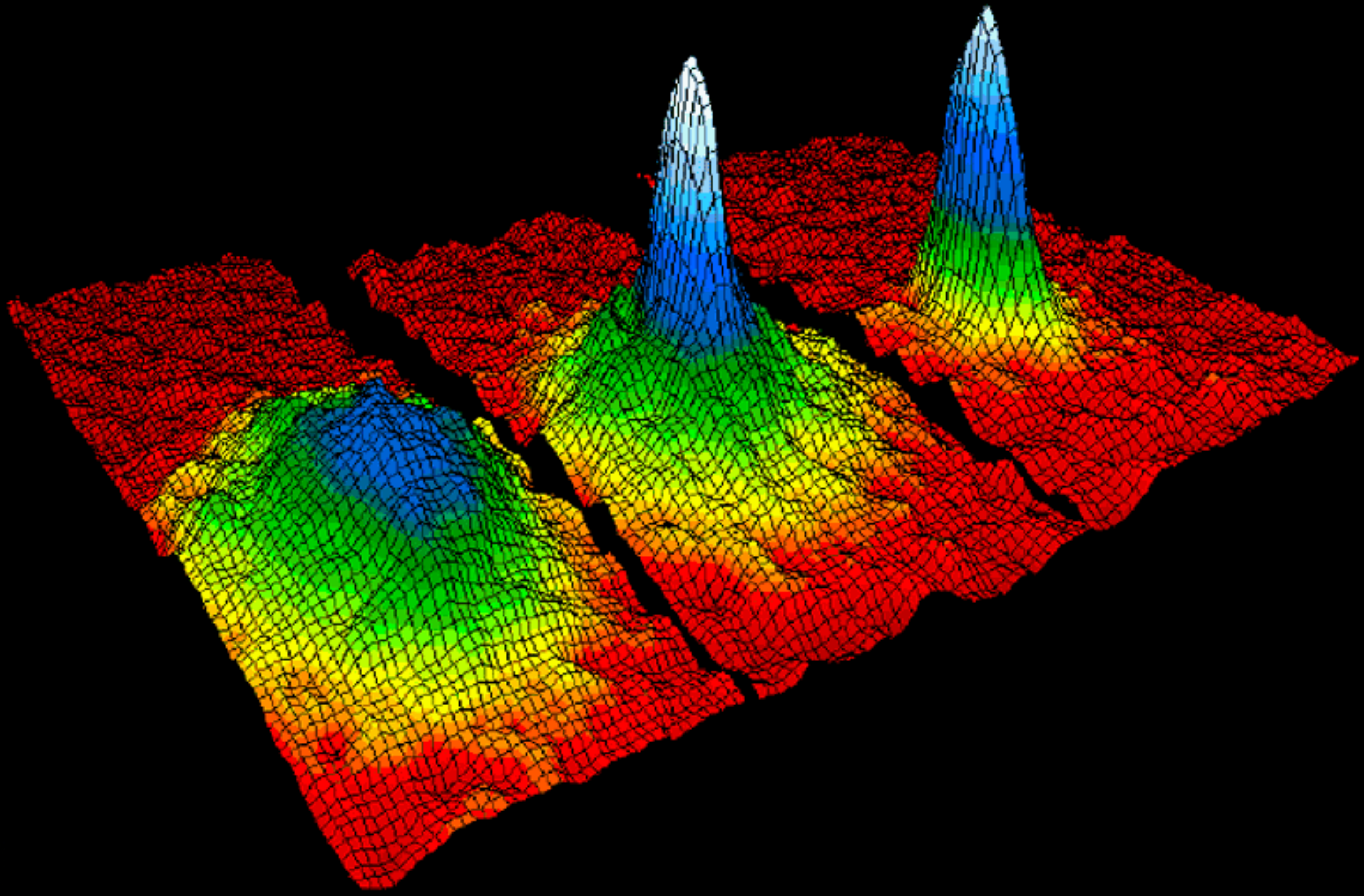
I will show you results that just a few years ago were (at least I thought!) impossible to obtain.

Context

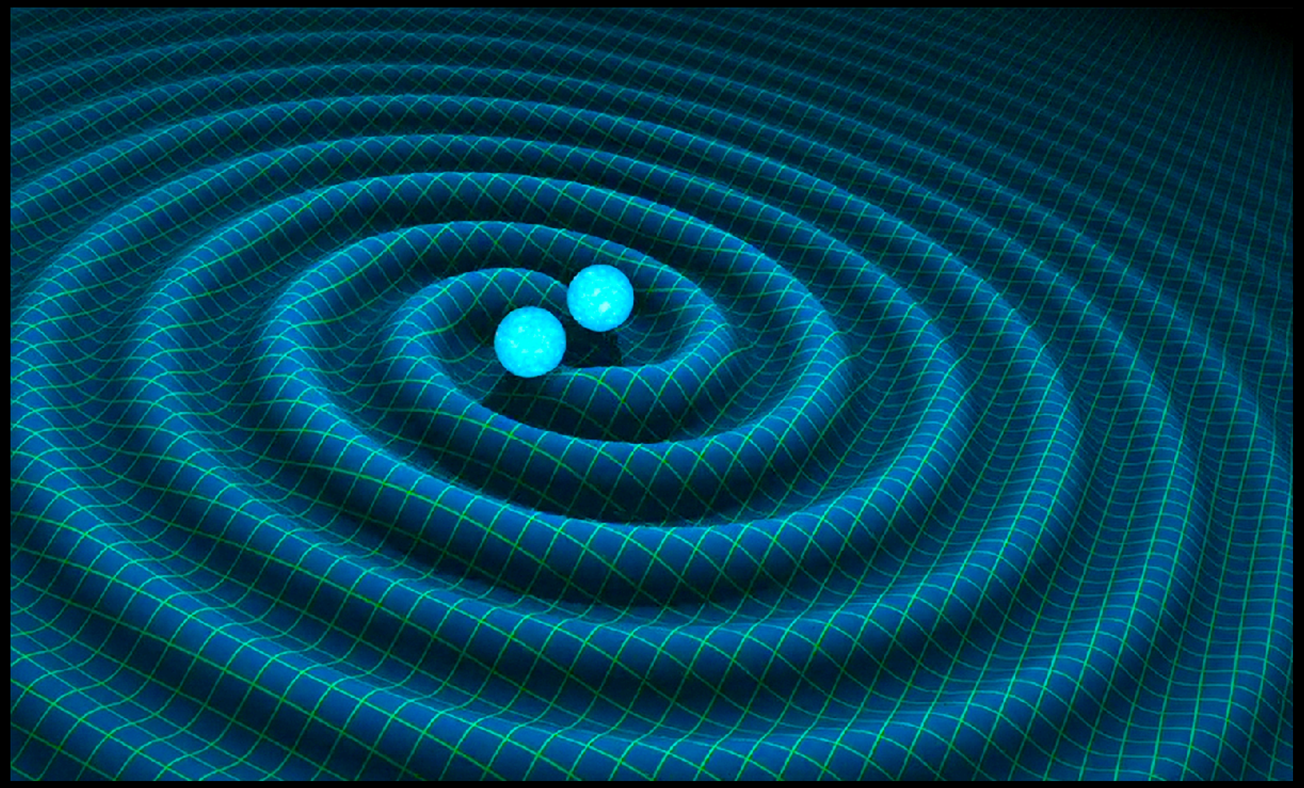
Nuclear astrophysics

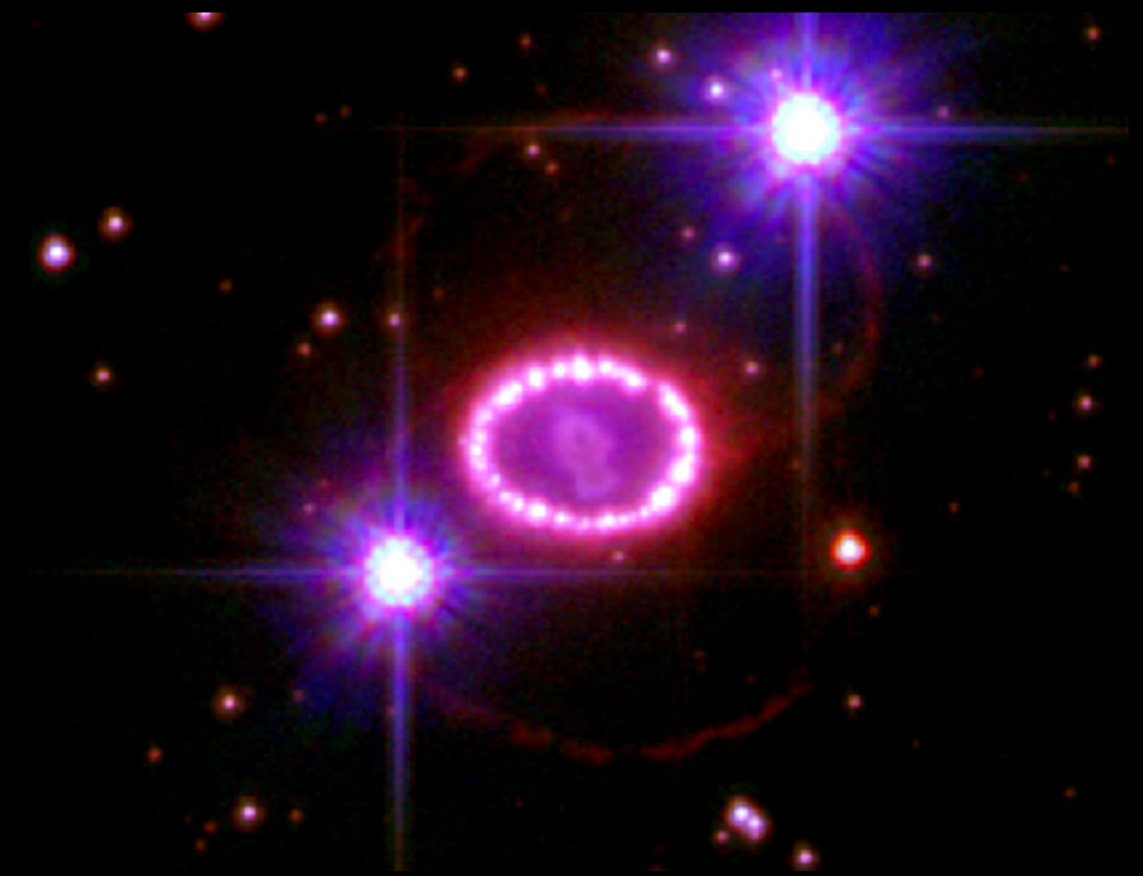


Ultracold atoms



Nuclear astrophysics





Neutron star mergers

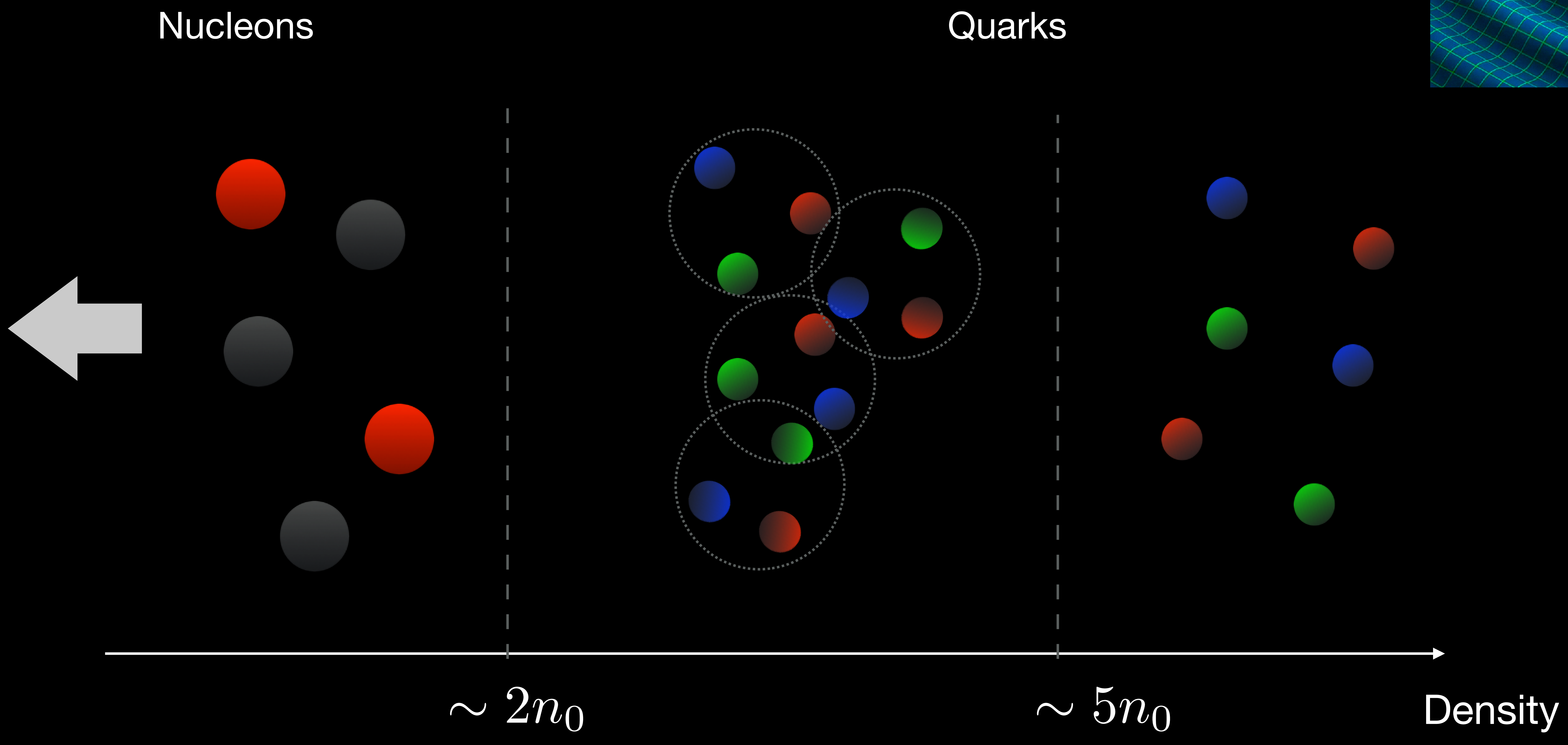
Core-collapse supernovae

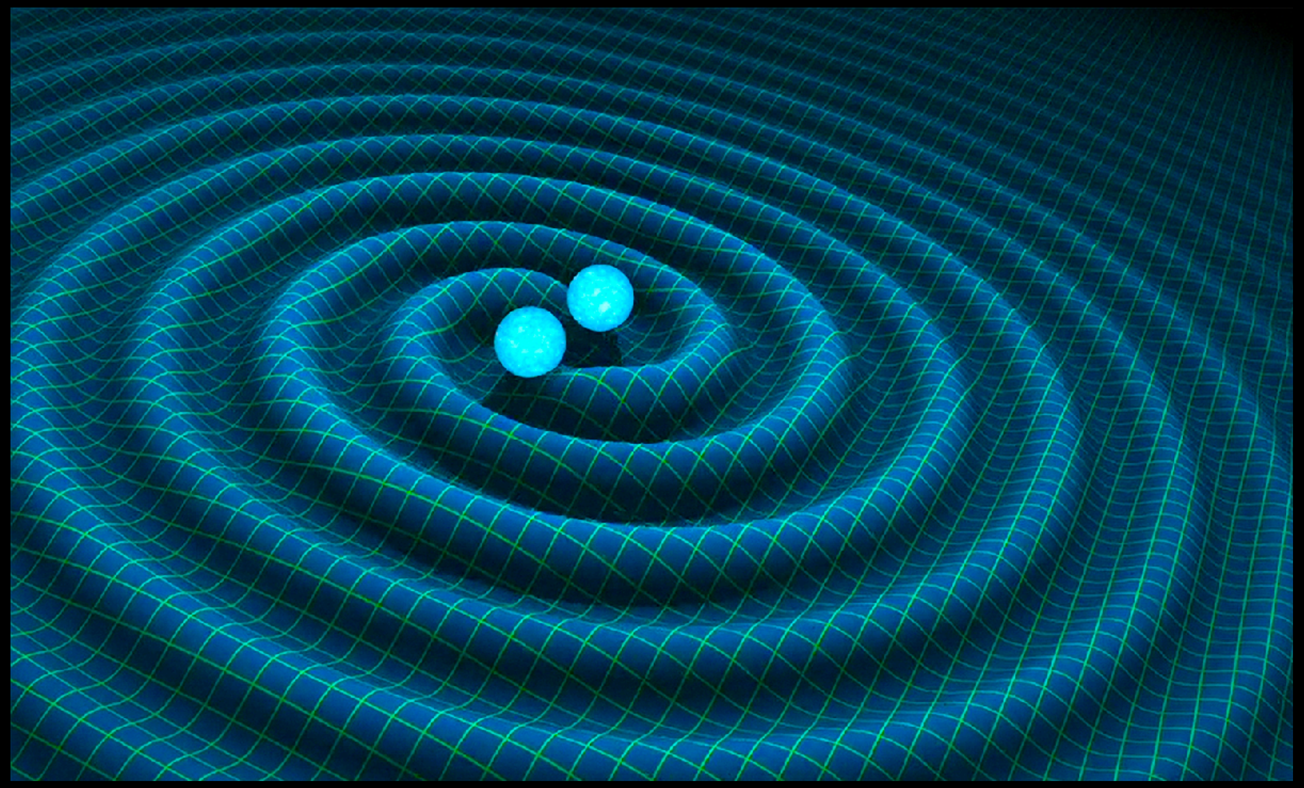
Studied with dynamical simulations;
require thermodynamic input from nuclear physics:

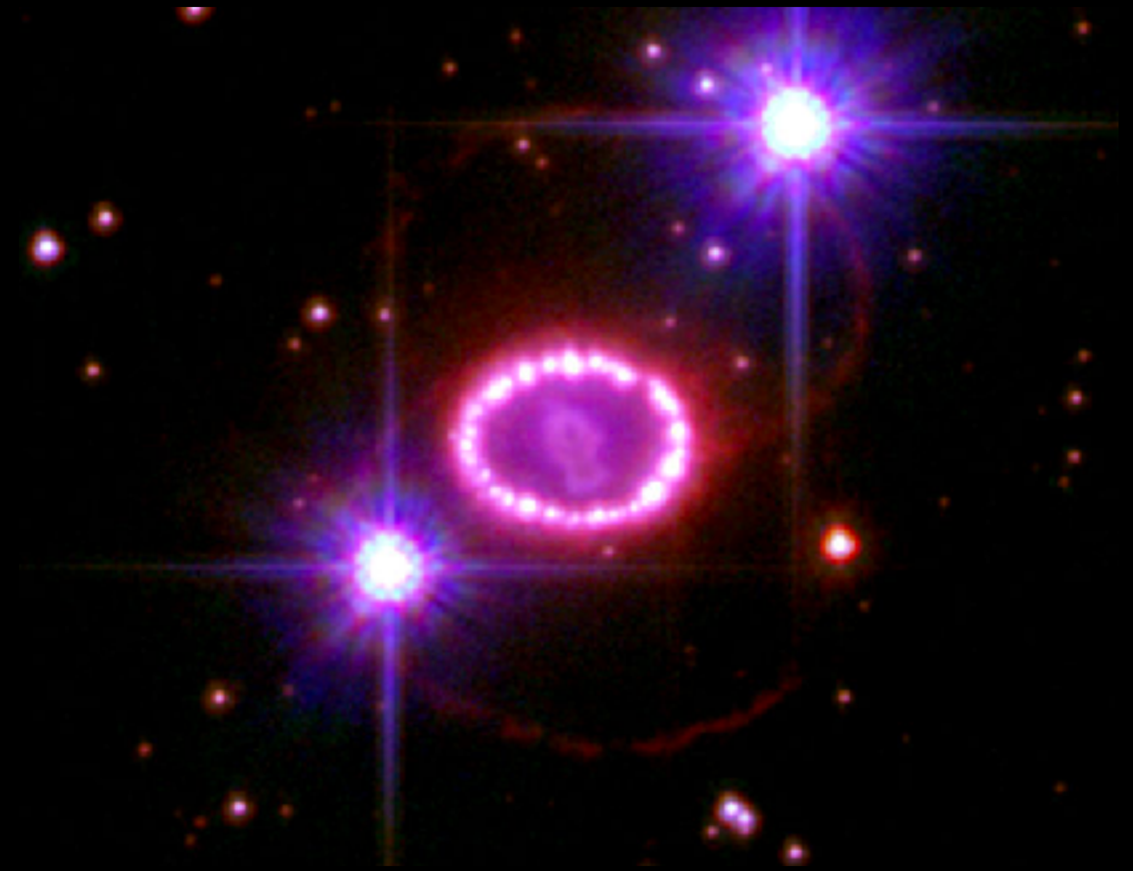
- Pressure-density EoS
- Quasiparticle spectrum
- Density and spin response
- Hydrodynamic response

… this is needed, in particular, at finite temperature.
(see Mark Alford's talk yesterday)

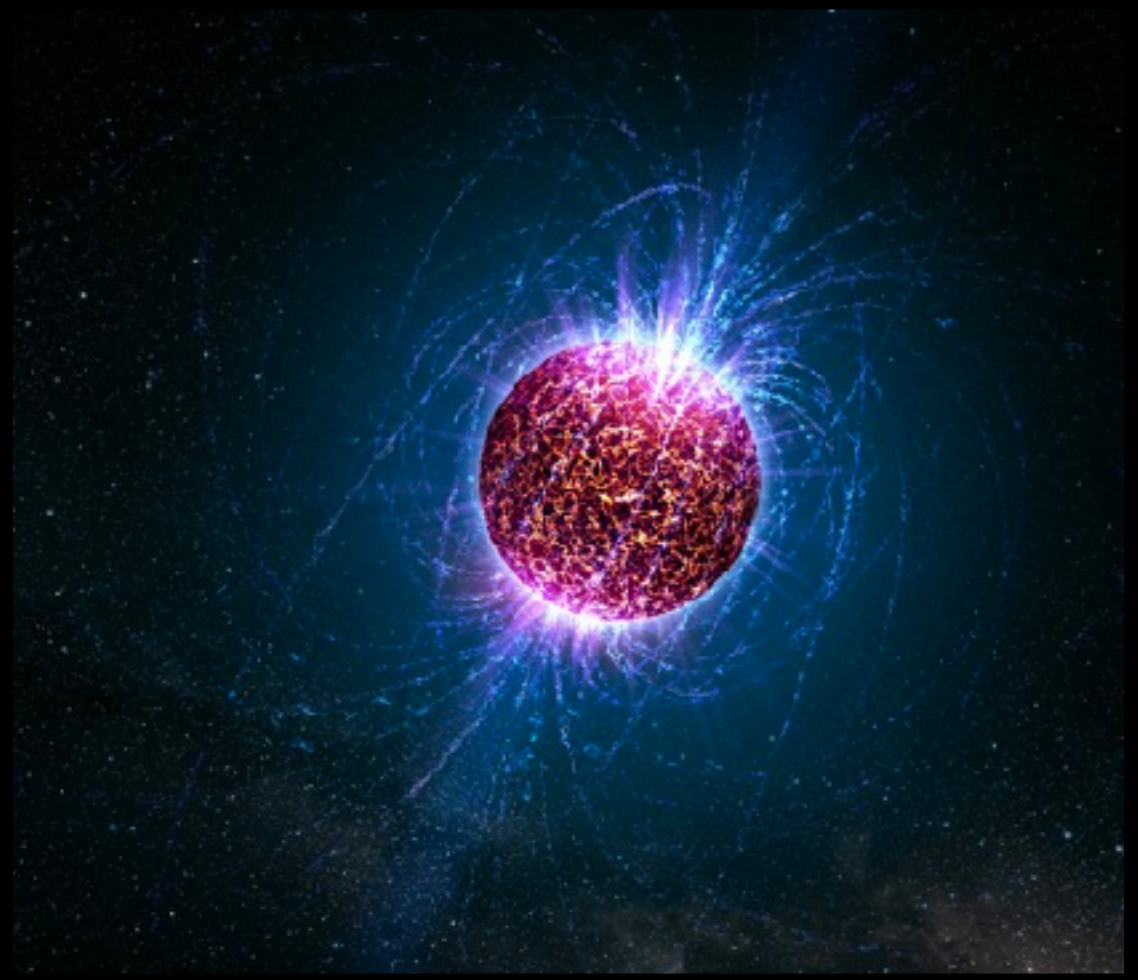
Nuclear astrophysics





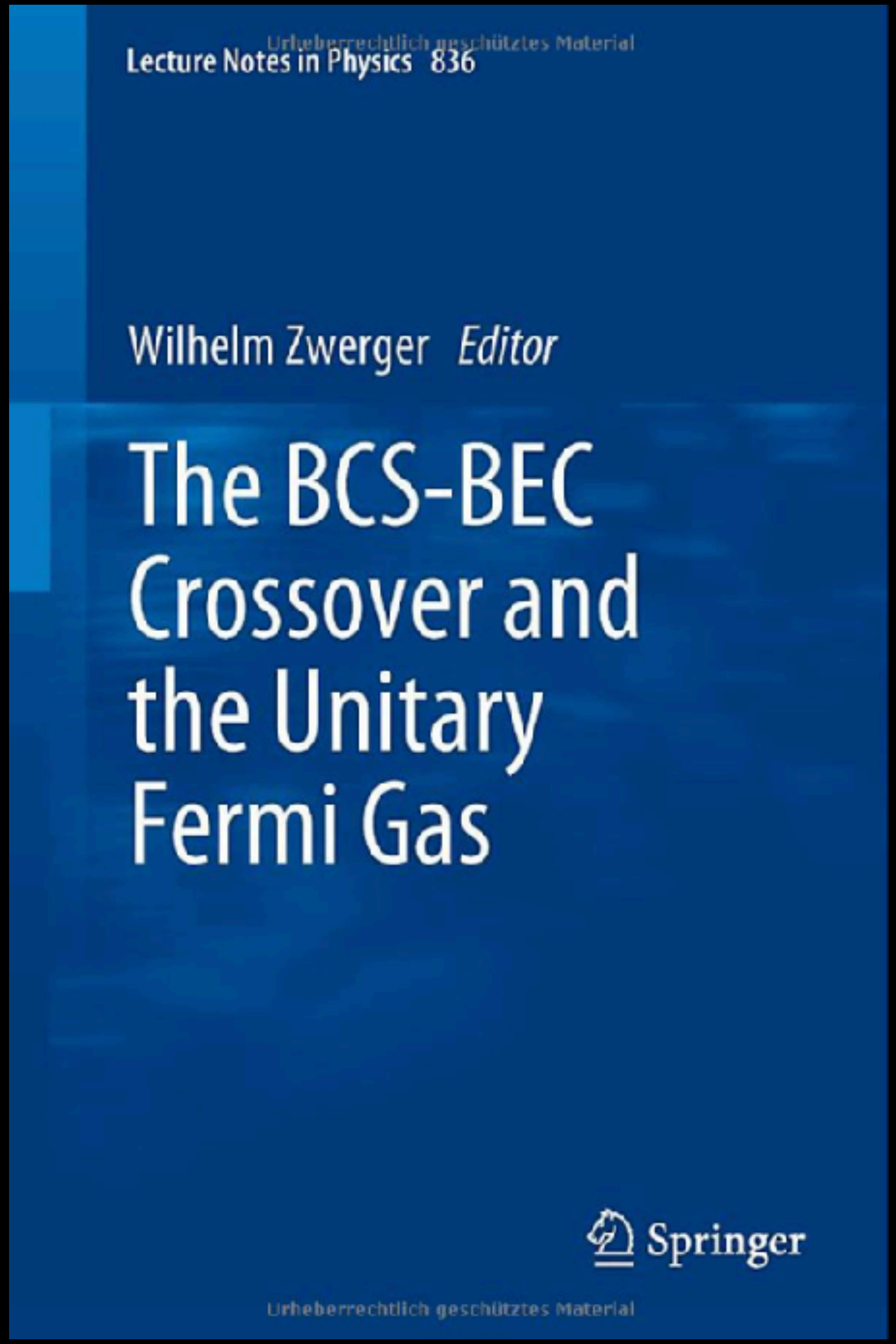


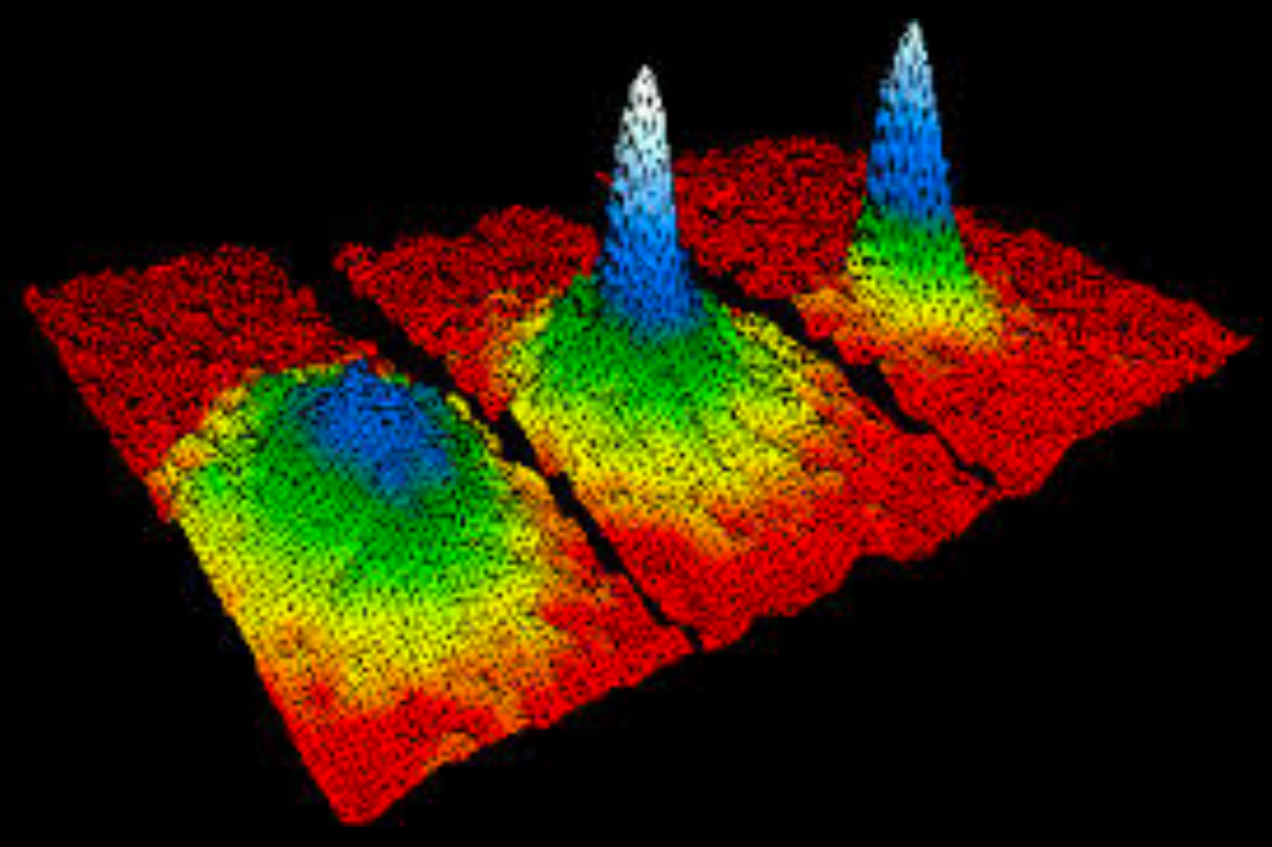
Dilute Fermi gases in universal regimes



Dilute neutron matter

$$a_s = -18.5 \text{ fm}$$
$$r_0 = 2.7 \text{ fm}$$





Dilute atoms

$$a_s = 10^4 \text{ Bohr}$$
$$r_0 = 20 \text{ Bohr}$$

(see also Joe Carlson's talk yesterday)

Idealized regime:

$$a_s \to \infty$$
$$r_0 \to 0$$

"Unitary limit"

No small parameters!

Dilute Fermi gases in universal regimes

Two species of fermions with a contact two-body force

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

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

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

Solve for energies

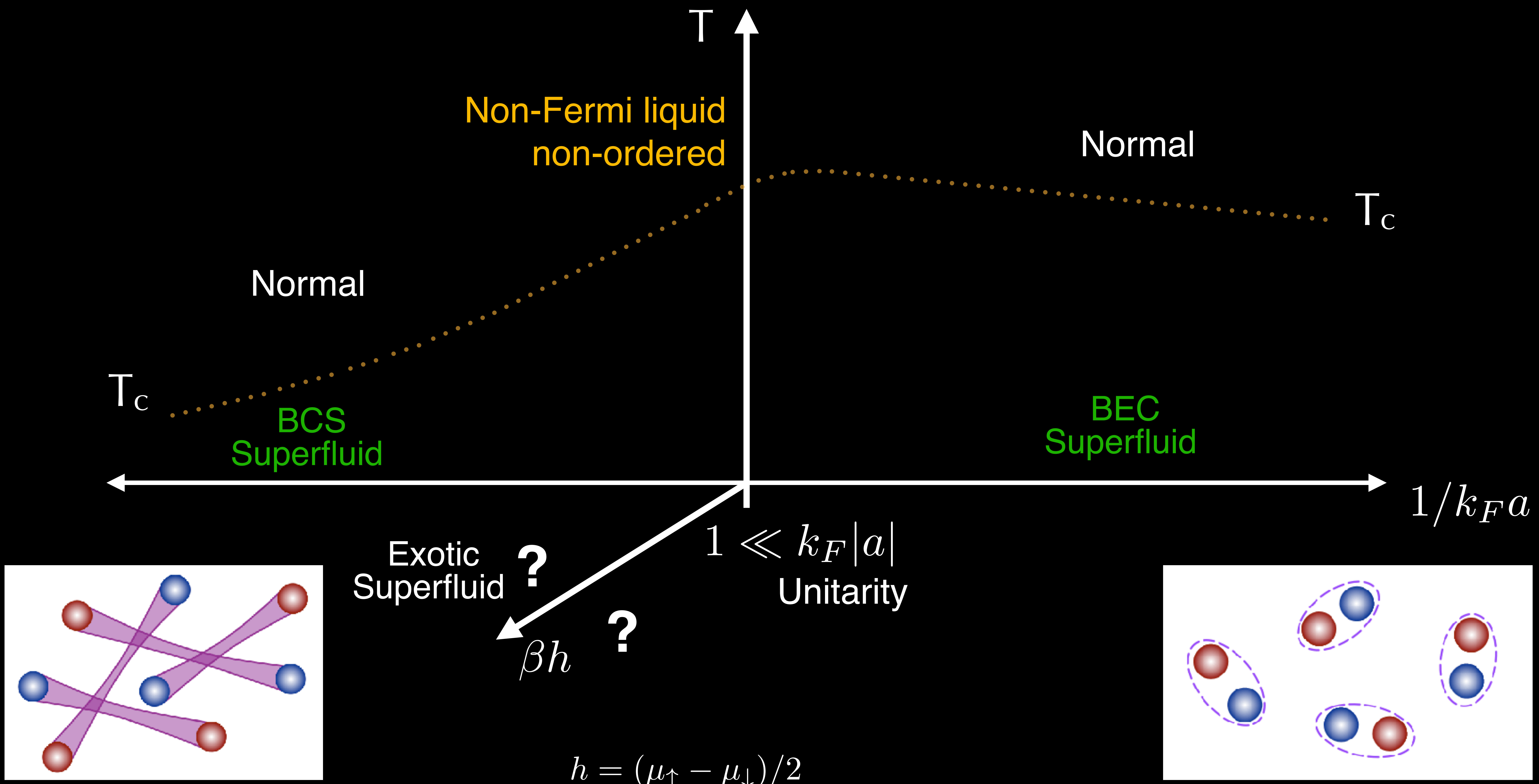
$$E = \frac{p^2}{2\bar{m}}$$

Plug in to determine scattering parameters

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

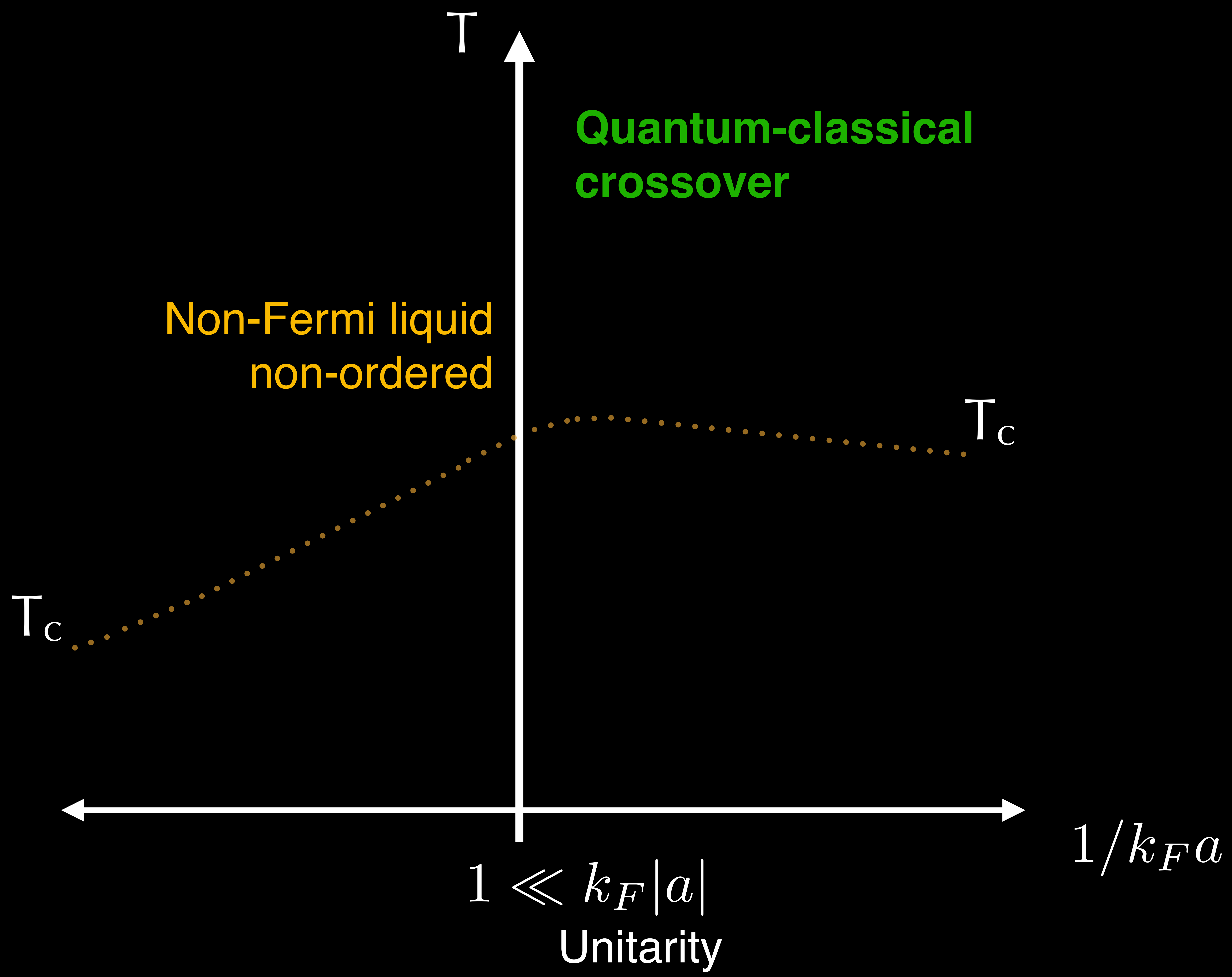
= 0 at unitarity

The many-body problem: BCS-BEC crossover



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

The many-body problem: BCS-BEC crossover



Technical details

The task and the challenge

Two species of fermions with a contact two-body force

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

Objective: Calculate the thermodynamics of this model
in an ab initio, non-perturbative fashion.

Thermodynamics and the virial expansion

Thermodynamics

$$-\beta\Omega = PV = \ln \mathcal{Z}$$

Grand-canonical partition function

$$\mathcal{Z} = \sum_{N=0}^{\infty} Q_N z^N$$

Fugacity

$$z = e^{\beta\mu}$$

Interaction effects

$$-\beta\Delta\Omega = \ln(\mathcal{Z}/\mathcal{Z}_0) = Q_1 \sum_{n=2}^{\infty} \Delta b_n z^n$$

Canonical partition functions

$$Q_N = \mathrm{Tr}_N \left[e^{-\beta \hat{H}} \right]$$

“Small-fugacity” expansion: **virial expansion**

Virial coefficients $\Delta b_n = b_n - b_n^{(0)}$ obtained from n-body problem

The thermodynamics and static response are encoded in these numbers!

Thermodynamics and the virial expansion

$$\Delta b_2 = \frac{\Delta Q_2}{Q_1}$$

Beth-Uhlenbeck formula (1937)

$$\Delta b_3 = \frac{\Delta Q_3}{Q_1} - Q_1 \Delta b_2$$

Precise calculations only in 21st century and in very specific cases

$$\Delta b_4 = \frac{\Delta Q_4}{Q_1} - \Delta\left(b_3 + \frac{b_2^2}{2}\right) Q_1 - \frac{\Delta b_2}{2} Q_1^2$$

Precise only in last decade also in very specific cases

$$\vdots$$

Access to the Q_N gives us access to the virial coefficients, but…

$$Q_N \sim O(V^N)$$

Delicate volume cancellations required at each order!

Very challenging to accomplish with Monte Carlo

We proceed analytically, but still aided by computers.

Our approach to calculating virial coefficients

Temporal lattice approximation (a.k.a. Suzuki-Trotter factorization)

$$e^{-\beta(\hat{T}+\hat{V})} = \lim_{k\to\infty}\left(e^{-\beta\hat{T}/k}e^{-\beta\hat{V}/k}\right)^k$$

fix k

$$Q_N = \mathrm{Tr}_N\left[e^{-\beta\hat{H}}\right] \longrightarrow \mathrm{Tr}_N\left[\left(e^{-\beta\hat{T}/k}e^{-\beta\hat{V}/k}\right)^k\right]$$

automate

$$\Delta b_N$$

extrapolate to large k

C. R. Shill, J. E. Drut
Phys. Rev. A **98**, 053615 (2018).

Y. Hou, A. Czejdo, J. DeChant, C.R. Shill, J. E. Drut
Phys. Rev. A **100**, 063627 (2019)

A. J. Czejdo, et al.
Phys. Rev. A **101**, 063630 (2020)

Y. Hou, J. E. Drut
Phys. Rev. A **102**, 033319 (2020)
Phys. Rev. Lett. **125**, 050403 (2020)
(Editor's suggestion)

K. Morrell, C. E. Berger, J. E. Drut
Phys. Rev. A **102**, 023309 (2020)

Our approach to calculating virial coefficients

What goes into the "automation" step? Gaussian integrals!

$$Q_N = \mathrm{Tr}_N \left[e^{-\beta \hat{H}} \right] \longrightarrow \mathrm{Tr}_N \left[\left(e^{-\beta \hat{T}/k} e^{-\beta \hat{V}/k} \right)^k \right]$$

Contact interaction $\Longleftrightarrow$ constant in momentum space

E.g. N=2 $\quad \langle p_1 p_2 | e^{-\beta \hat{V}} | p_1' p_2' \rangle = \delta_{p_1 p_1'} \delta_{p_2 p_2'} + C \, \delta_{p_1 + p_1', p_2 + p_2'}$

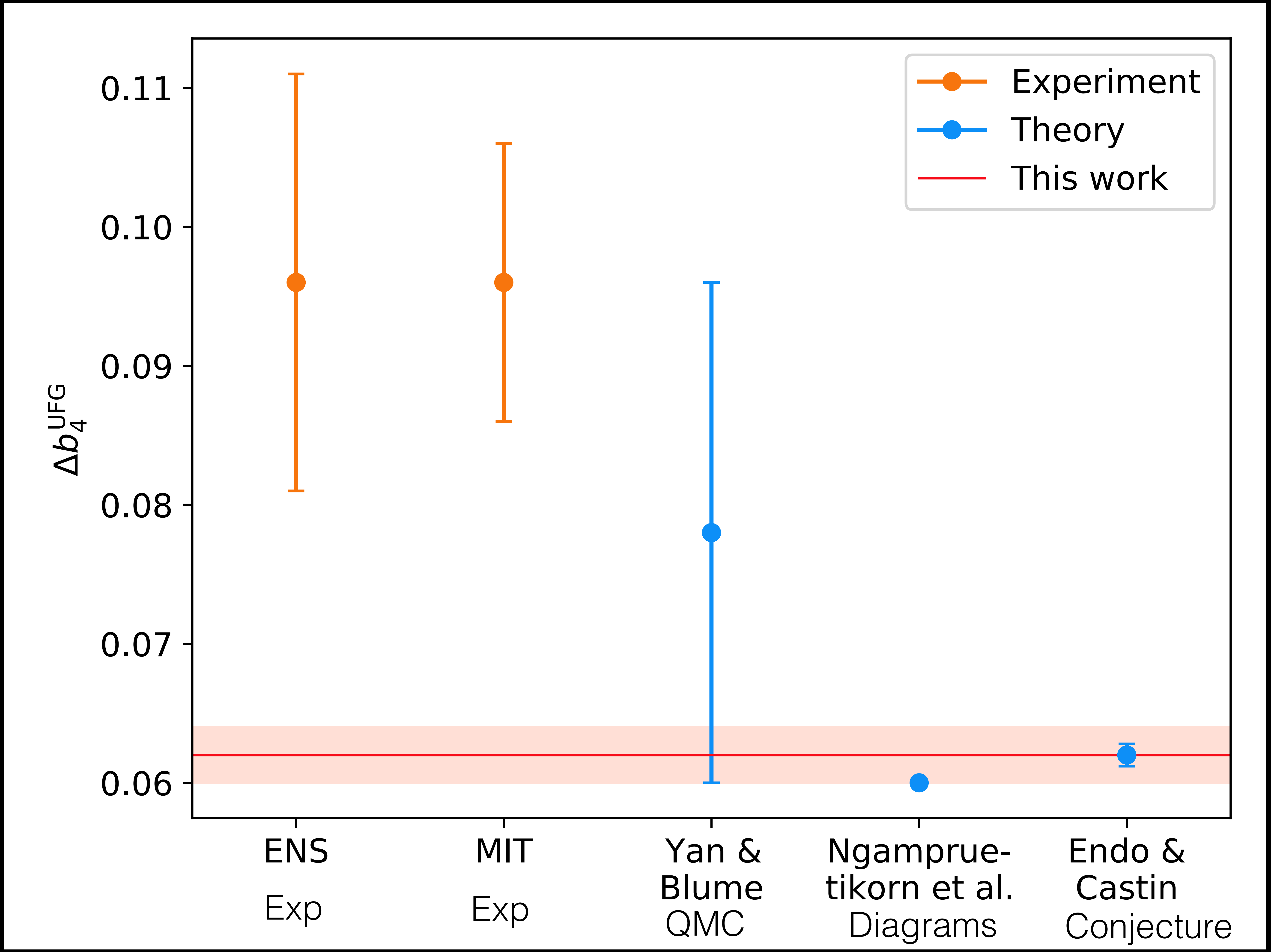
$\Longleftrightarrow$ only Gaussian integrals in momentum space

More complicated interaction? Write the above matrix element in a Gaussian basis.

Results

Results: virial coefficients

First result: Δb_4 at unitarity



Y. Hou, J. E. Drut
Phys. Rev. Lett. **125**, 050403 (2020)
Editor's suggestion

$a_s \to \infty$

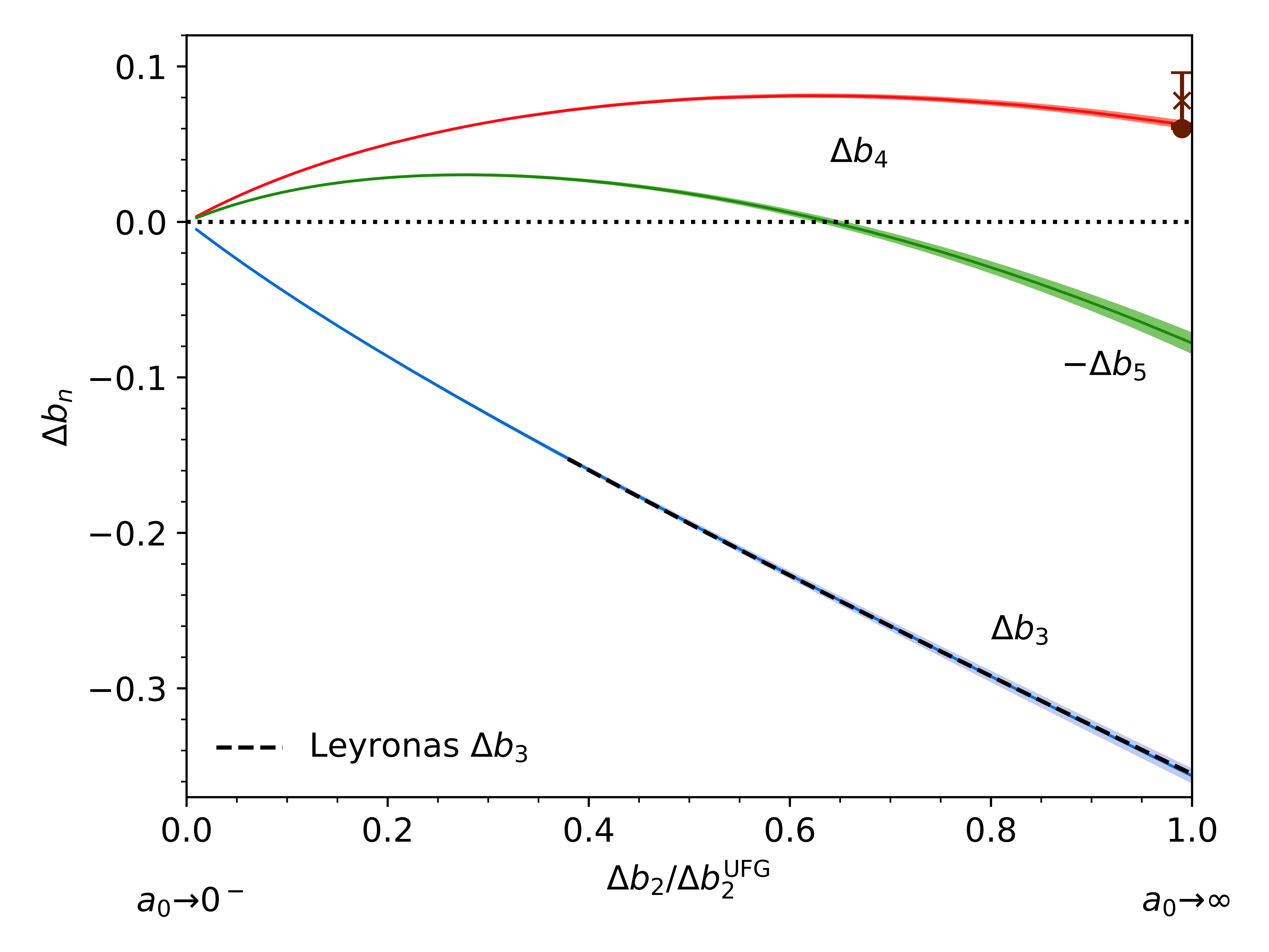
$r_0 \to 0$

Maximum k

Δb_4 : 12

Results: virial coefficients

Large-**k** extrapolated results for **3D** fermions in the BCS-BEC crossover



Y. Hou, J. E. Drut
Phys. Rev. Lett. **125**, 050403 (2020)
Editor's suggestion

Other results shown:

Δb_3 : Leyronas (exact)

Δb_4 : Endo & Castin (conjecture), Yan & Blume (QMC), Ngampruetikorn et al (diagrammatic approx).

Maximum k

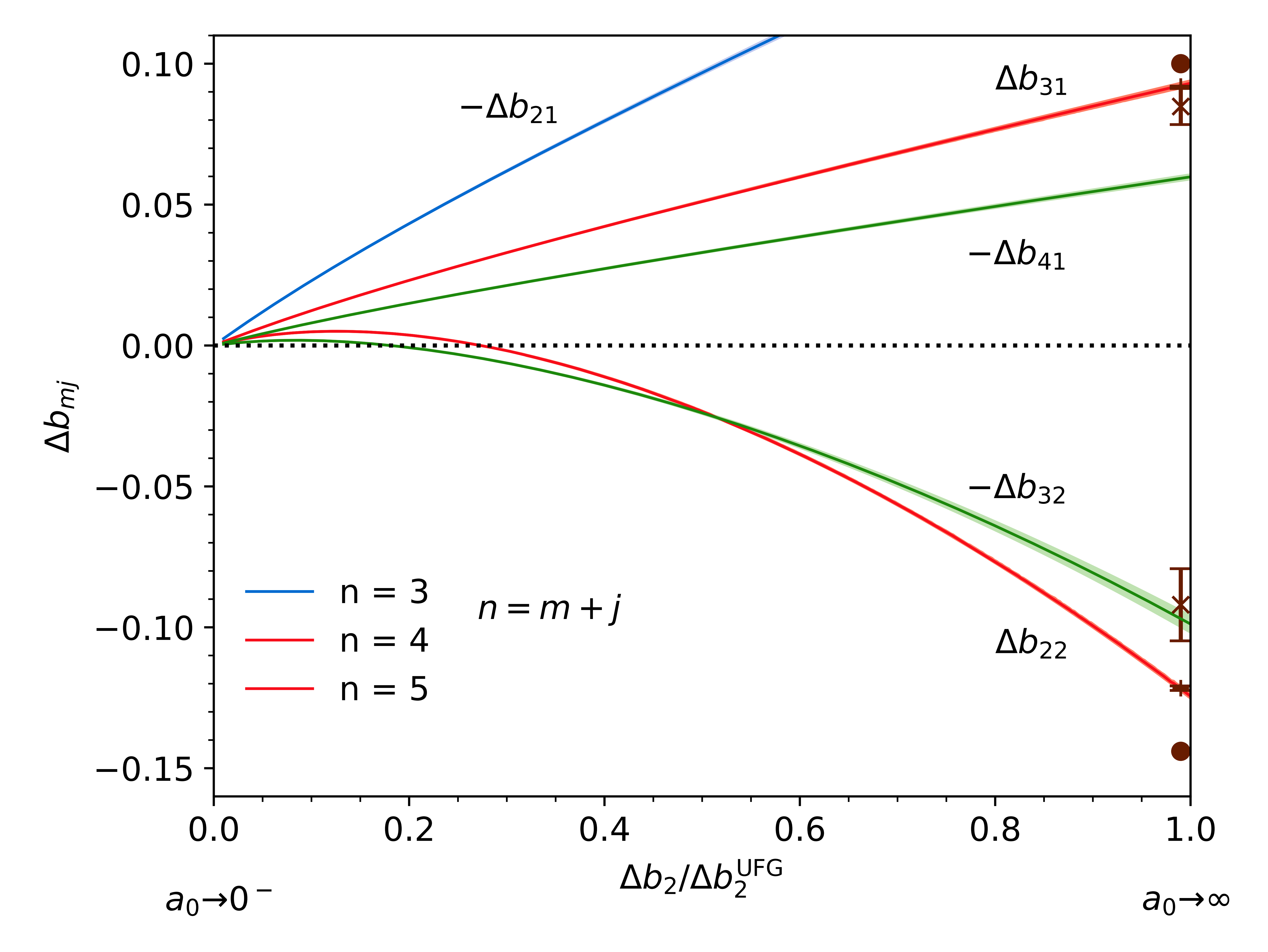
Δb_3 : 21

Δb_4 : 12

Δb_5 : 9

Results: virial coefficients

Large-**k** extrapolated results for **3D** fermions in the BCS-BEC crossover

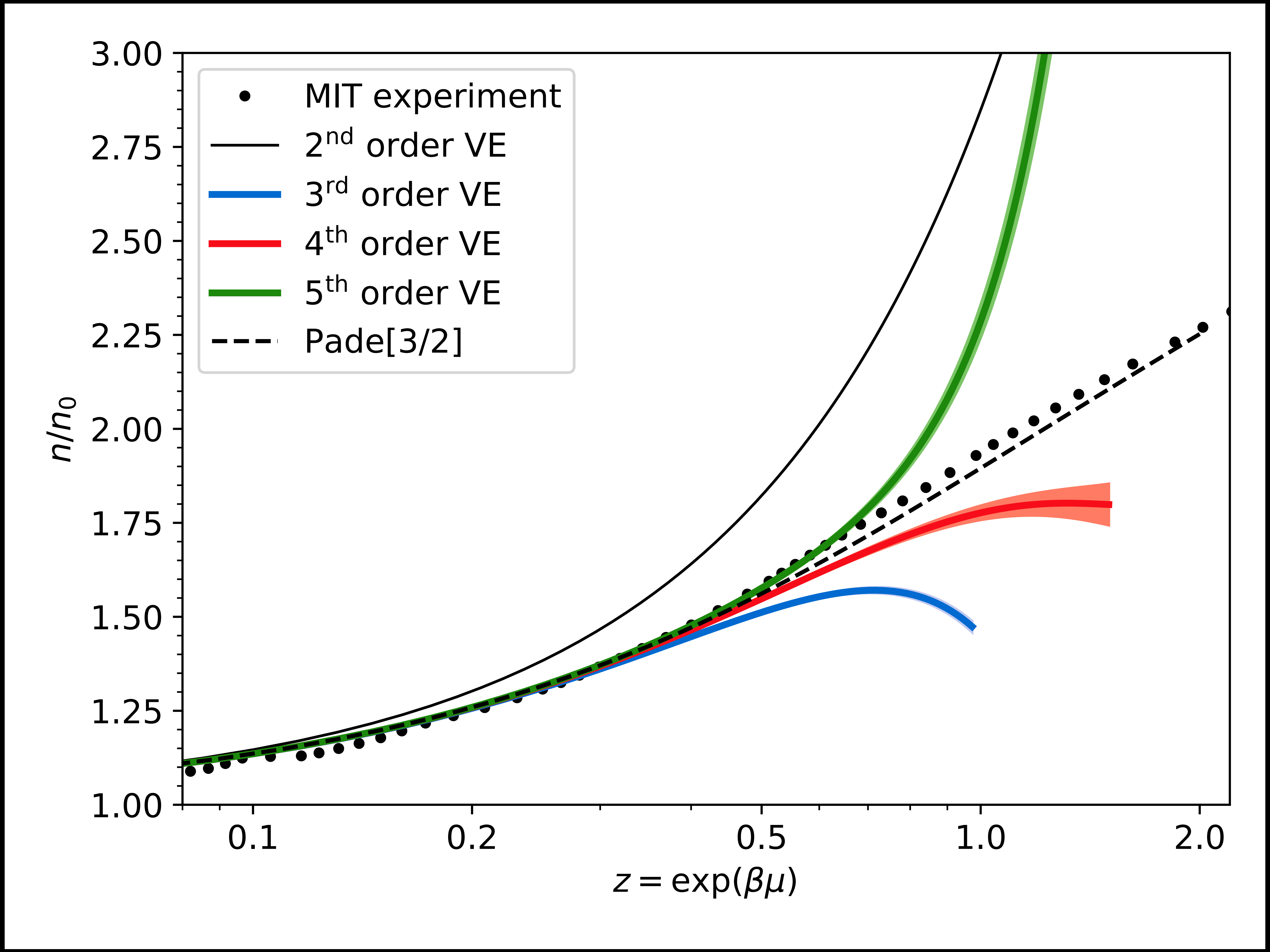


Y. Hou, J. E. Drut
Phys. Rev. Lett. **125**, 050403 (2020)
Editor's suggestion

$$\Delta b_2 \leftarrow \Delta b_{11}$$
$$\Delta b_3 \leftarrow \Delta b_{21}$$
$$\Delta b_4 \leftarrow \Delta b_{31},\ \Delta b_{22}$$
$$\Delta b_5 \leftarrow \Delta b_{41},\ \Delta b_{32}$$
$$\vdots$$

Results: density EoS from virial coefficients

3D fermions at unitarity

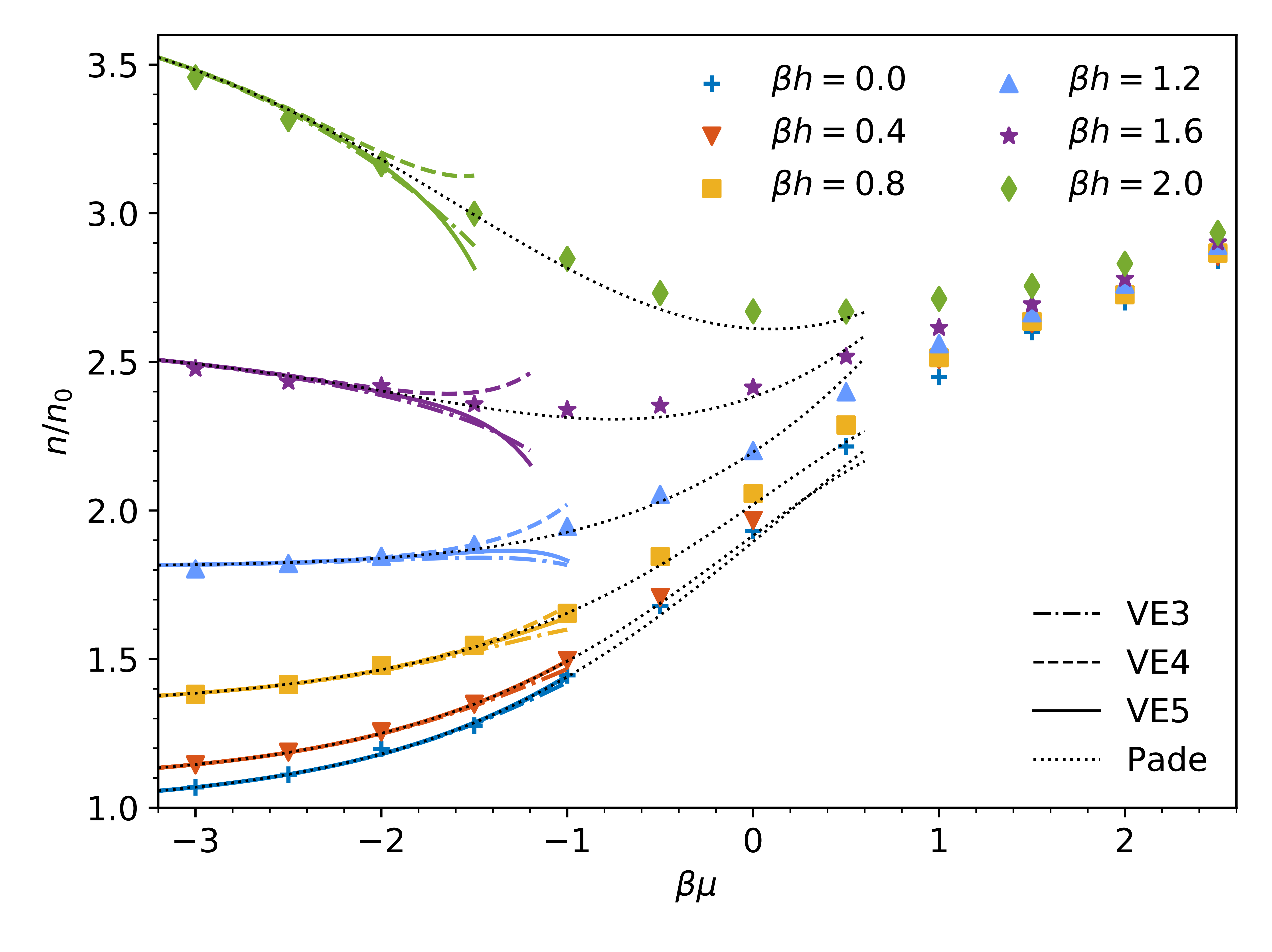


Y. Hou, J. E. Drut
Phys. Rev. Lett. **125**, 050403 (2020)
Editor's suggestion

MIT experiment:
Ku et al.
Science **335**, 563 (2012)

Results: polarized EoS from virial coefficients

3D fermions at unitarity



Y. Hou, J. E. Drut
Phys. Rev. A **102**, 033319 (2020)
resummation techniques
& generalization to 1D, 2D, 3D.

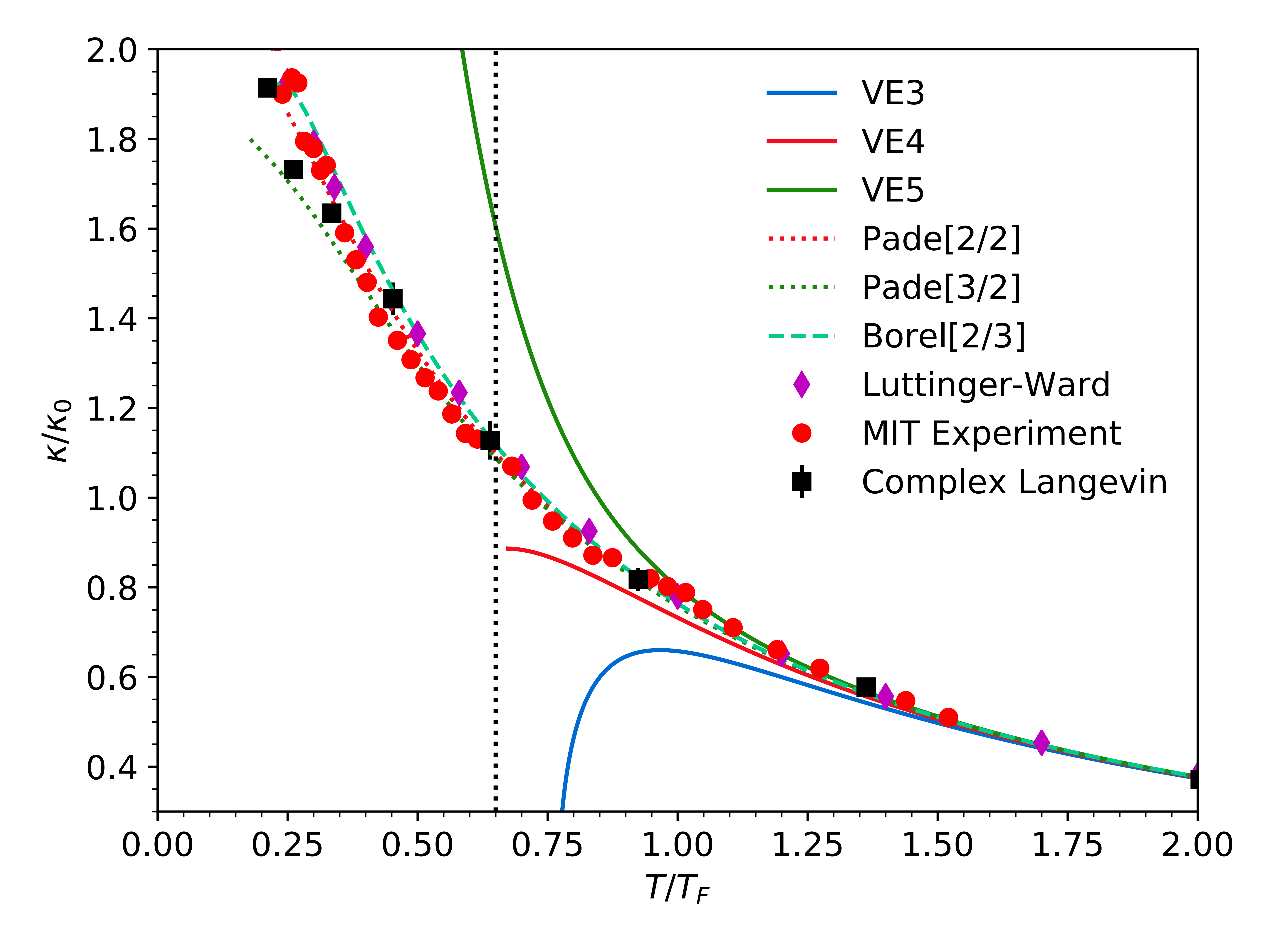
Complex Langevin:
Rammelmueller et al.
Phys. Rev. Lett. **121**, 173001 (2018)

$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$

$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

Results: compressibility

3D fermions at unitarity



Y. Hou, J. E. Drut
Phys. Rev. A **102**, 033319 (2020)

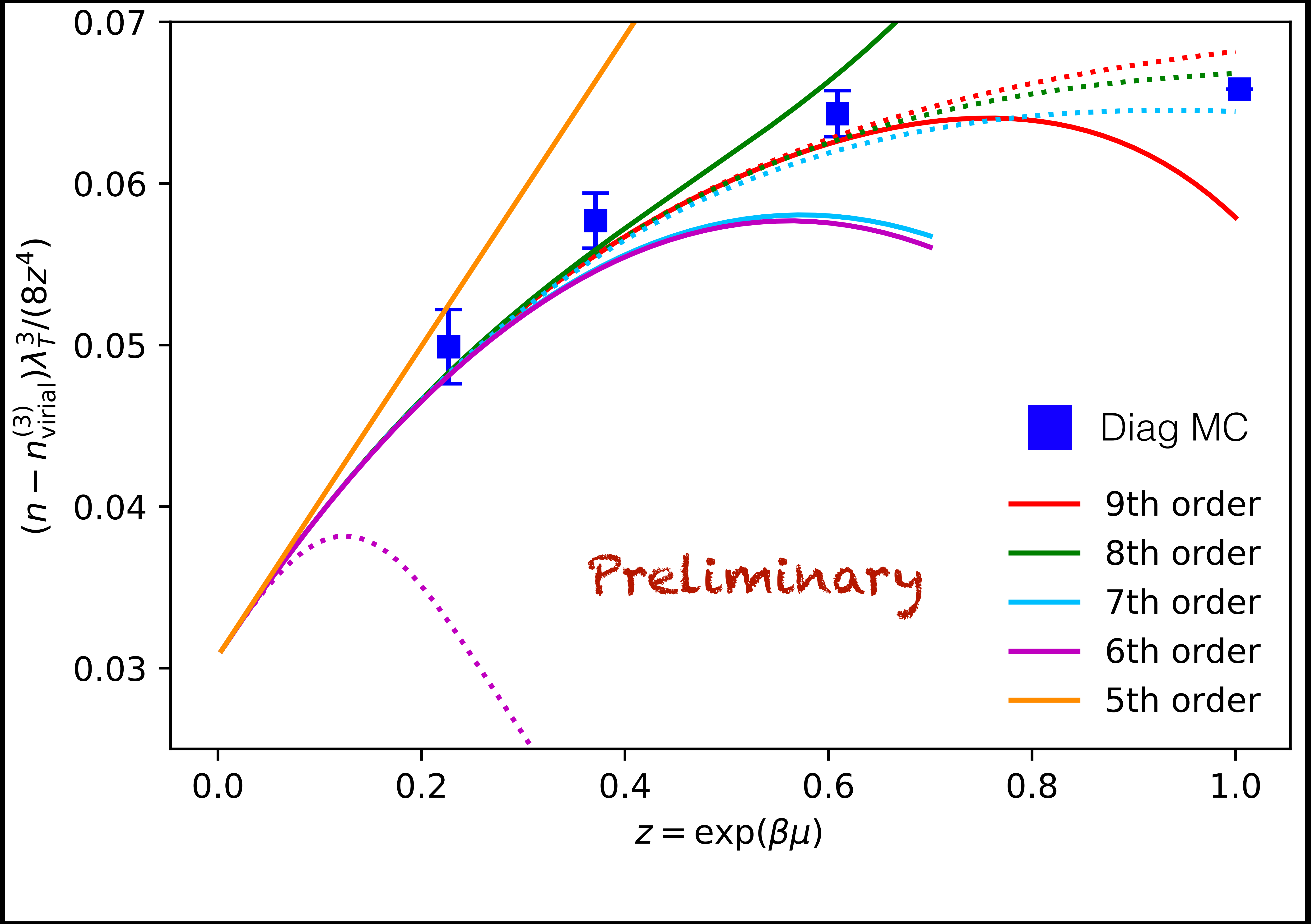
Luttinger-Ward:
Enss & Haussmann
Phys. Rev. Lett. **109**, 195303 (2012)

MIT experiment:
Ku et al.
Science **335**, 563 (2012)

Complex Langevin:
Rammelmueller et al.
Phys. Rev. Lett. **121**, 173001 (2018)

The future: Beyond 5th order

3D fermions at unitarity (unpublished high-order results)



Y. Hou, J. E. Drut
unpublished

Compared with
Rossi et al
Phys. Rev. Lett **121**, 130405 (2018)

Maximum k

$\Delta b_3 : 23$

$\Delta b_4 : 15$

$\Delta b_5 : 12$

$\Delta b_6 : 8$

$\Delta b_7 : 6$

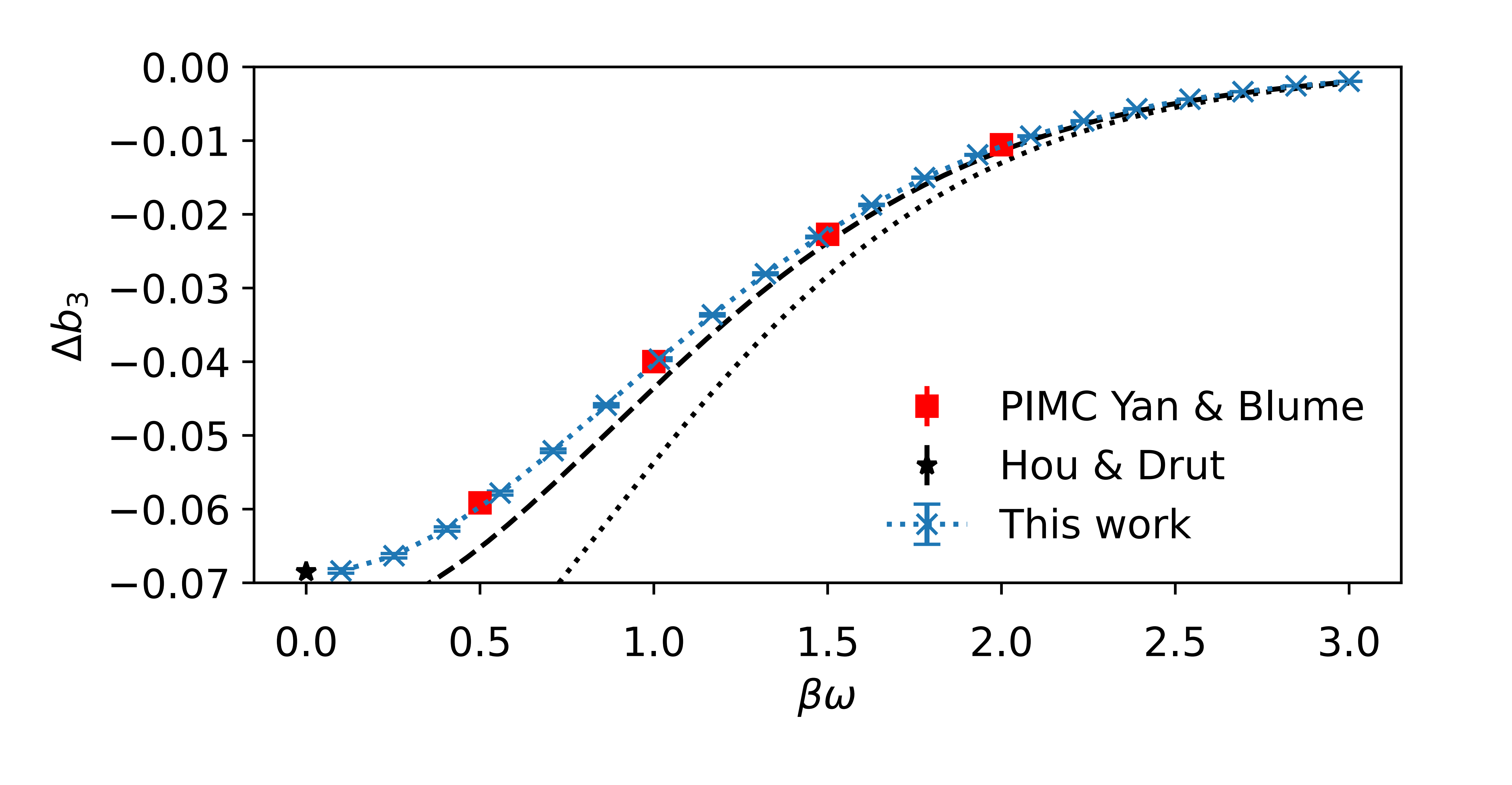
$\Delta b_8 : 5$

$\Delta b_9 : 4$

The future: Harmonically trapped case

3D fermions at unitarity (Phys. Rev. Research, in print)

Y. Hou, A. Czejdo, K. Morrell, J. E. Drut
Phys. Rev. Research (in print)



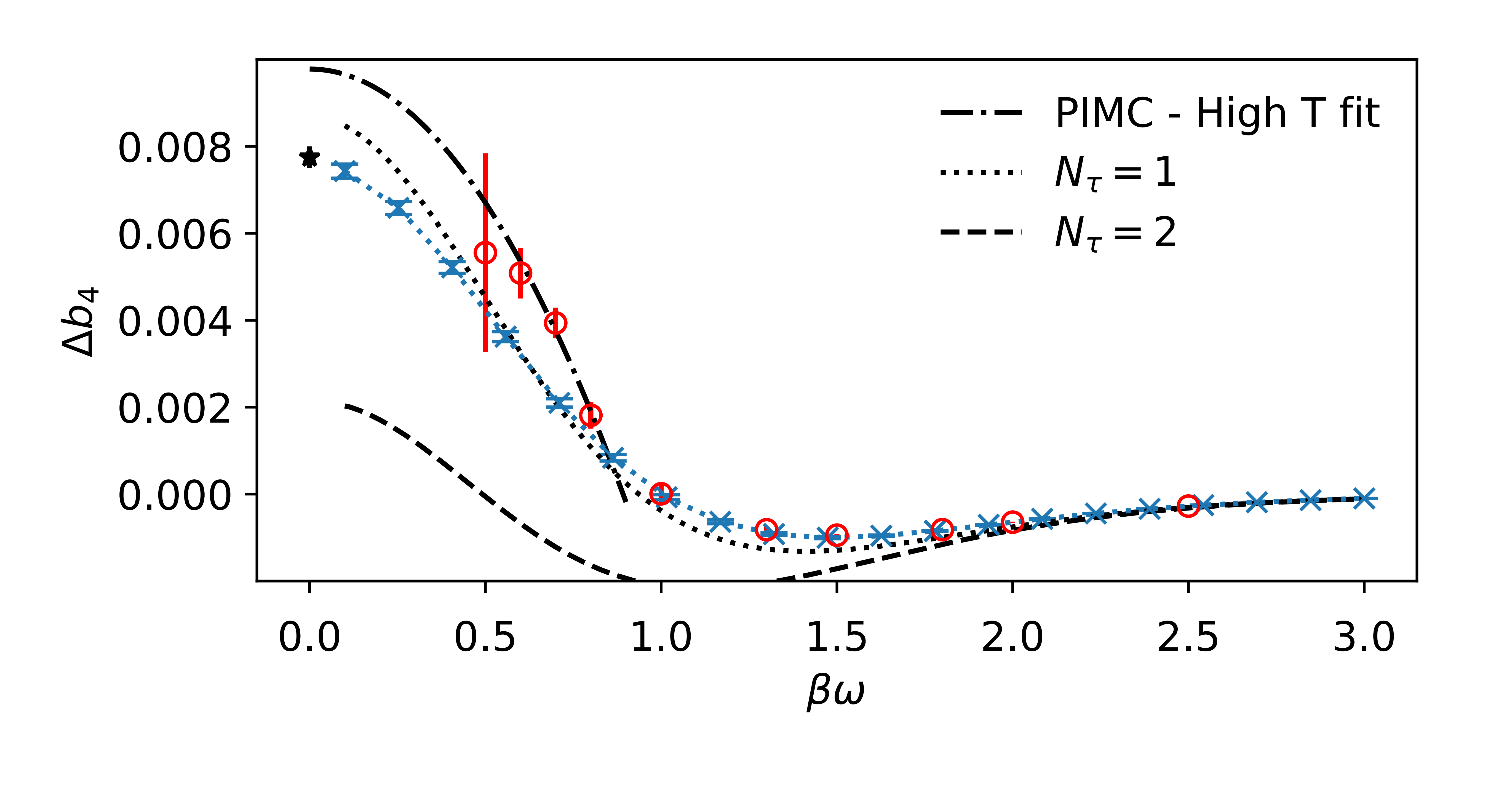
Maximum k: 20

Compared with PIMC
Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

The future: Harmonically trapped case

3D fermions at unitarity (Phys. Rev. Research, in print)

Y. Hou, A. Czejdo, K. Morrell, J. E. Drut
Phys. Rev. Research (in print)

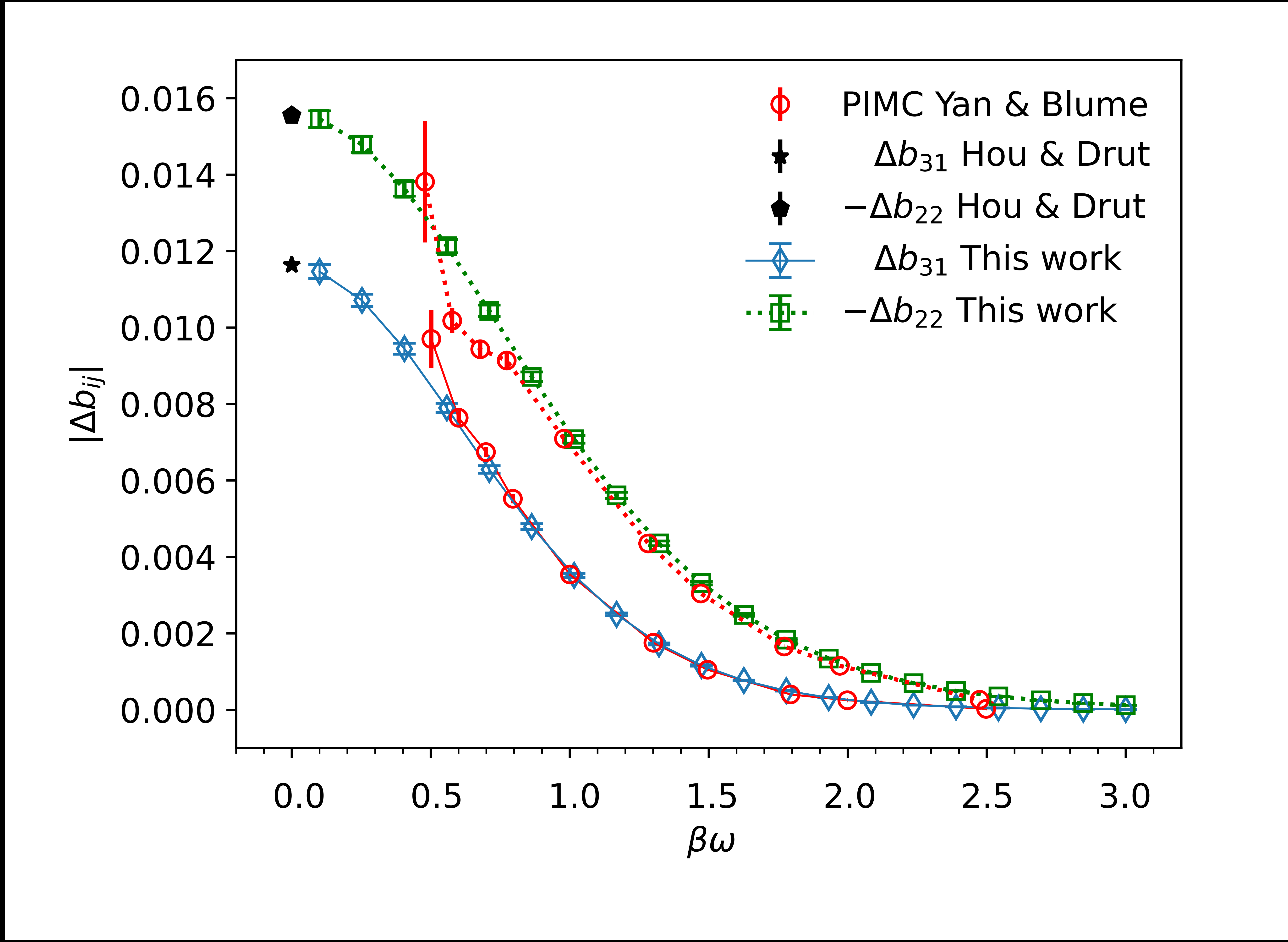


Maximum k: 16, 12

Compared with PIMC
Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

The future: Harmonically trapped case

3D fermions at unitarity (Phys. Rev. Research, in print)



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Phys. Rev. Research (in print)

Maximum k: 16, 12

Compared with PIMC
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Phys. Rev. Lett. **116**, 230401 (2016)

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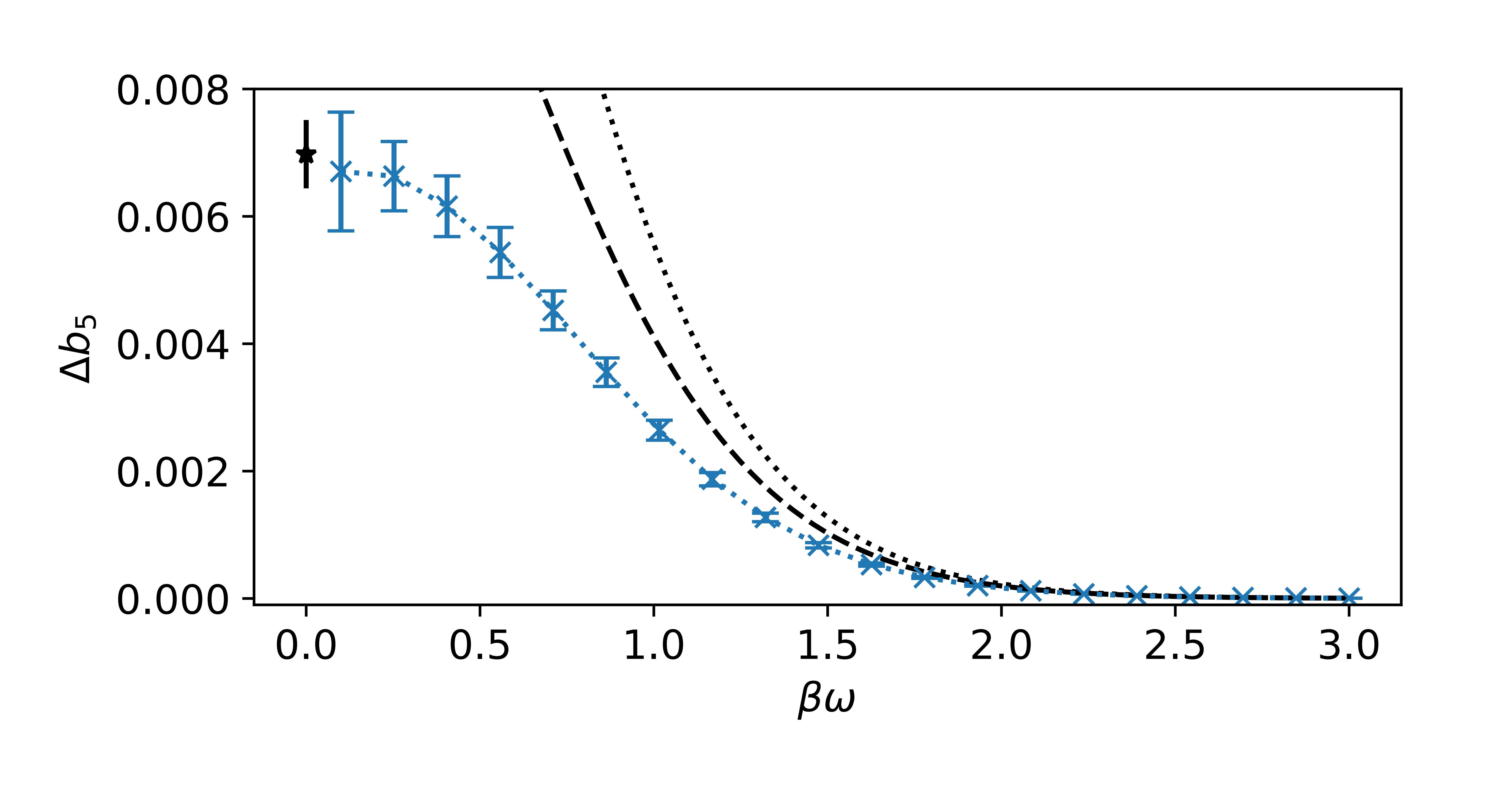

Maximum k: 12, 8

Compared with PIMC
Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

Summary

- Nuclear astrophysics and ultracold atoms need finite-temperature quantum many-body theory;

- We are exploring a computational idea to bridge between entirely numerical and entirely analytic approaches to quantum many-body physics, namely automated algebra;

- That idea has allowed us to push the virial expansion to new limits, also shedding light where previous methods came short;

- We used the results, complemented with resummation techniques, to access the thermodynamics of strongly coupled matter.

The future

- We are generalizing automated-algebra methods to other physical situations (attractive Bose gases, harmonically trapped systems, nuclear matter) and observables beyond thermodynamics;

- Calculations at higher orders in the VE are possible and desirable to apply resummation methods.

Thank you!