THERMODYNAMICS OF THE SPIN-POLARIZED UNITARY FERMI GAS

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Michigan State University, October 5th, 2018

[LR, Loheac, Drut, Braun *in preparation*]
[LR, Loheac, Drut, Braun arXiv:1807.04664 *(accepted in Phys. Rev. Lett.)*]
[LR, Porter, Drut, Braun *Phys. Rev. D* 96, 094506, 2017]

HGS-HIRe for FAIR
Helmholtz Graduate School for Hadron and Ion Research

Center for Scientific Computing Frankfurt

HIC for FAIR
Helmholtz International Center

TECHNISCHE UNIVERSITÄT DARMSTADT

ultracold quantum gases

densities: ~$\mathbf{10^{14}\,cm^{-3}}$
temperatures: few nK

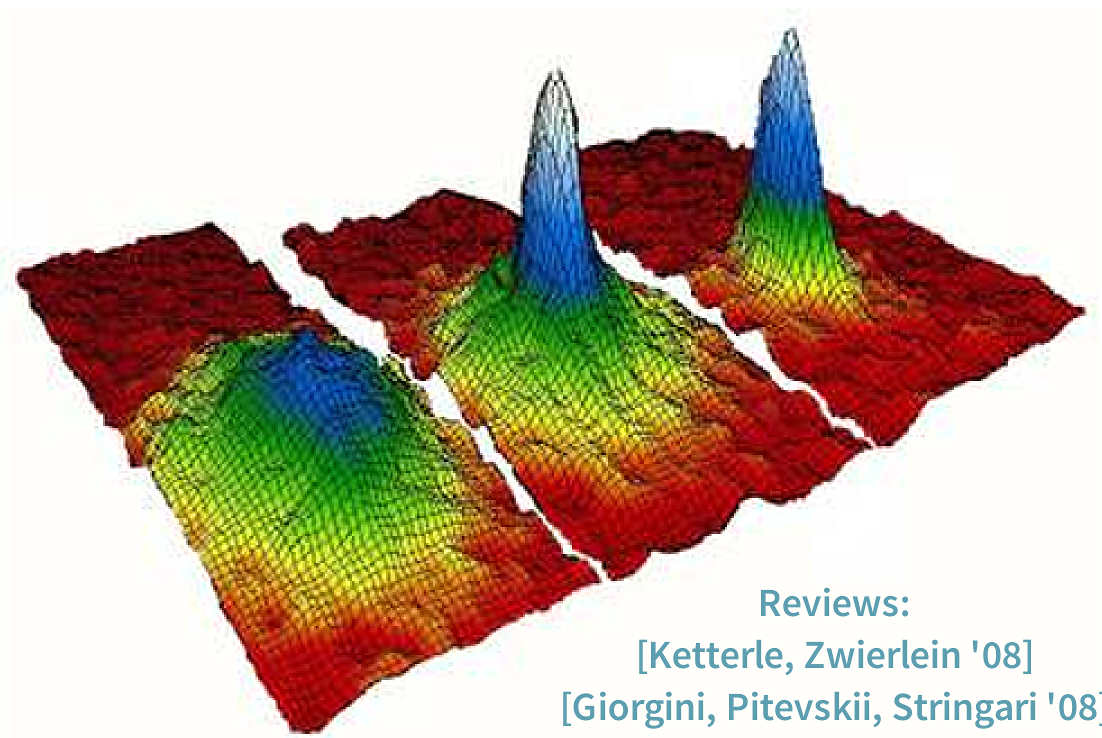
$\boldsymbol{\lambda_T}$ on the order of interparticle distance

quantum regime

experiments: precise control over physical parameters

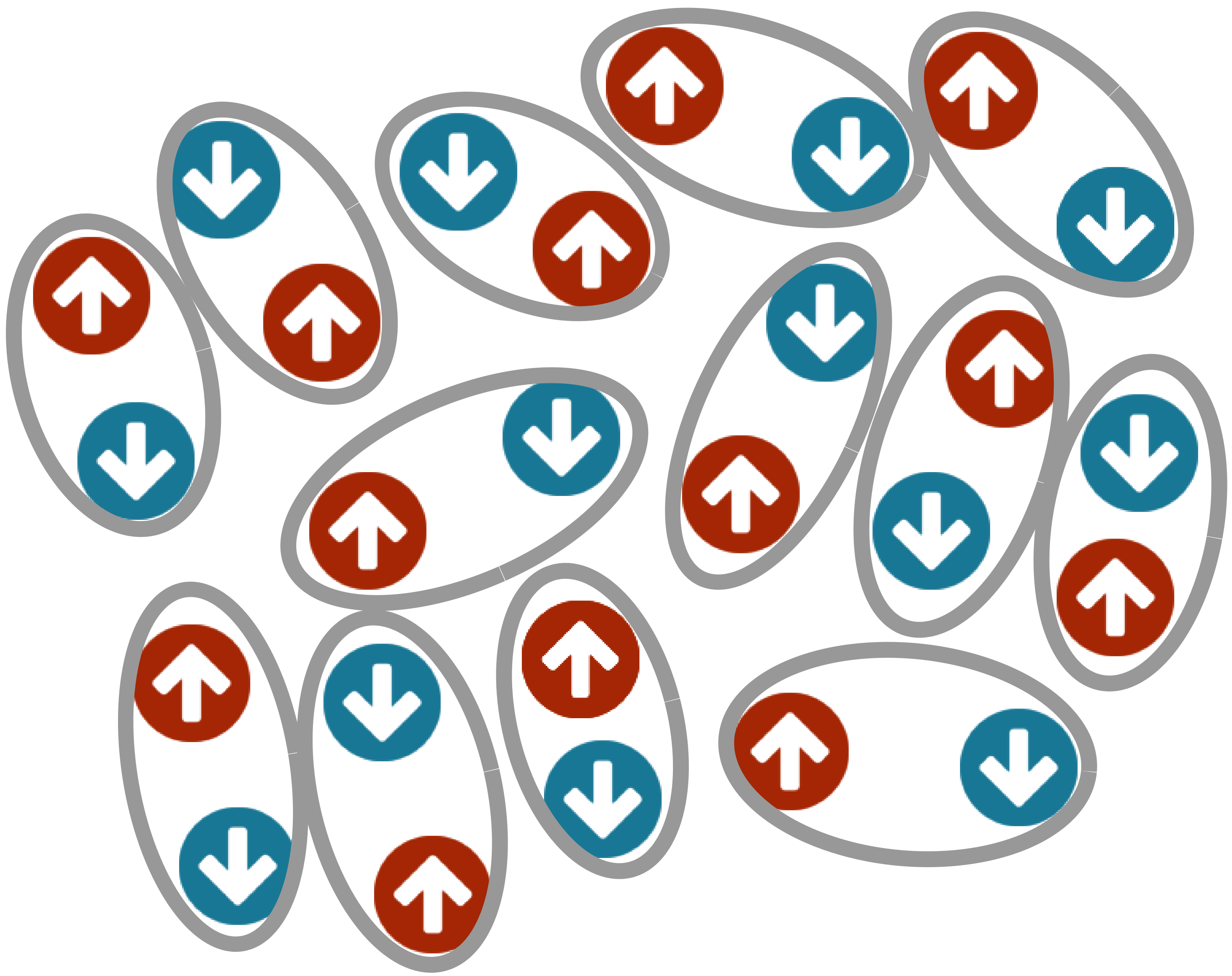
- **interaction** (Feshbach resonances)
- temperature (laser cooling, evaporative cooling ..)
- trapping potential (harmonic, box, lattice ..)
- spatial dimension (anisotropic potentials)
- statistics (**fermions**, bosons, mixtures..)
- **polarization** & mass-imbalance

rich phenomenology!



Reviews:
[Ketterle, Zwierlein '08]
[Giorgini, Pitevskii, Stringari '08]
[Bloch, Dalibard, Zwerger '08]

balanced Fermi gas

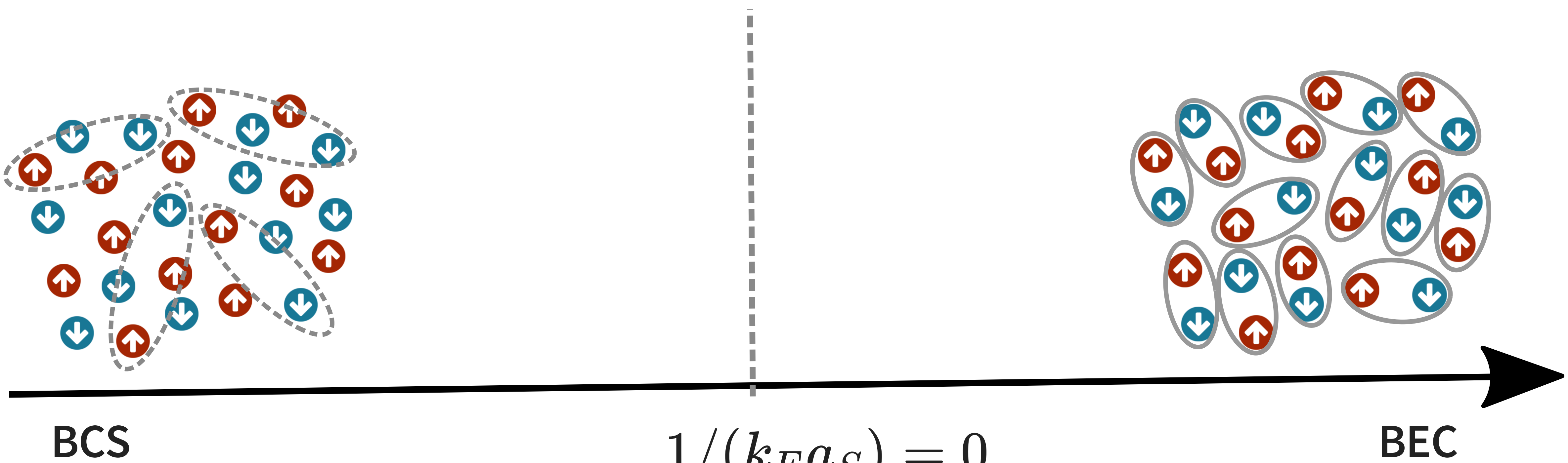


BEC pairing

the unitary Fermi gas

[reviews: Zwerger '12; Mukaiyama,Ueda '13]

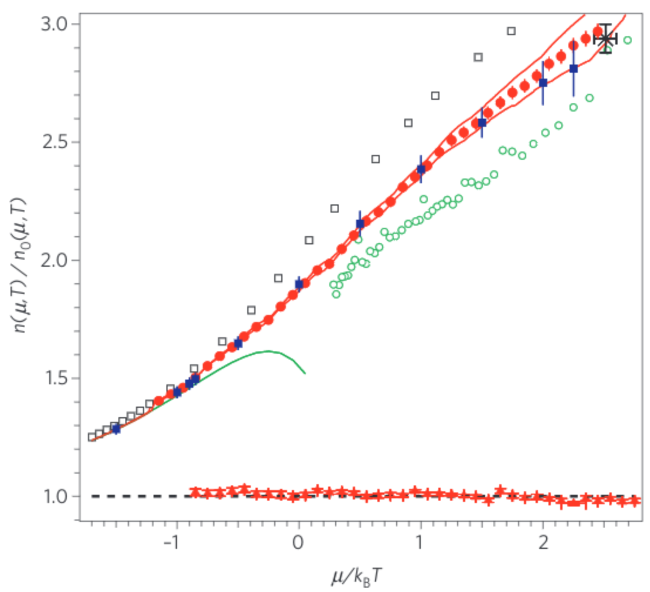
$$a_S \gg n^{-1/3} \gg r_0$$



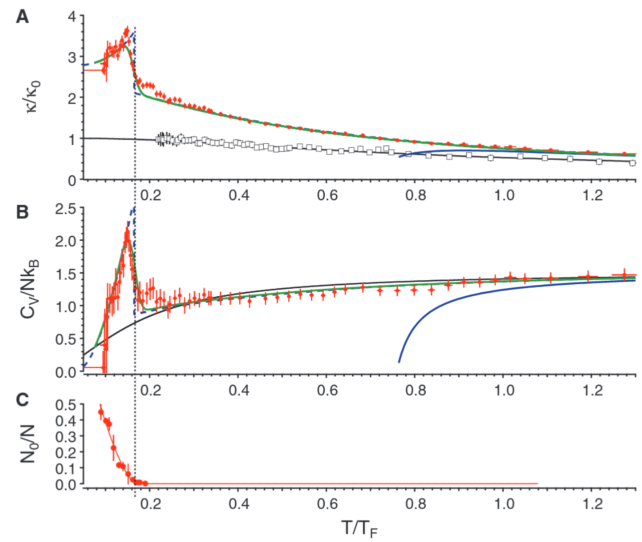
density & temperature are only dimensionful scales in the system

universal scaling: $E = E_0 \; f_E(\beta\mu), P = P_0 \; f_P(\beta\mu) \cdots$

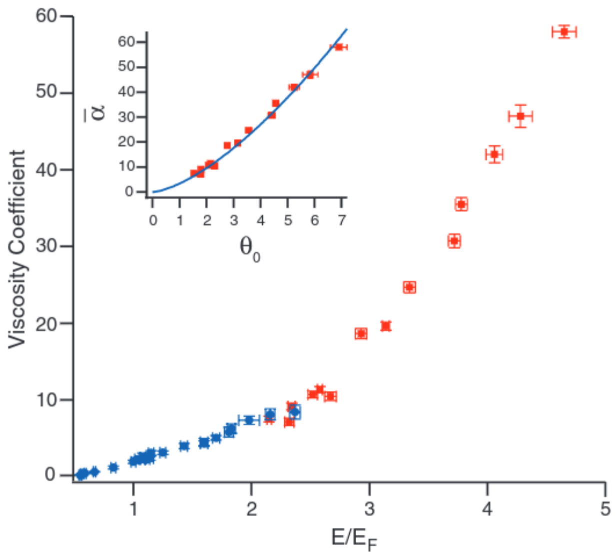
the unitary Fermi gas: many experiments



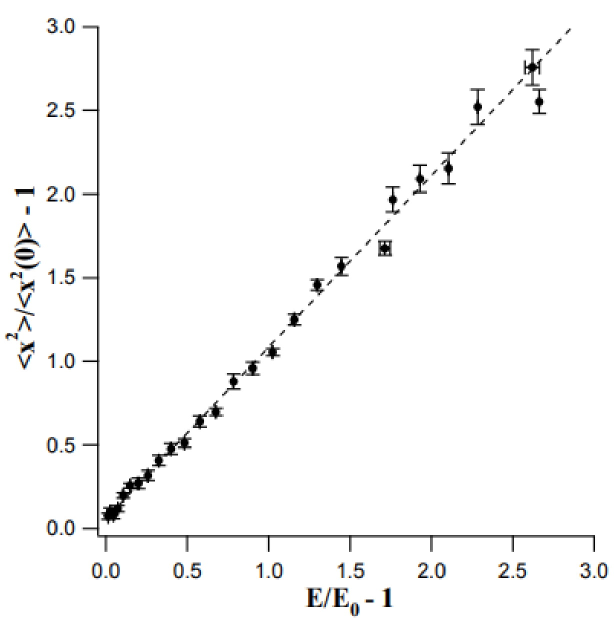
[van Houcke et al. '12]



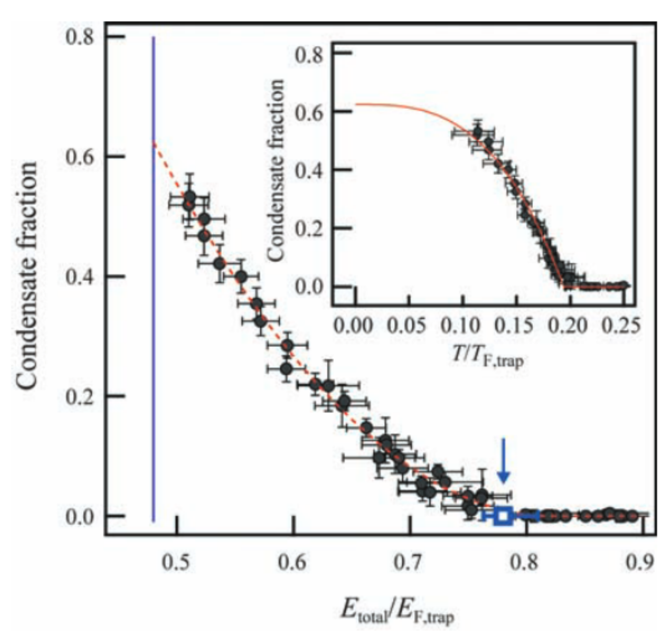
[Ku et al. '12]



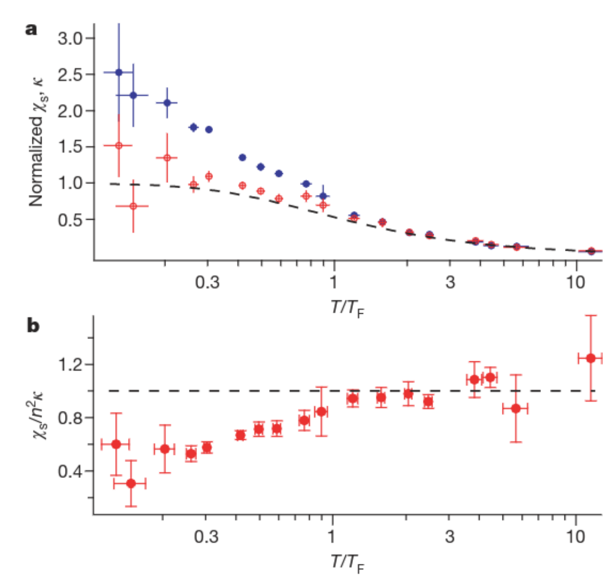
[Cao et al. '11]



[Thomas, Kinast, Turpalov '05]

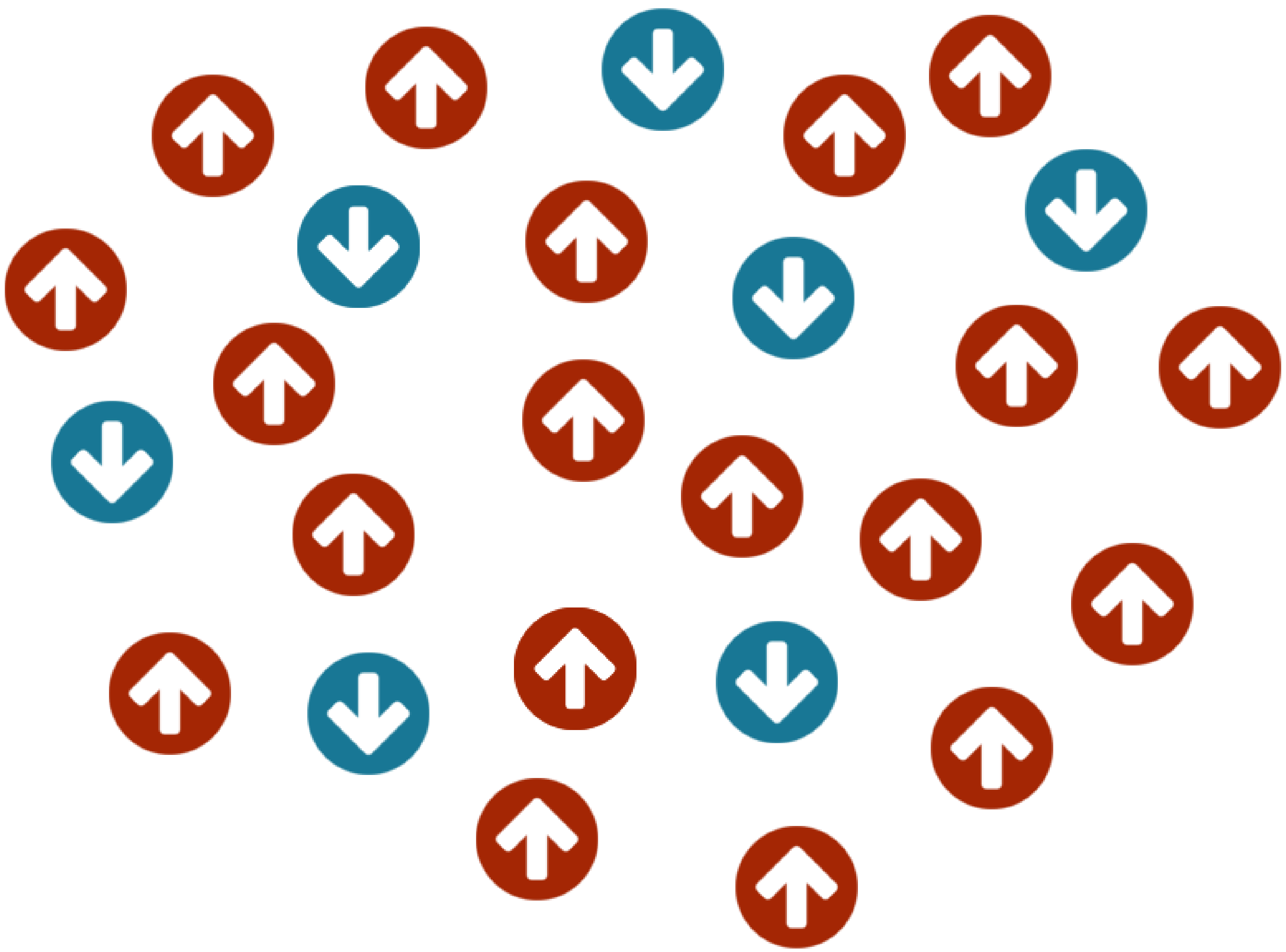


[Horikoshi et al. '10]



[Sommer et al. '11]

spin polarization



[reviews: Chevy '10; Gubbels,Stoof '13]

THE PLAN:
AB INITIO THERMODYNAMICS OF THE UFG

method:

why is it challenging and what to do about it?

key questions:

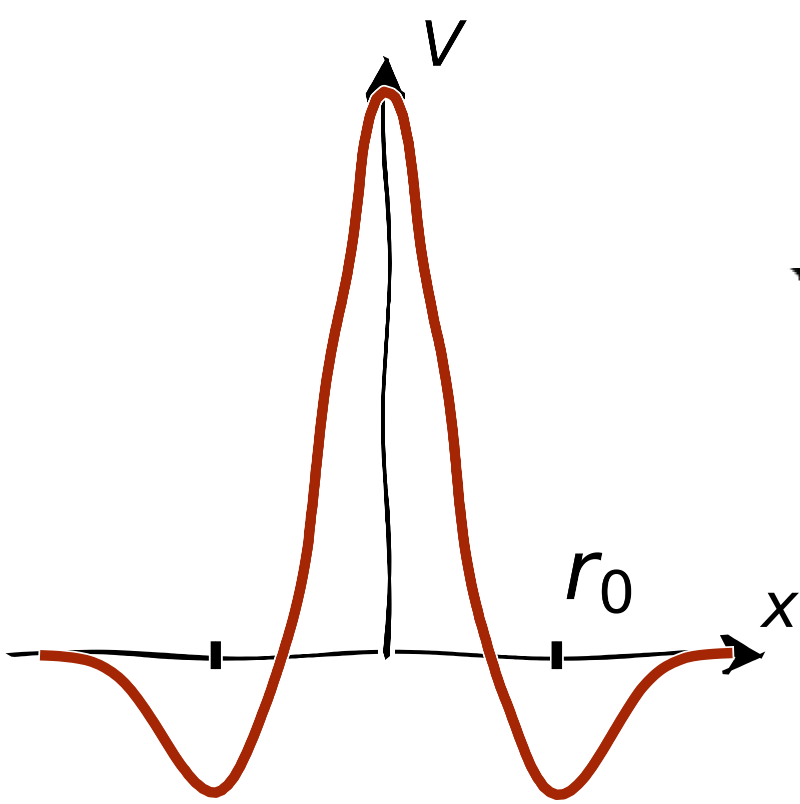
can we get the EOS for polarized systems?

how does T_C change with polarization?

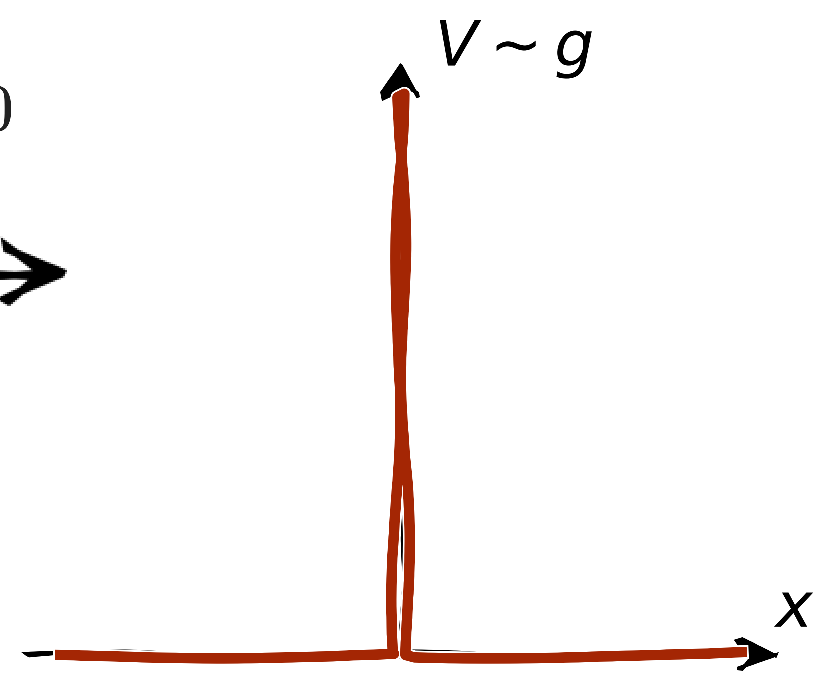
model: contact interaction

$$\hat{H} = -\sum_{s=\uparrow,\downarrow} \int d^d x \; \hat{\psi}^\dagger_s(\vec{x}) \left(\frac{\hbar^2 \vec{\nabla}^2}{2m_s} \right) \hat{\psi}_s(\vec{x})$$

$$+ \, g \int d^d x \; \hat{\psi}^\dagger_\uparrow(\vec{x}) \, \hat{\psi}_\uparrow(\vec{x}) \, \hat{\psi}^\dagger_\downarrow(\vec{x}) \, \hat{\psi}_\downarrow(\vec{x})$$



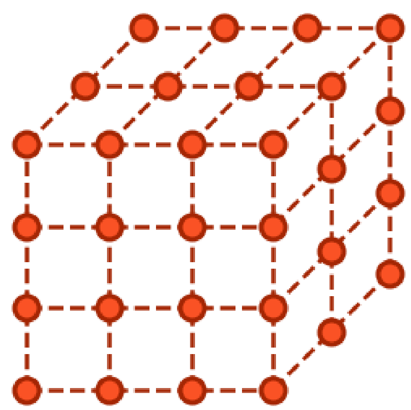
$$k_F^{-1} \gg r_0$$



what do we need to compute?

$$\mathcal{Z} = \mathrm{Tr}[\mathrm{e}^{-\beta\hat{H}}] = \mathrm{Tr}[\mathrm{e}^{-\beta(\hat{T}+\hat{V})}]$$

$$\langle\mathcal{O}\rangle = \frac{1}{\mathcal{Z}}\mathrm{Tr}[\hat{\mathcal{O}}\,\mathrm{e}^{-\beta\hat{H}}]$$



+ Trotter decomposition

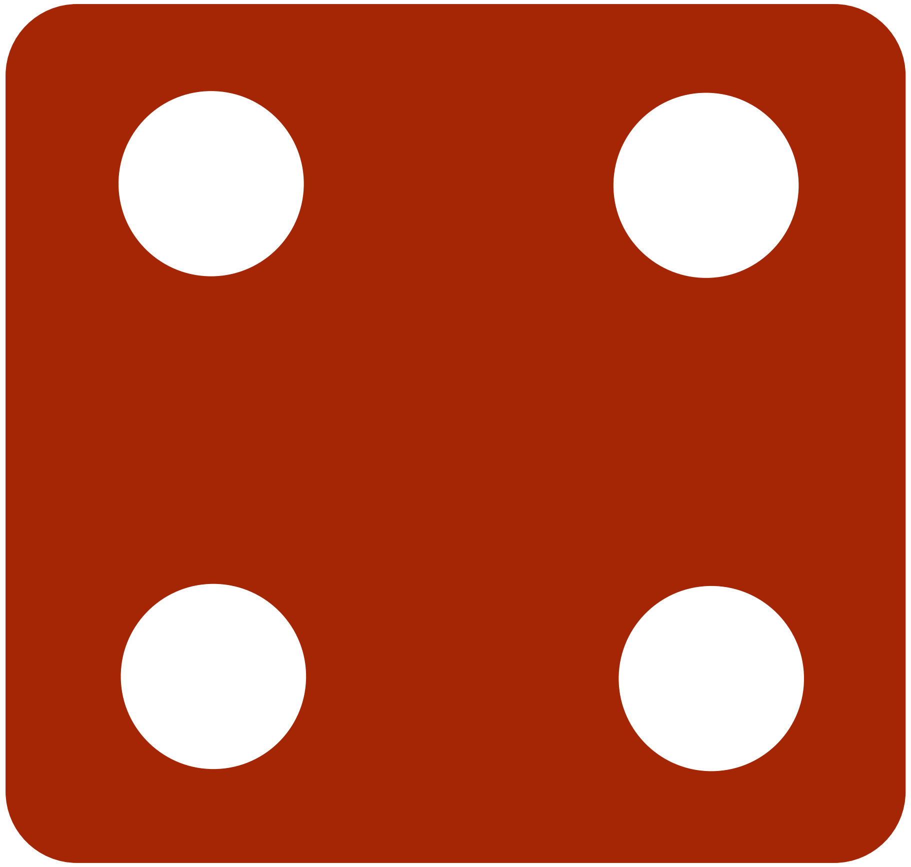
+ Hubbard-Stratonovich transformation

rewrite the problem as a path-integral:

$$\mathcal{Z} = \int\mathcal{D}\phi\;\det M_\phi^{\uparrow}\;\det M_\phi^{\downarrow} \equiv \int\mathcal{D}\phi\,\mathrm{e}^{-S[\phi]}$$

[lattice methods: Lee '09; Drut,Nicholson '13]

roll some dice



(create random auxiliary field configurations)

Monte Carlo in a nutshell

$$\langle \mathcal{O} \rangle = \int \mathcal{D}\phi \, P[\phi] \, \mathcal{O}[\phi]$$

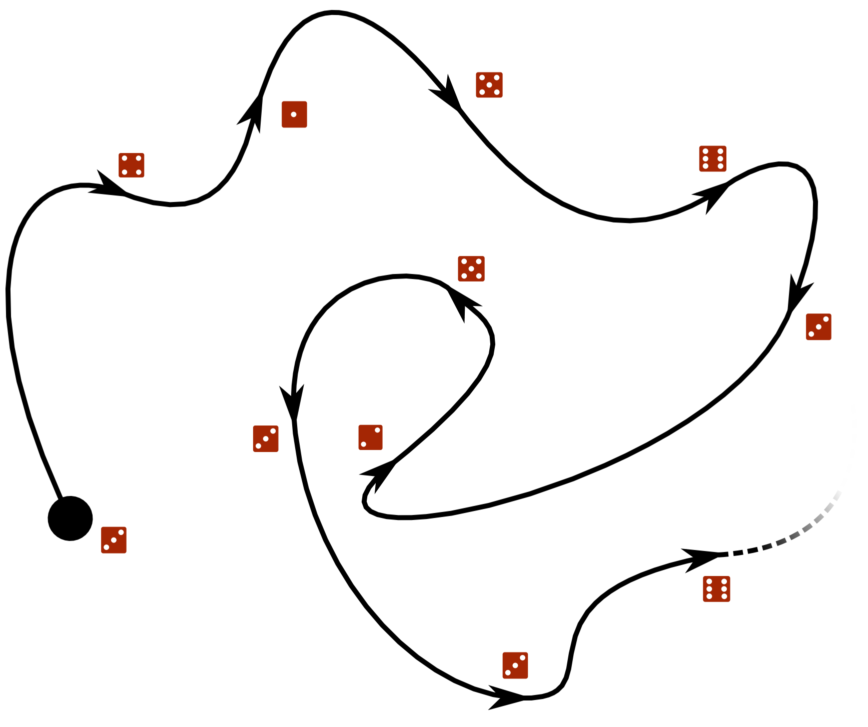
$$P[\phi] = \frac{1}{\mathcal{Z}} \det M_\phi^\uparrow \, \det M_\phi^\downarrow$$

i. produce a random sample of the auxiliary field ϕ

ii. evaluate the integrand with that value

iii. save result & repeat

iv. stop after *enough samples* and compute the average

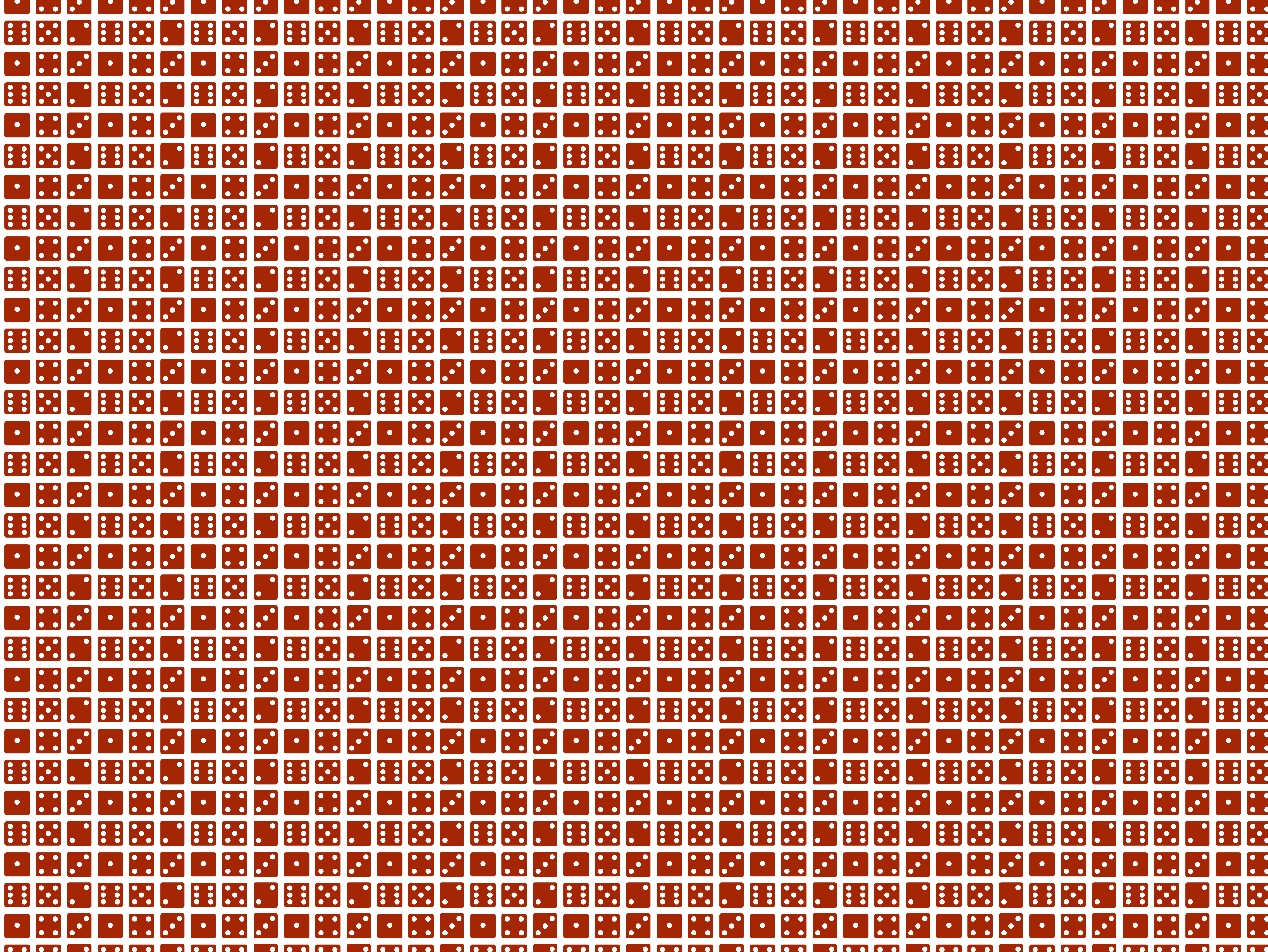


Markov chain typically produced with Metropolis algorithm (accept/reject step)

workhorse of lattice QCD: hybrid Monte Carlo (HMC)

[Duane, Kennedy, Pendleton, Roweth '87]

statistical uncertainty $\propto 1/\sqrt{\#\text{ of (uncorrelated) samples}}$



THE SIGN PROBLEM

(computational effort increases exponentially with system size)

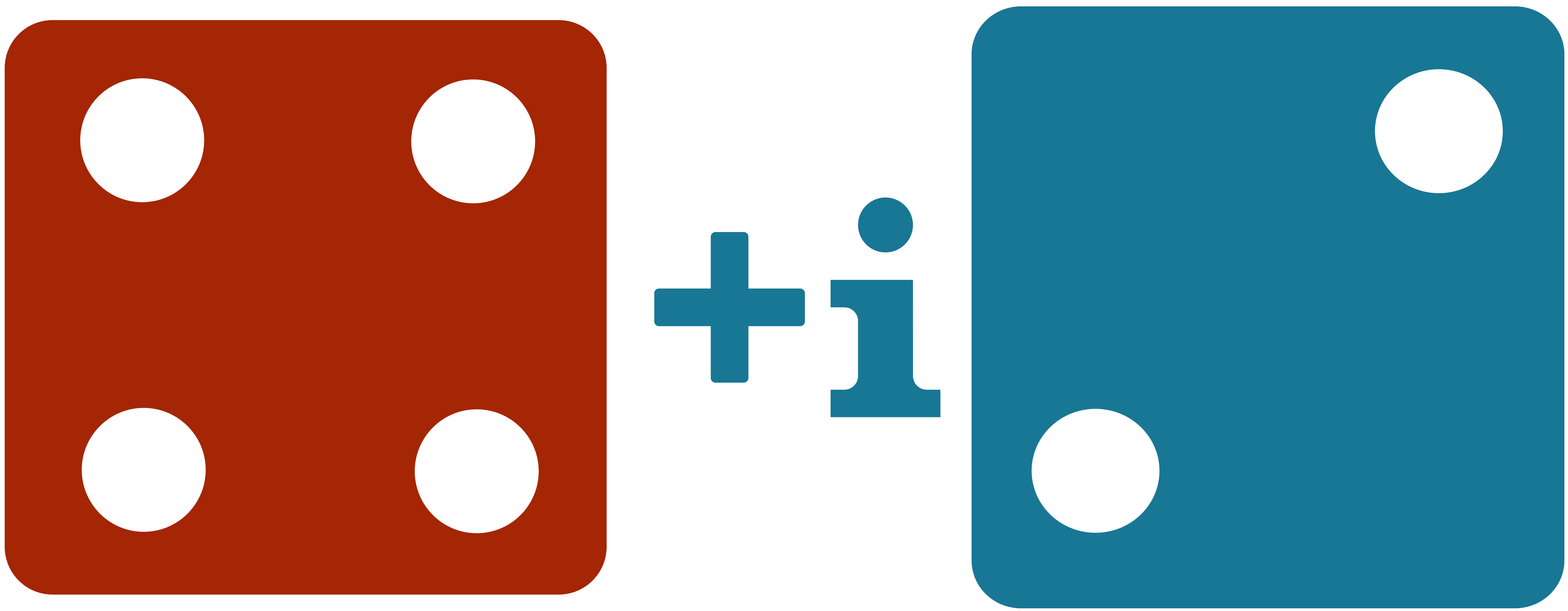
[Troyer, Wiese '05]

$$\mathcal{Z} = \int \mathcal{D}\phi \, \det M_\phi^\uparrow \, \det M_\phi^\downarrow$$

probability measure **not positive (semi-)definite** if any of these conditions applies:

$$N_\uparrow \neq N_\downarrow$$
$$\mu_\uparrow \neq \mu_\downarrow$$
$$m_\uparrow \neq m_\downarrow$$
$$g > 0$$

roll dice with imaginary sides



(complexified auxiliary fields)

stochastic quantization

stochastic quantization: equilibrium distribution of a $(d+1)$-dimensional random process is identified with the probability measure of our d-dimensional path integral

random walk governed by Langevin equation (Brownian motion):

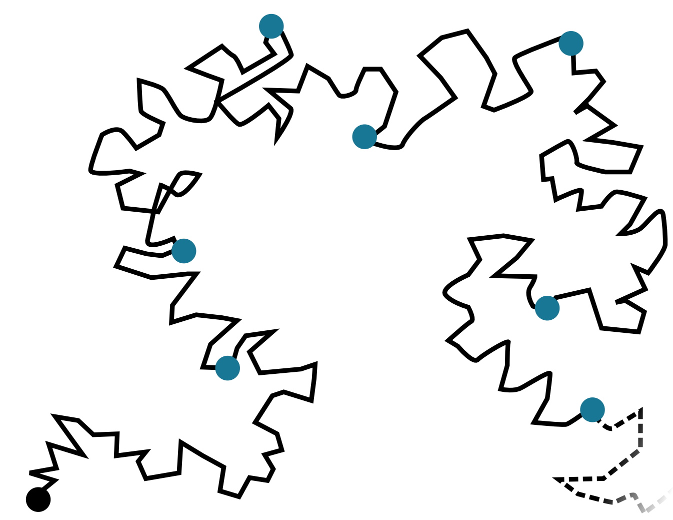
$$\frac{\partial \phi}{\partial t} = -\frac{\delta S[\phi]}{\delta \phi} + \eta_t$$

ficticious time (not physical)

$$\langle \eta \rangle = 0$$
$$\langle \eta_t \eta_{t'} \rangle = 2\delta(t-t')$$

[Parisi, Wu '81; Damgaard,Huffel '87]
[Aarts '09; Seiler '17]
[Loheac, Drut '17; LR, Porter, Drut, Braun '17]

complex Langevin (CL)



use discrete Langevin equations
to produce a Markov chain:

$$\phi_{n+1} = \phi_n + \Delta\phi$$

$$\Delta\phi_R = -\mathrm{Re}\left[\frac{\delta S[\phi]}{\delta\phi}\right]\Delta t + \eta_t\sqrt{\Delta t} \;\; + 2\xi\phi_R\Delta t$$

$$\Delta\phi_I = -\mathrm{Im}\left[\frac{\delta S[\phi]}{\delta\phi}\right]\Delta t \;\; + 2\xi\phi_I\Delta t$$

**introduce
a "regulator"**

[Loheac, Drut '17]

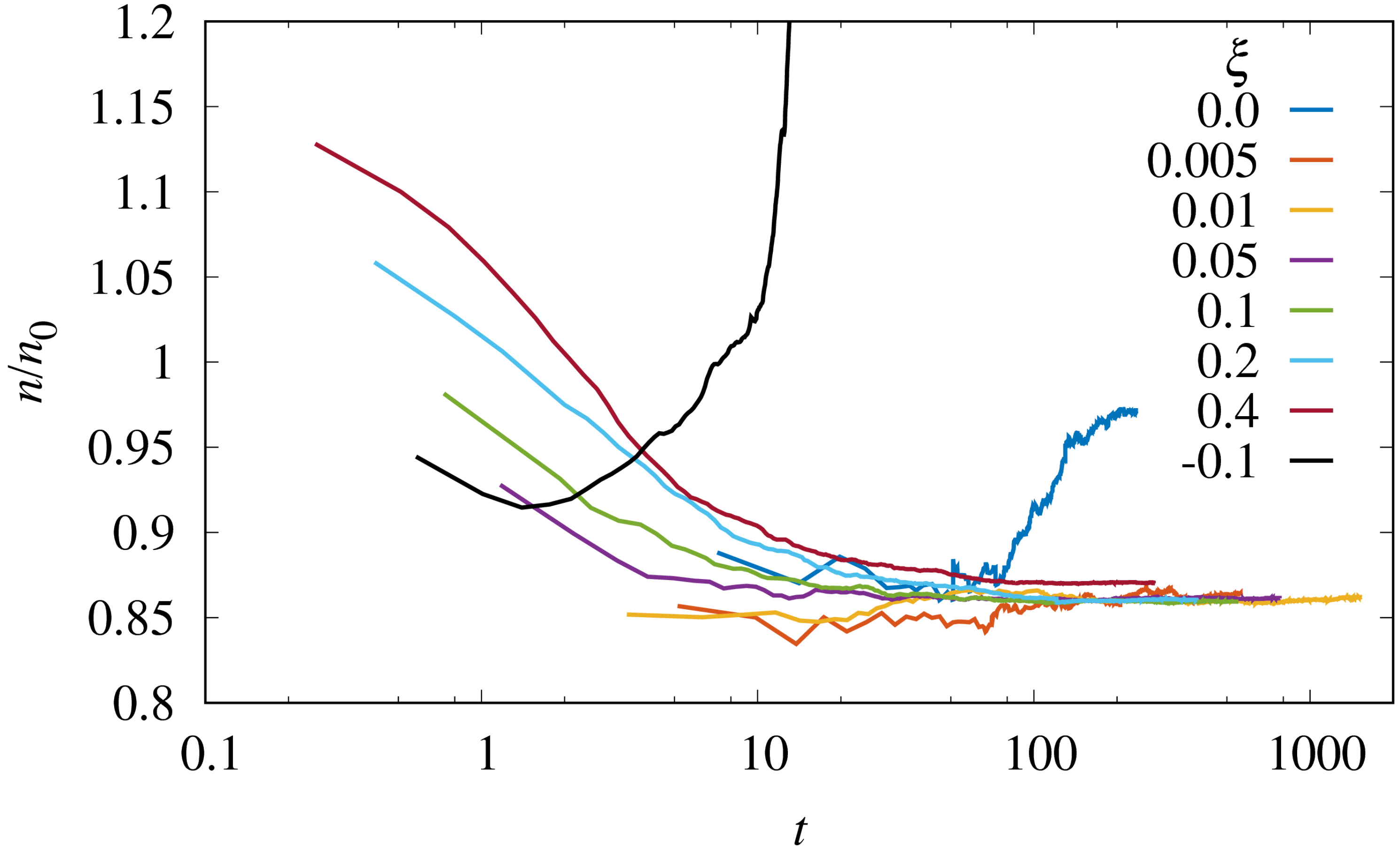
problematic: zeros in the fermion determinant!

$$S[\phi] \;\equiv \ln\left(\det M_\phi^{\uparrow}\; \det M_\phi^{\downarrow}\right)$$

effect of the regulator

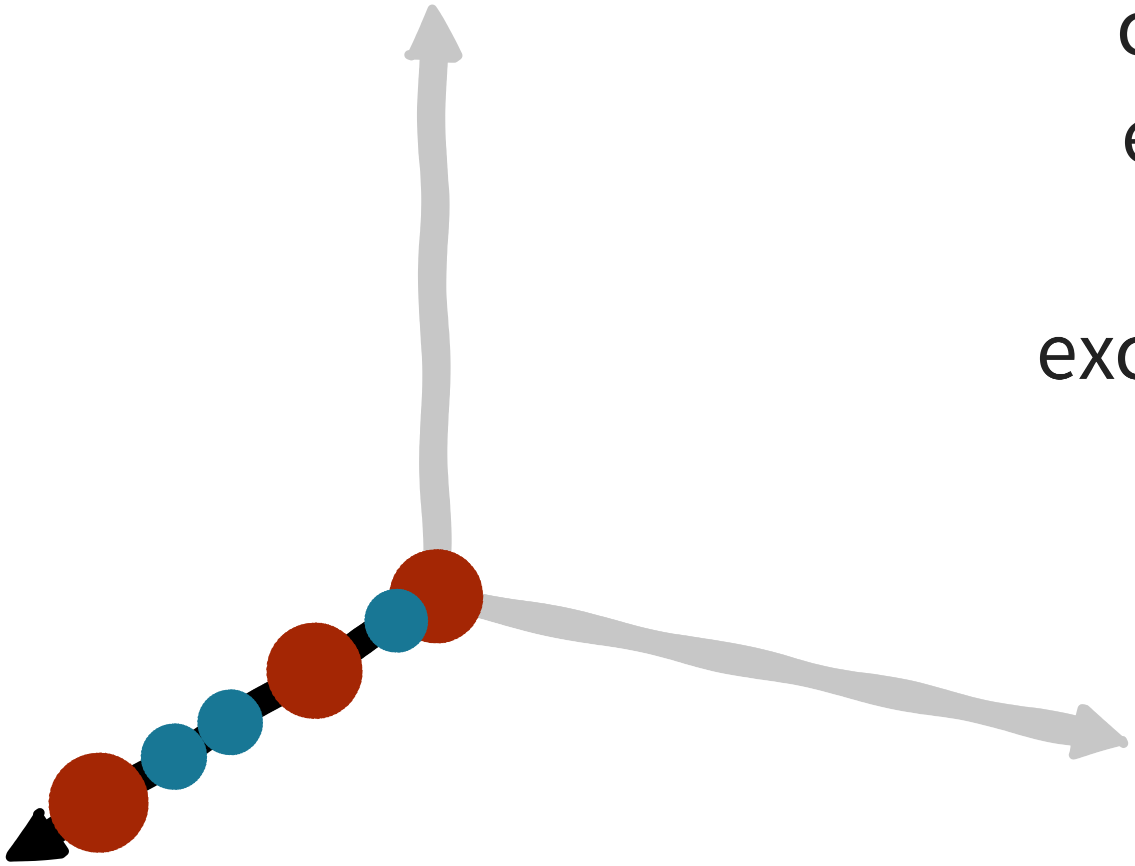
[Loheac,Drut '17]

unregulated runs tend to fail: **ξ stabilizes CL trajectories**



similar approach in QCD: "dynamic stabilization" [Attanasio,Jäger '18]

one-dimensional systems



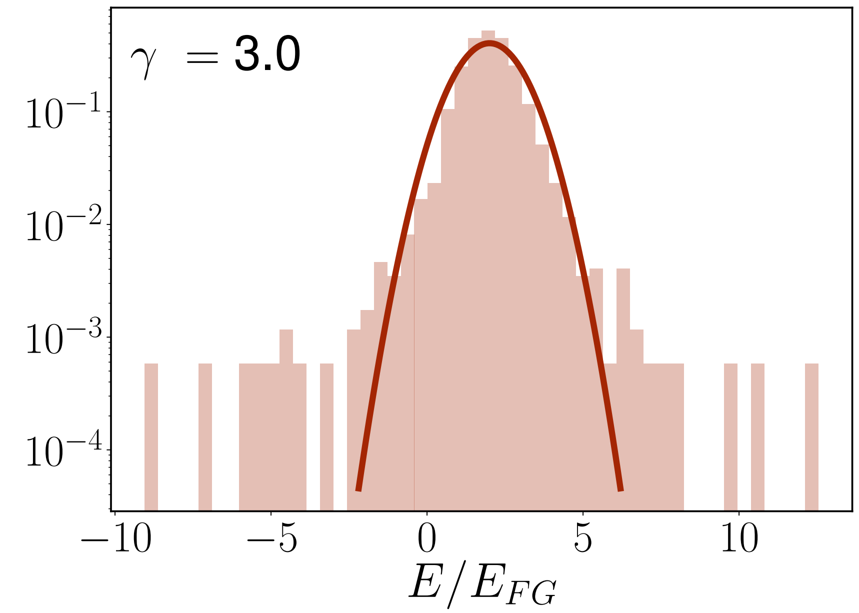
computationally cheap &
exact solutions available
=
excellent benchmark systems

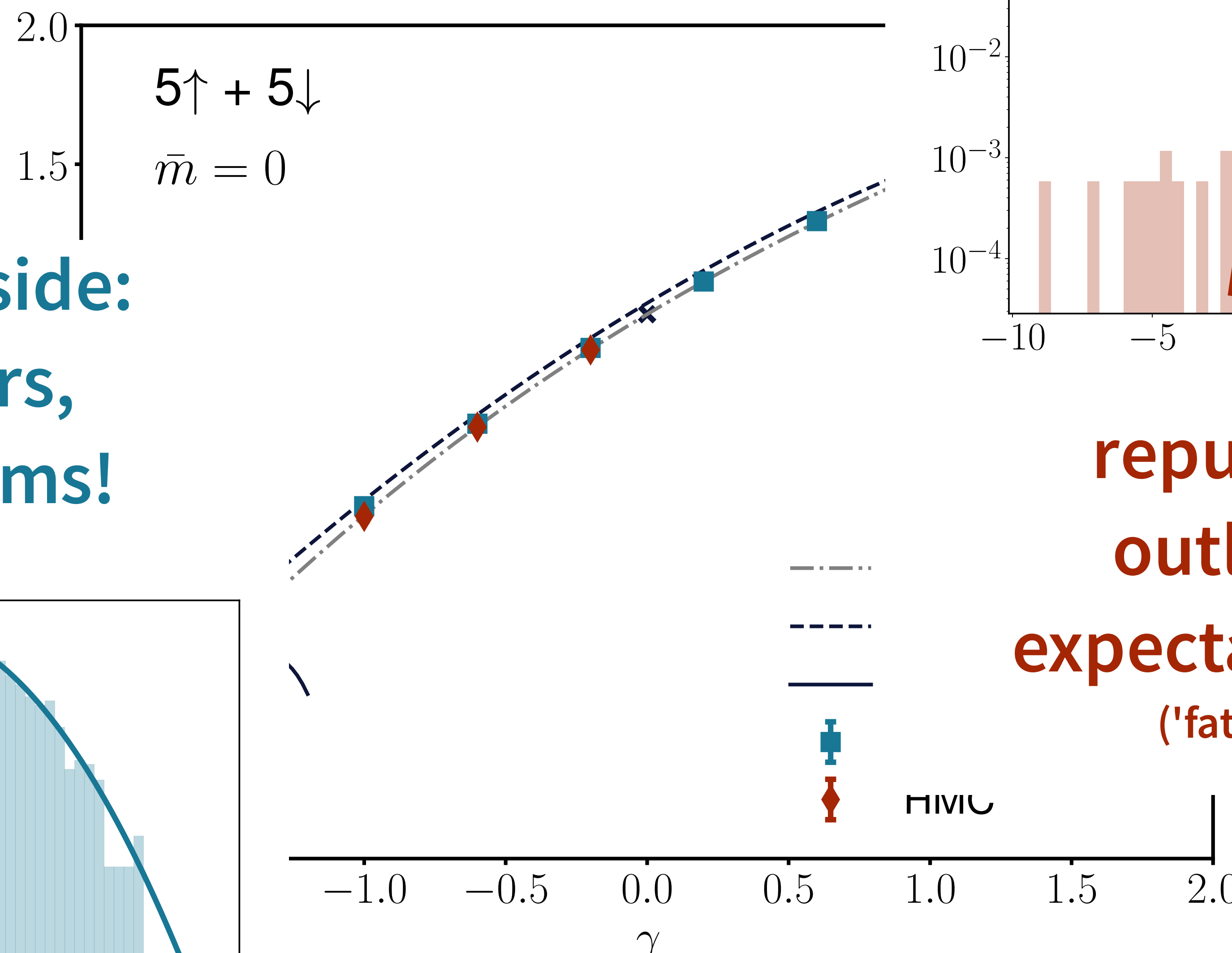
also accessible in experiment

[e.g. Liao et al. '10; Wenz et al. '13; Zürn et al. '13; Murmann et al. '15]

first step: compare to other methods

[LR, Porter, Drut, Braun '17]

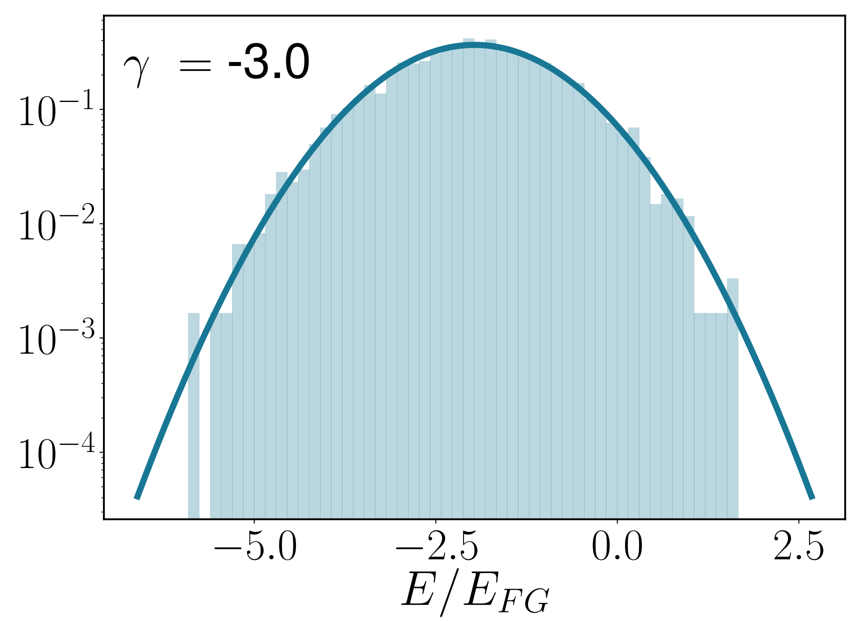




attractive side:
no outliers,
no problems!

repulsive side:
outliers skew
expectation values!
('fat tail' problem)

$$\gamma = g/n$$

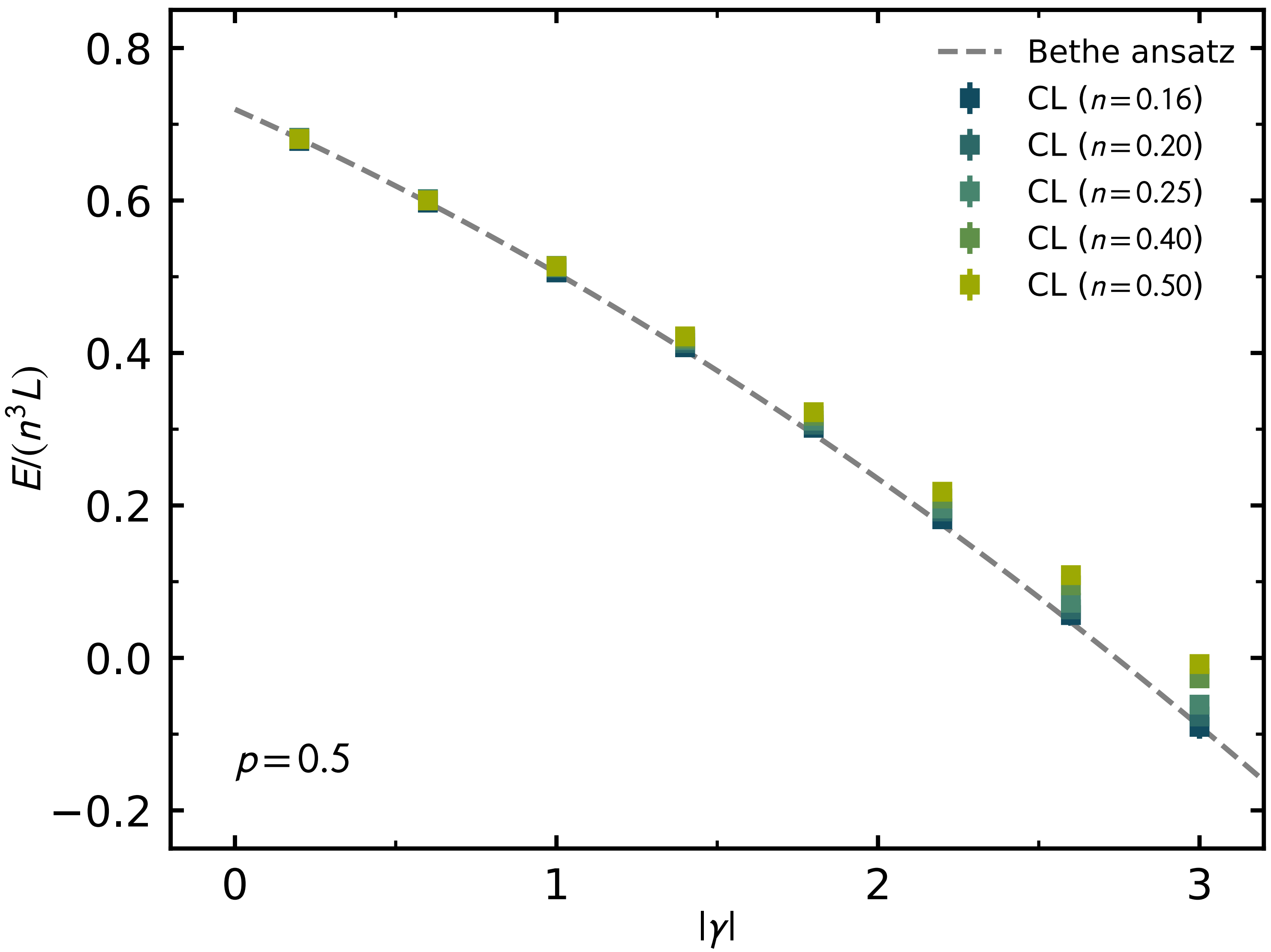


[BA: Iida, Wadati '07; Tracy, Widom '16]
[DFT-RG: Kemler, Pospiech, Braun '17; Kemler '17]
[HMC: LR, Porter, Loheac, Drut '15]

polarized 1D fermions: equation of state

[LR, Drut, Braun *in preparation*]

excellent agreement at low densities (zero-range limit)



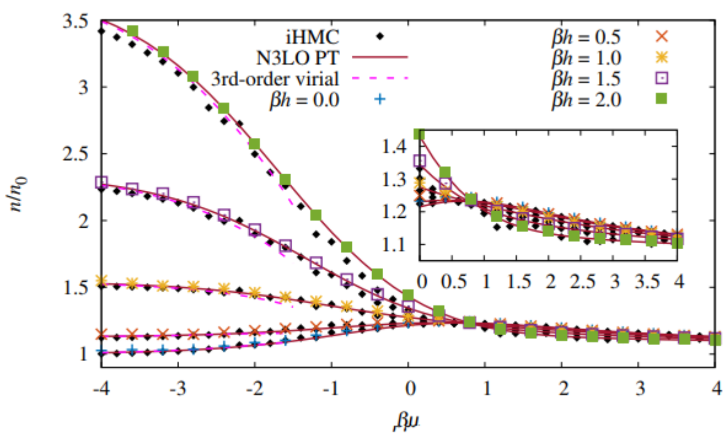
$$\gamma = g/n$$

$$p = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

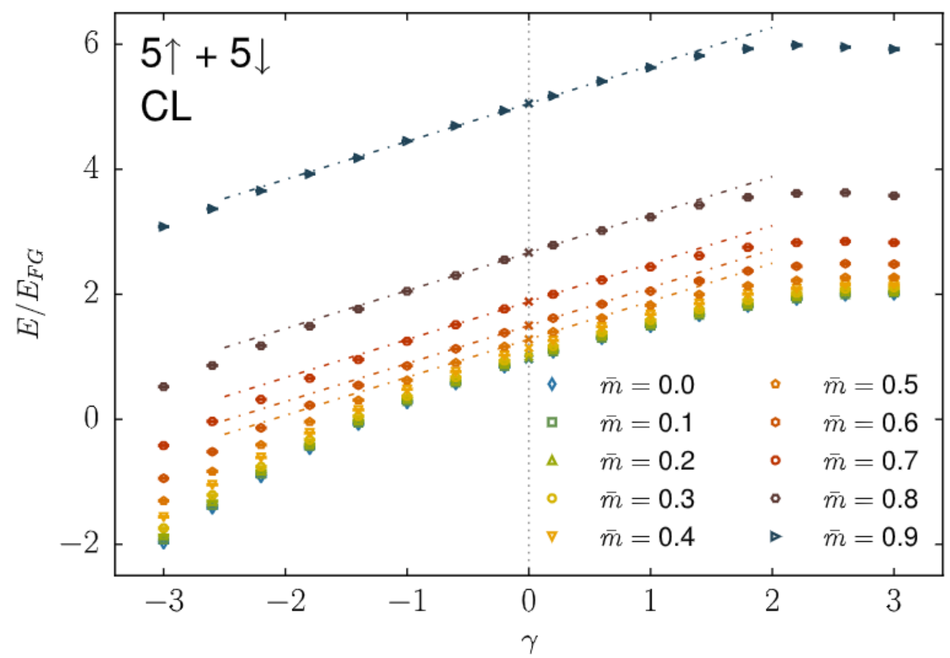
[BA: Iida, Wadati '07; Tracy, Widom '16]

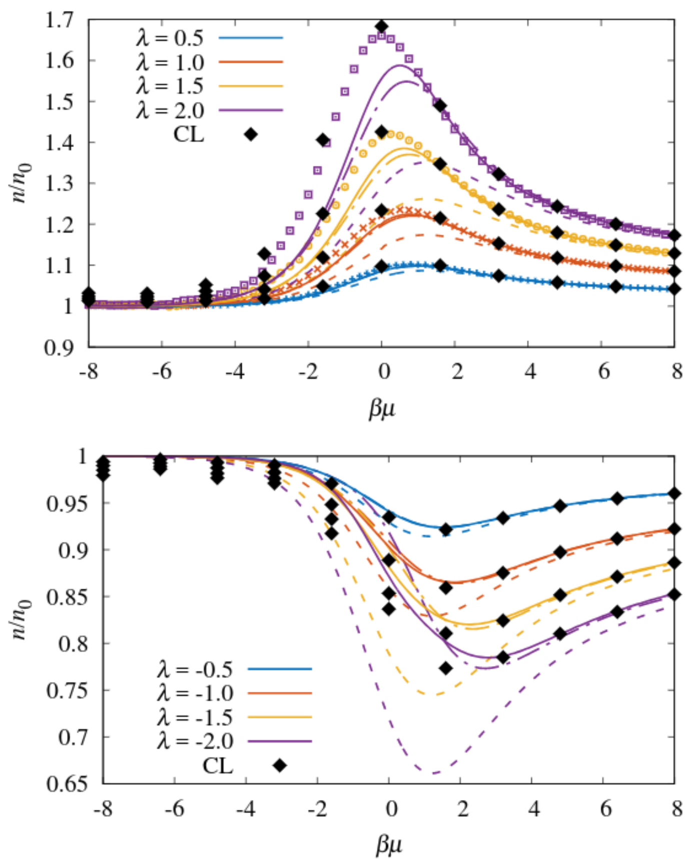
but wait: there's more!

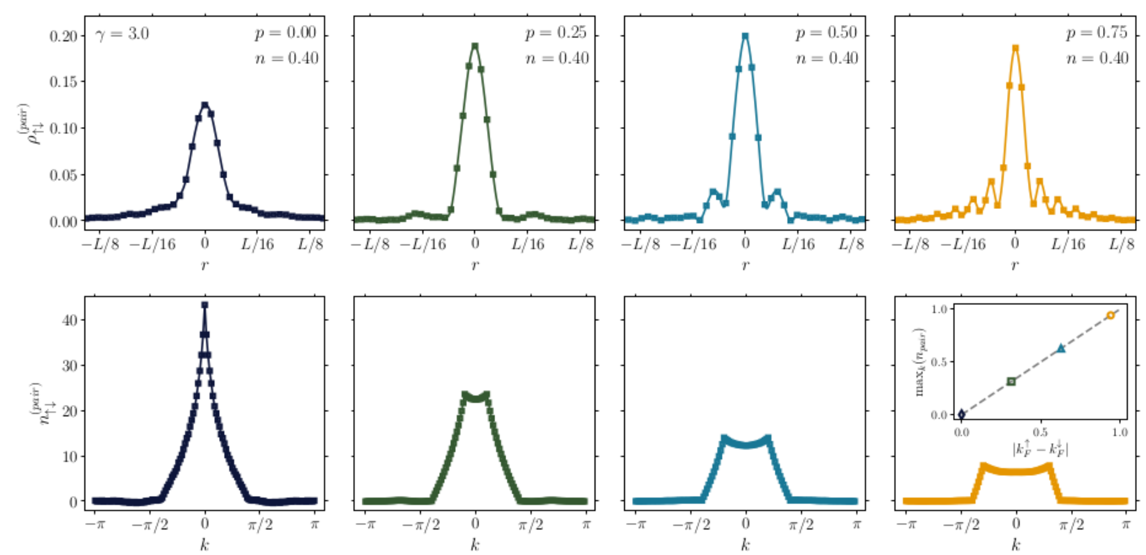
[Loheac,Drut '17]



[LR,Porter,Drut,Braun '17]



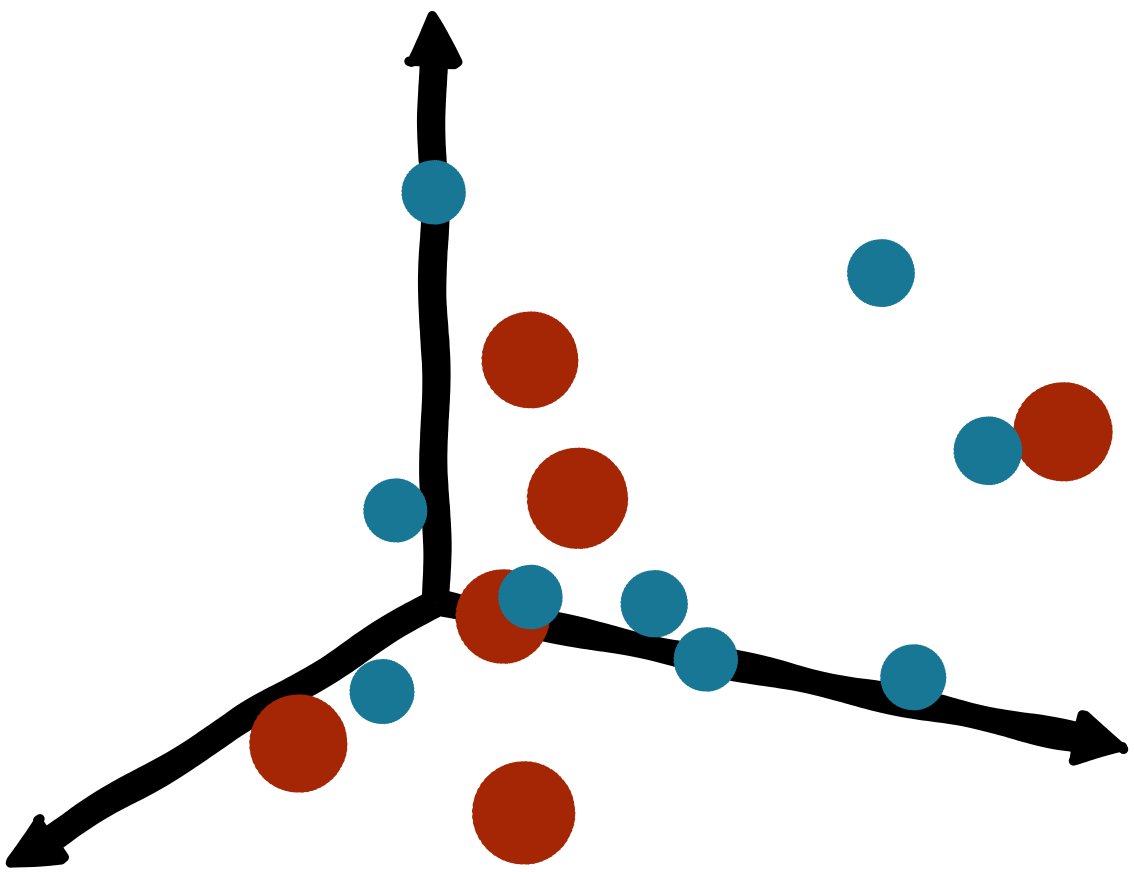




[Loheac,Braun,Drut '18]

[LR,Drut,Braun *in preparation*]

three dimensional systems at $T > 0$

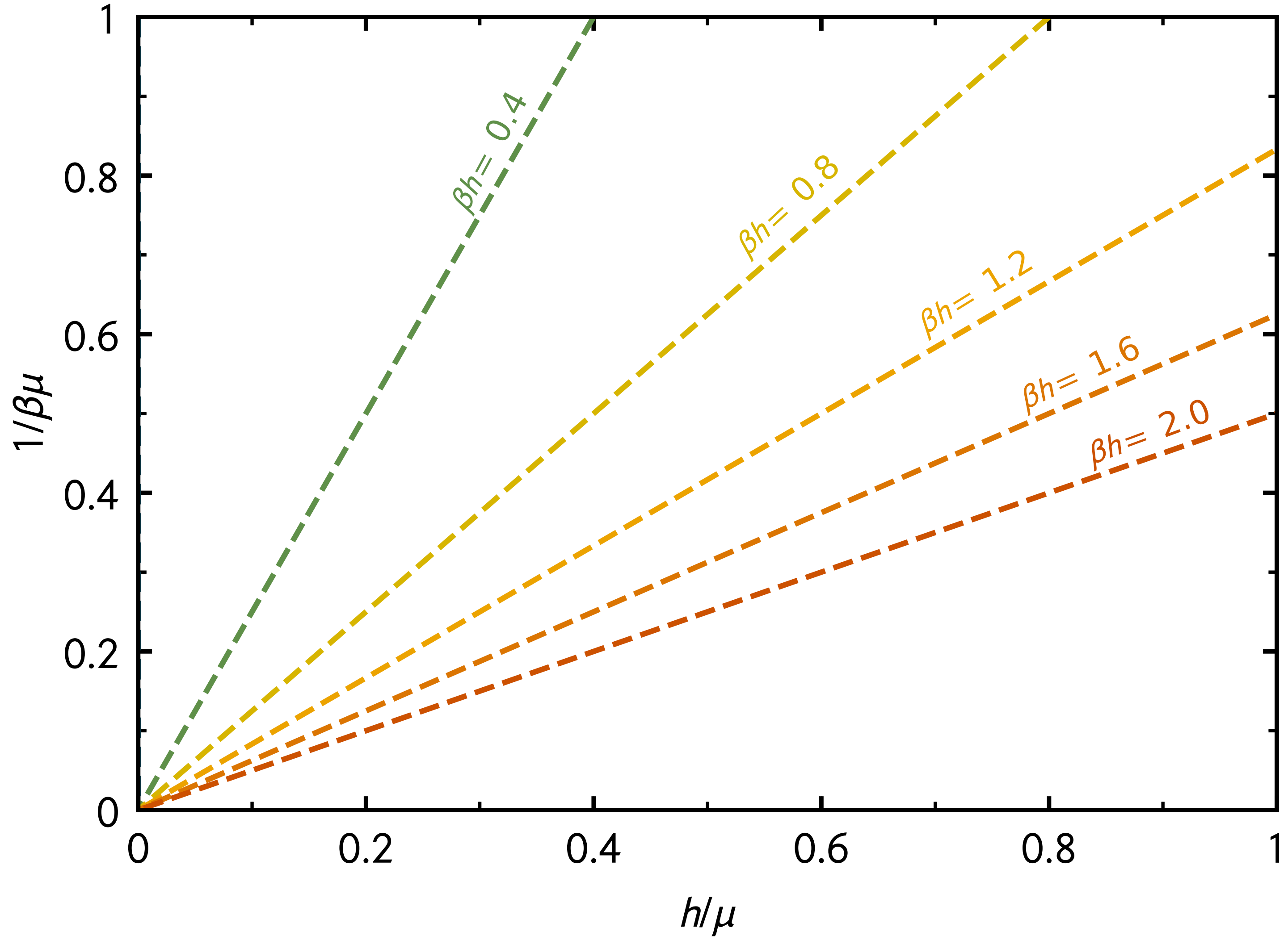


$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu_\uparrow\hat{N}_\uparrow-\mu_\downarrow\hat{N}_\downarrow)}\right]$$
$$= \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N}-h\hat{M})}\right]$$

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

computationally challenging (but feasible)

temperature vs. polarization "phase diagram"



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

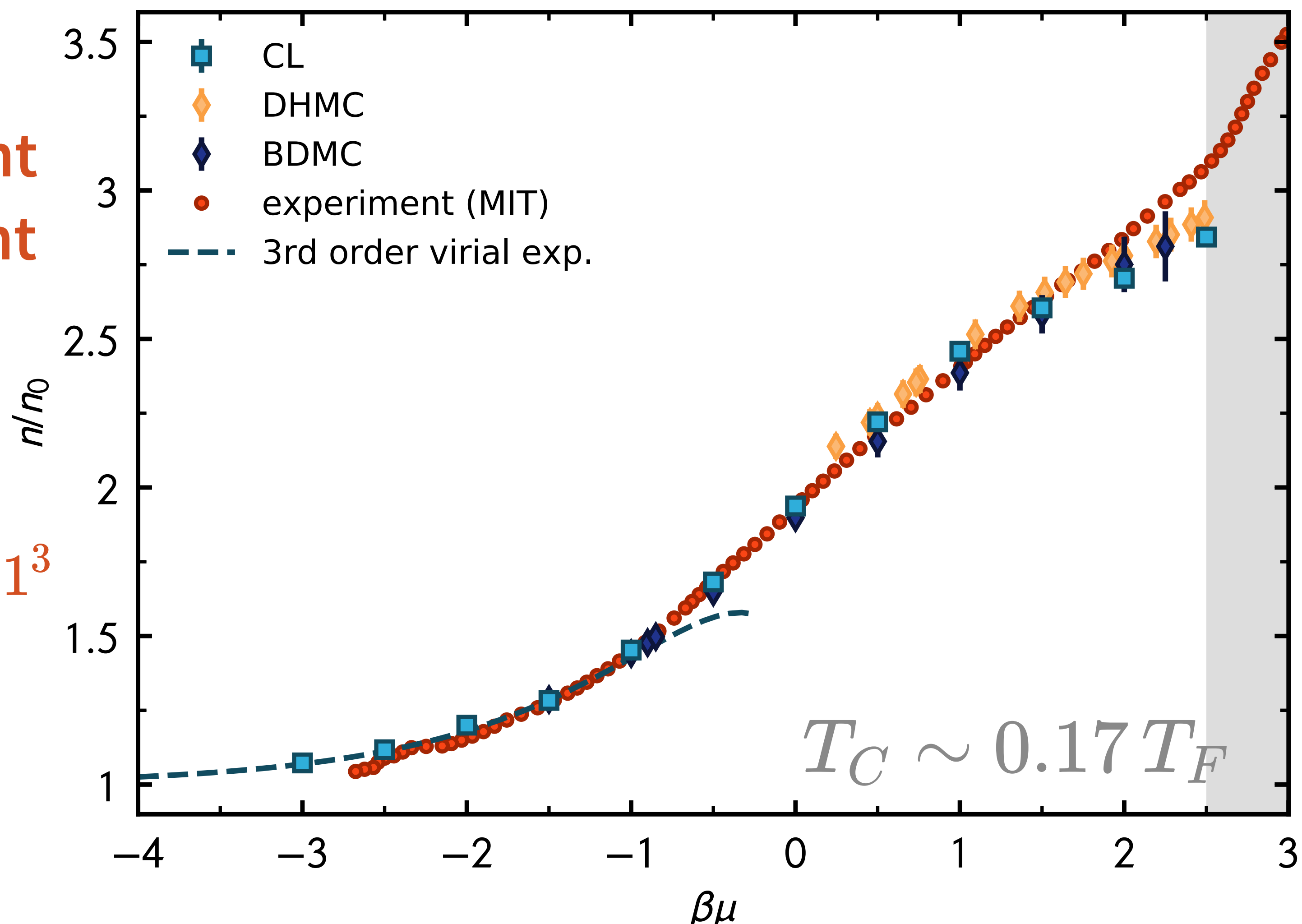
density equation of state

[LR, Loheac, Drut, Braun '18]

[experiment/BDMC: van Houcke et al. '12]
[DHMC: Drut, Lähde, Wlazlowski, Magierski '12]

good agreement with experiment and other methods!

CL results:
finite lattice $V = 11^3$



low temperatures:
λ_T increases
($\lambda_T \ll V^{1/3}$ must be fulfilled)

classical regime

$k_B T$ dominates

quantum regime

E_F dominates

interlude: the virial expansion

dilute gases: few-body correlations dominate

idea: describe the system as expansion in few-body clusters

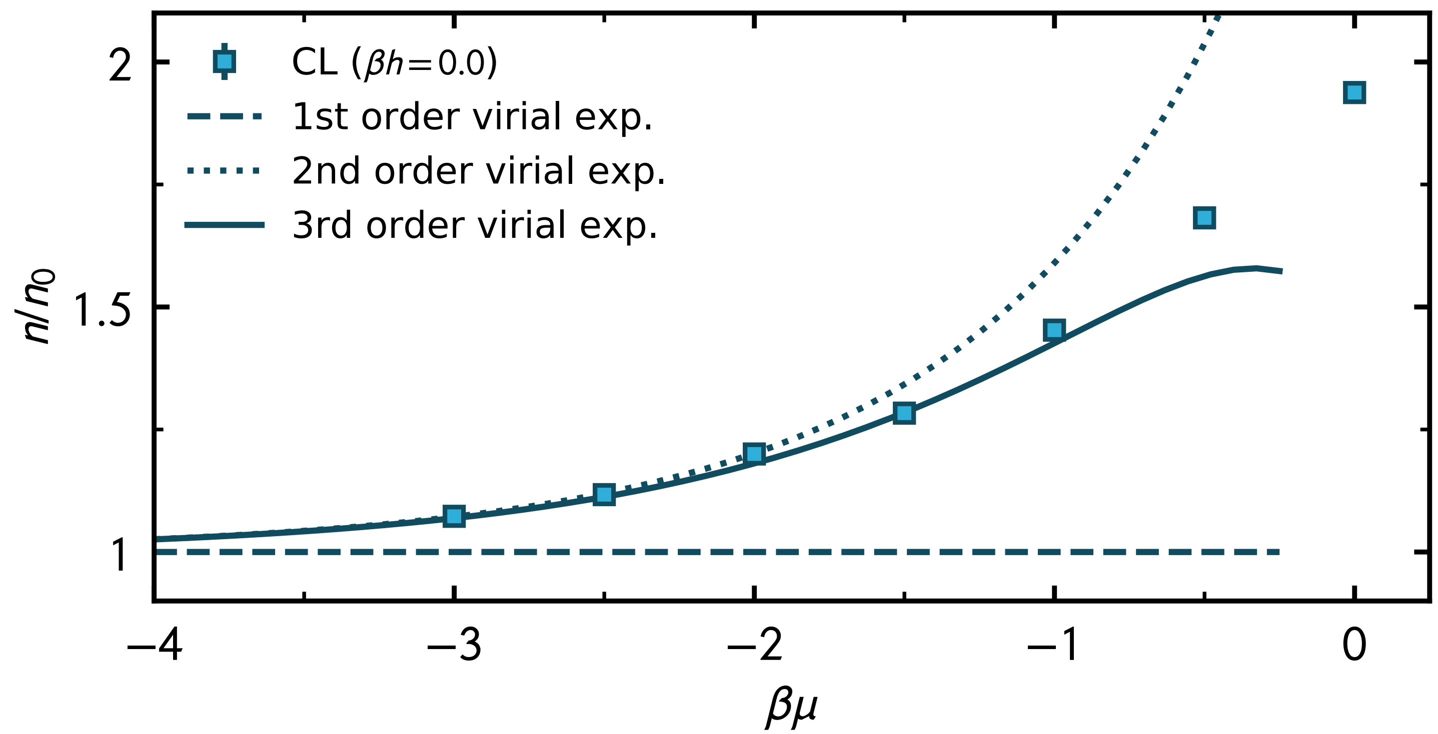
$$z = e^{\beta\mu}$$

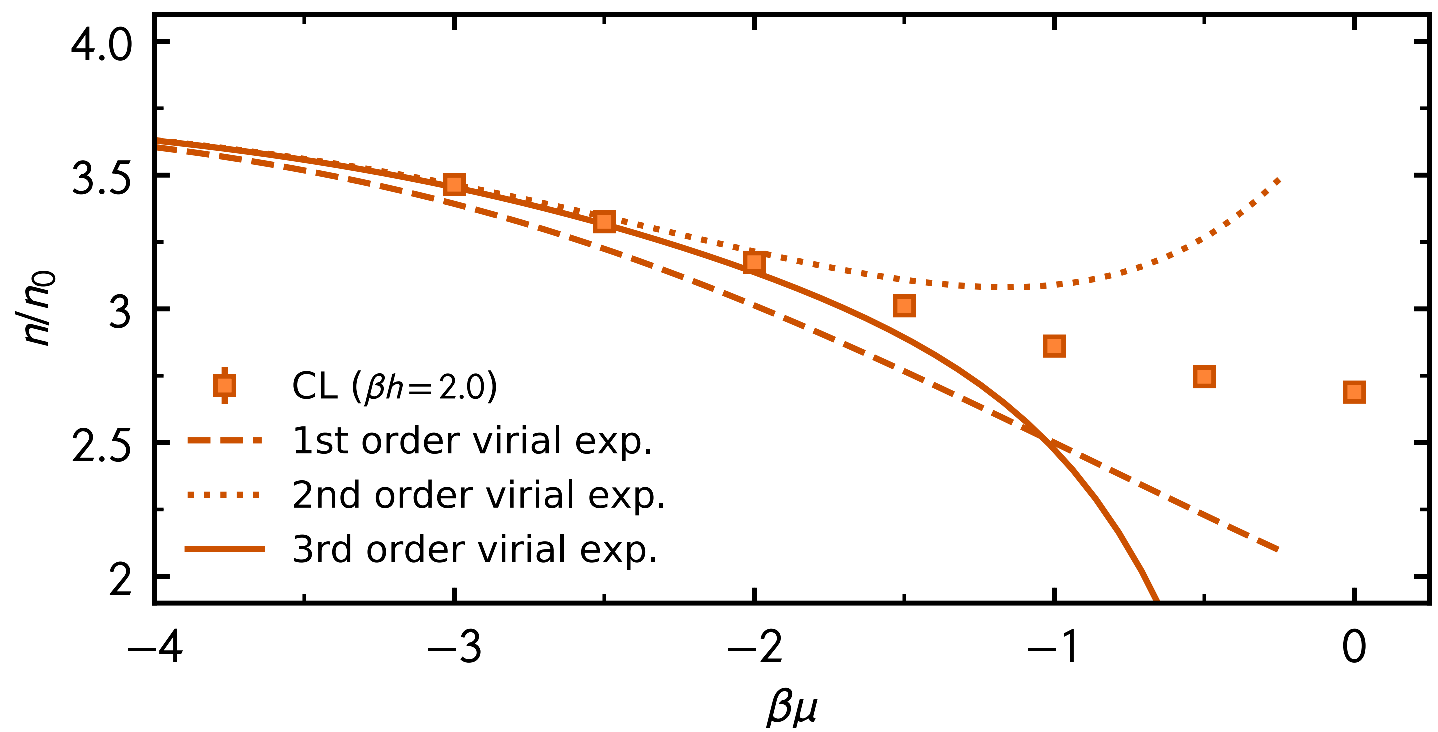
$$\ln \mathcal{Z} = \mathcal{Q}_1 \sum_n z^n b_n$$

density EOS (virial regime)

[LR, Loheac, Drut, Braun '18]

VE approaches the CL results order-by-order

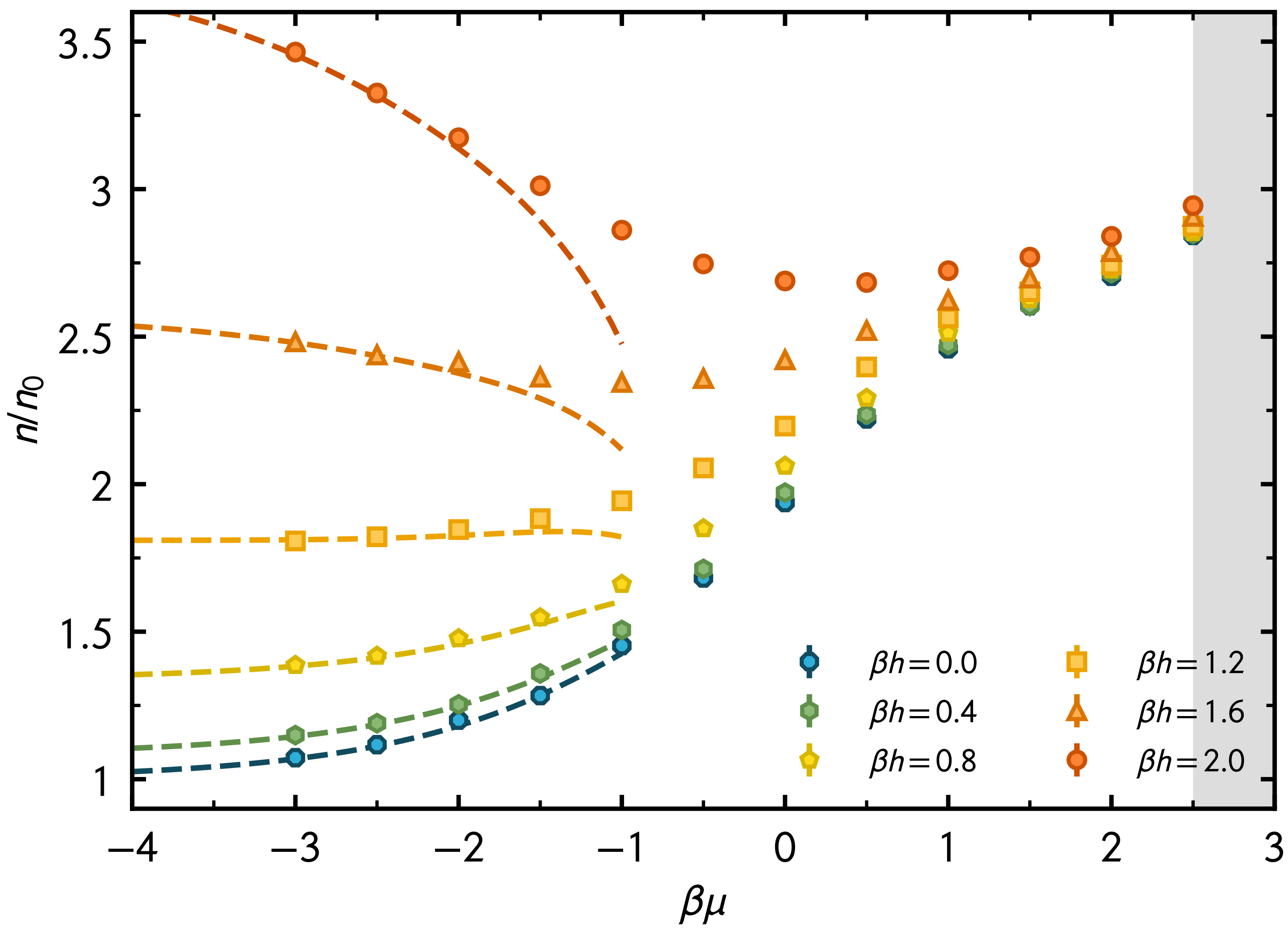




VE deviates earlier for polarized systems

density EOS at finite polarization

[LR, Loheac, Drut, Braun '18]



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

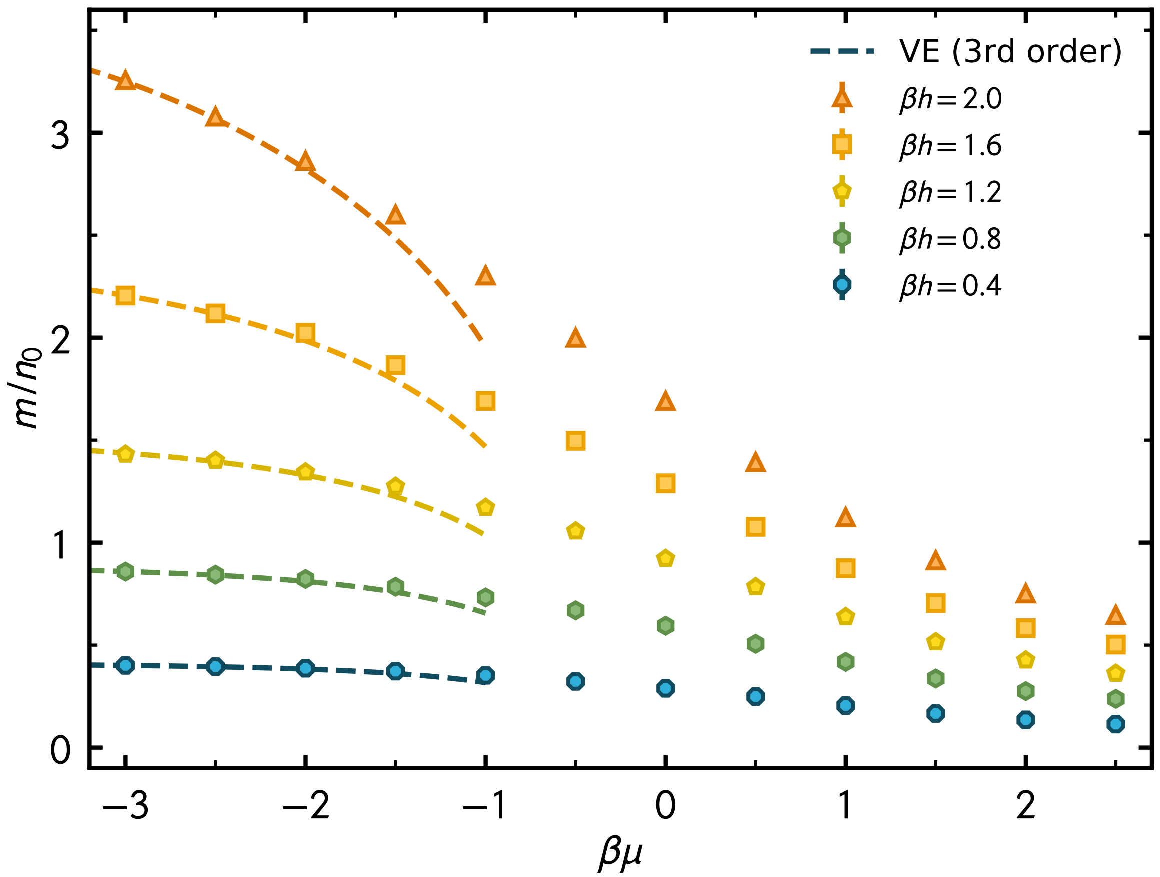
excellent agreement with virial expansion for all polarizations

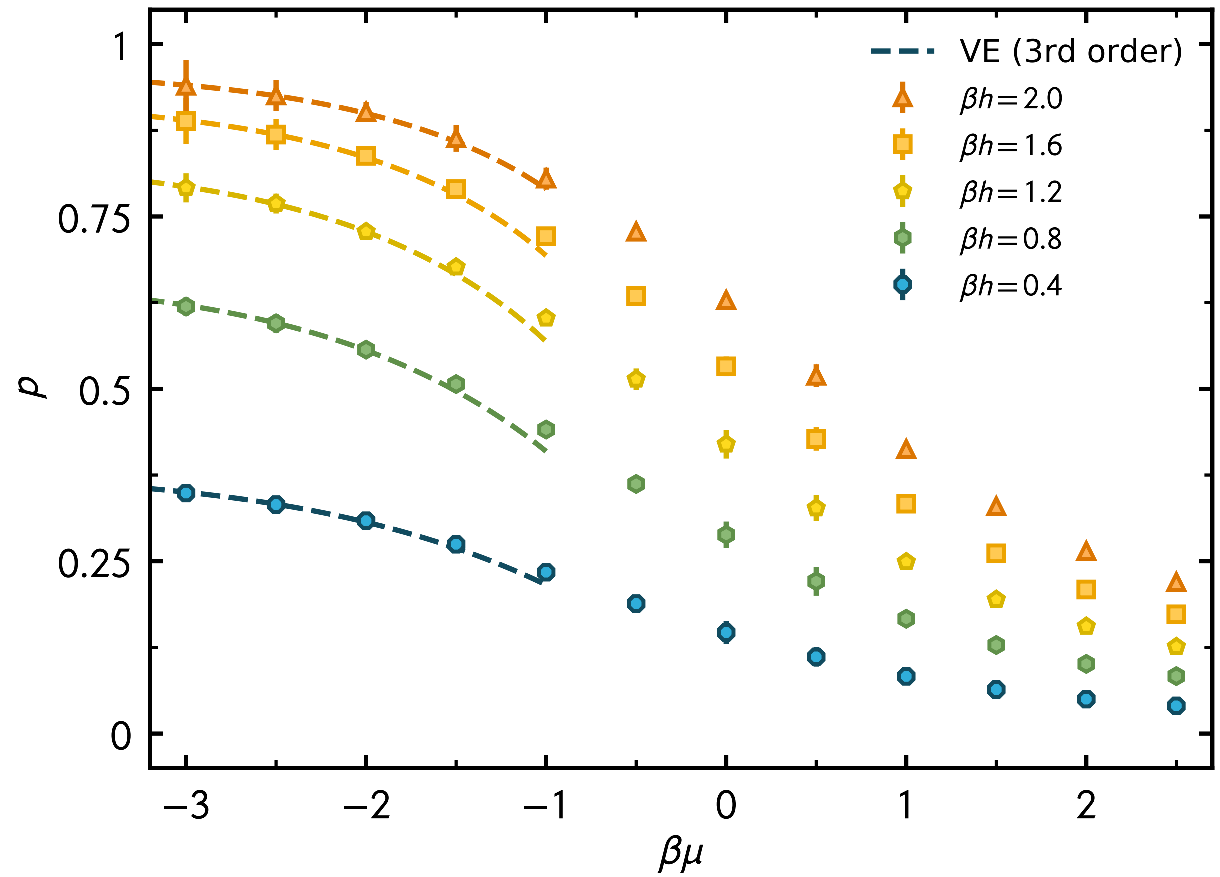
magnetization & polarization

[LR, Loheac, Drut, Braun '18]

$$m = n_\uparrow - n_\downarrow = \frac{\partial \ln \mathcal{Z}}{\partial(\beta h)}$$

$$p = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow} = \frac{m}{n}$$

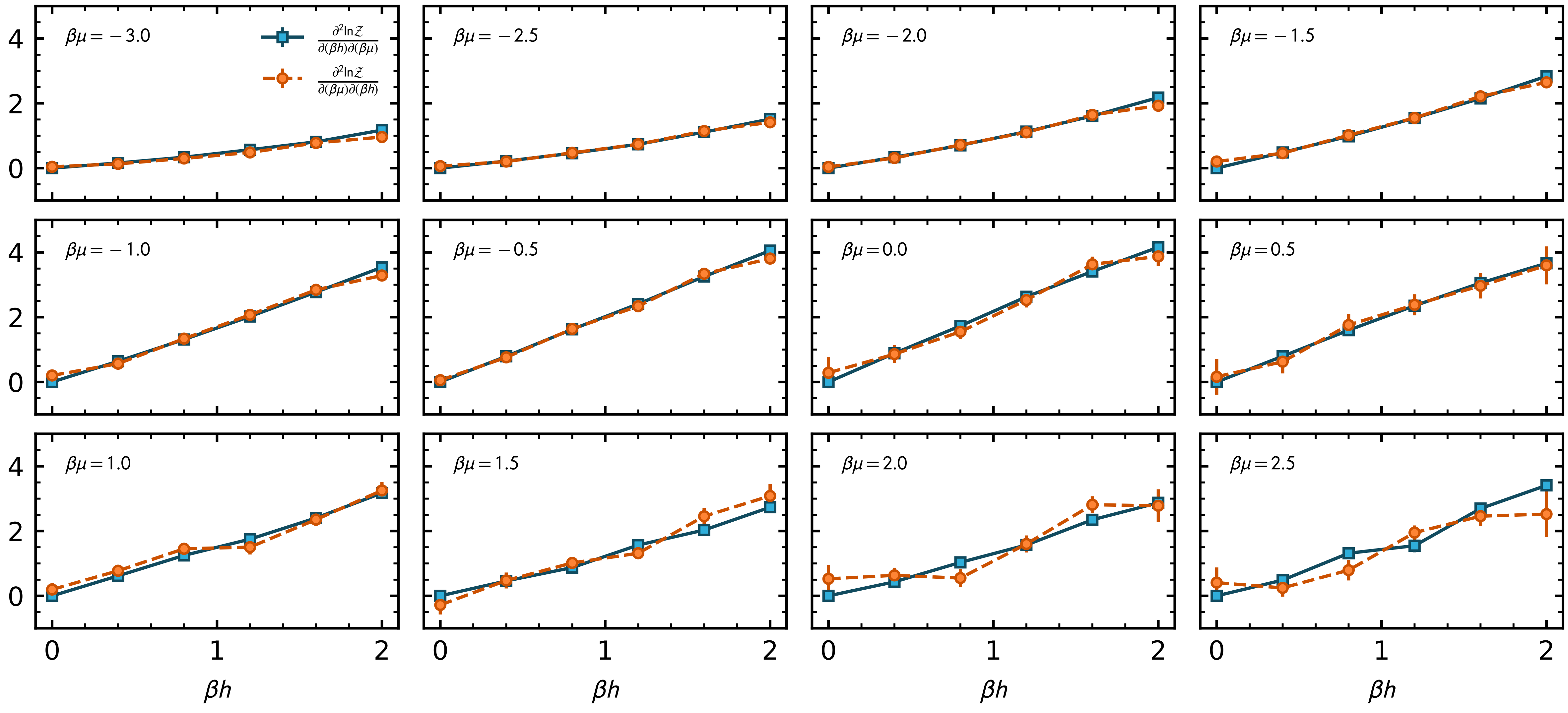




Maxwell relations: consistency check

[LR, Loheac, Drut, Braun '18]

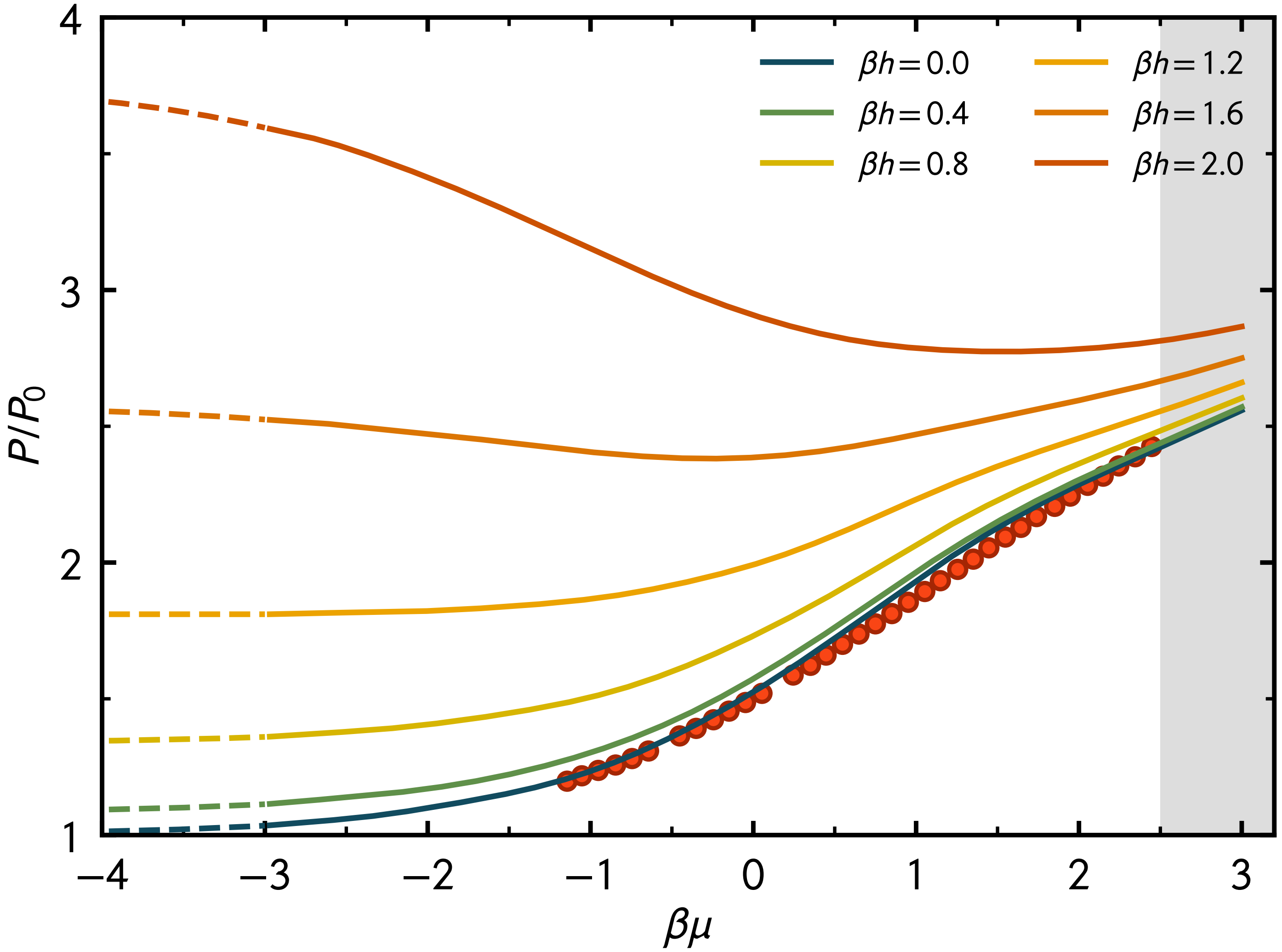
$$\left(\frac{\partial n}{\partial(\beta h)}\right)_{\beta\mu} \stackrel{!}{=} \left(\frac{\partial m}{\partial(\beta \mu)}\right)_{\beta h}$$



pressure equation of state

[LR, Loheac, Drut, Braun '18]

$$P(\beta\mu) = \frac{1}{\beta}\int_{-\infty}^{\beta\mu} n(x)\,dx$$

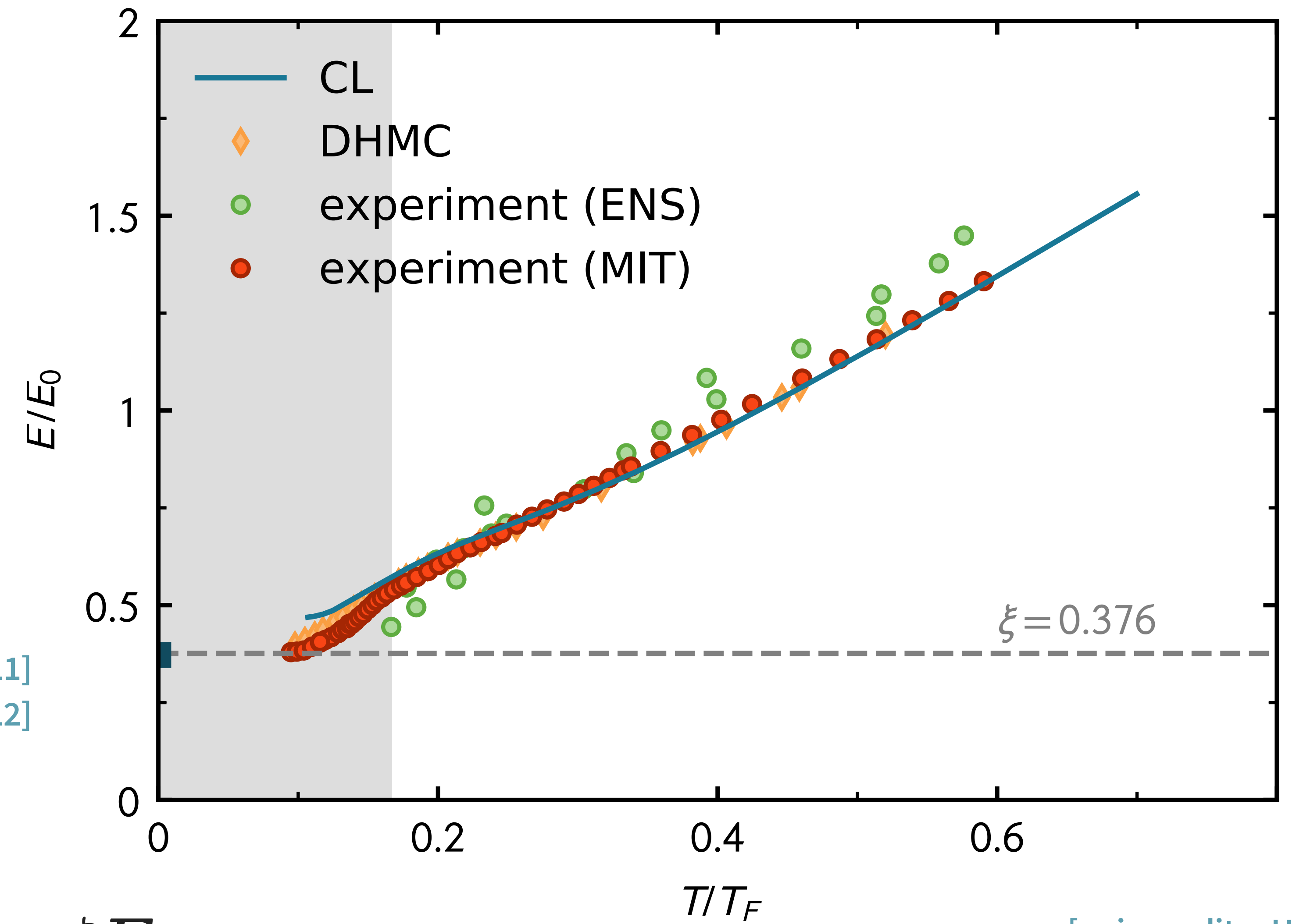


[experiment: Ku et al. '12]

energy equation of state

[LR, Loheac, Drut, Braun '18]

$$E = \frac{3}{2} PV$$



improvement at low T: larger lattices, improved operators

[Endres et al. '11; Drut '12]

[ξ, theory: Carlson et al. '11]
[ξ, experiment: Ku et al. '12]

$$E(T=0) = \xi E_0$$

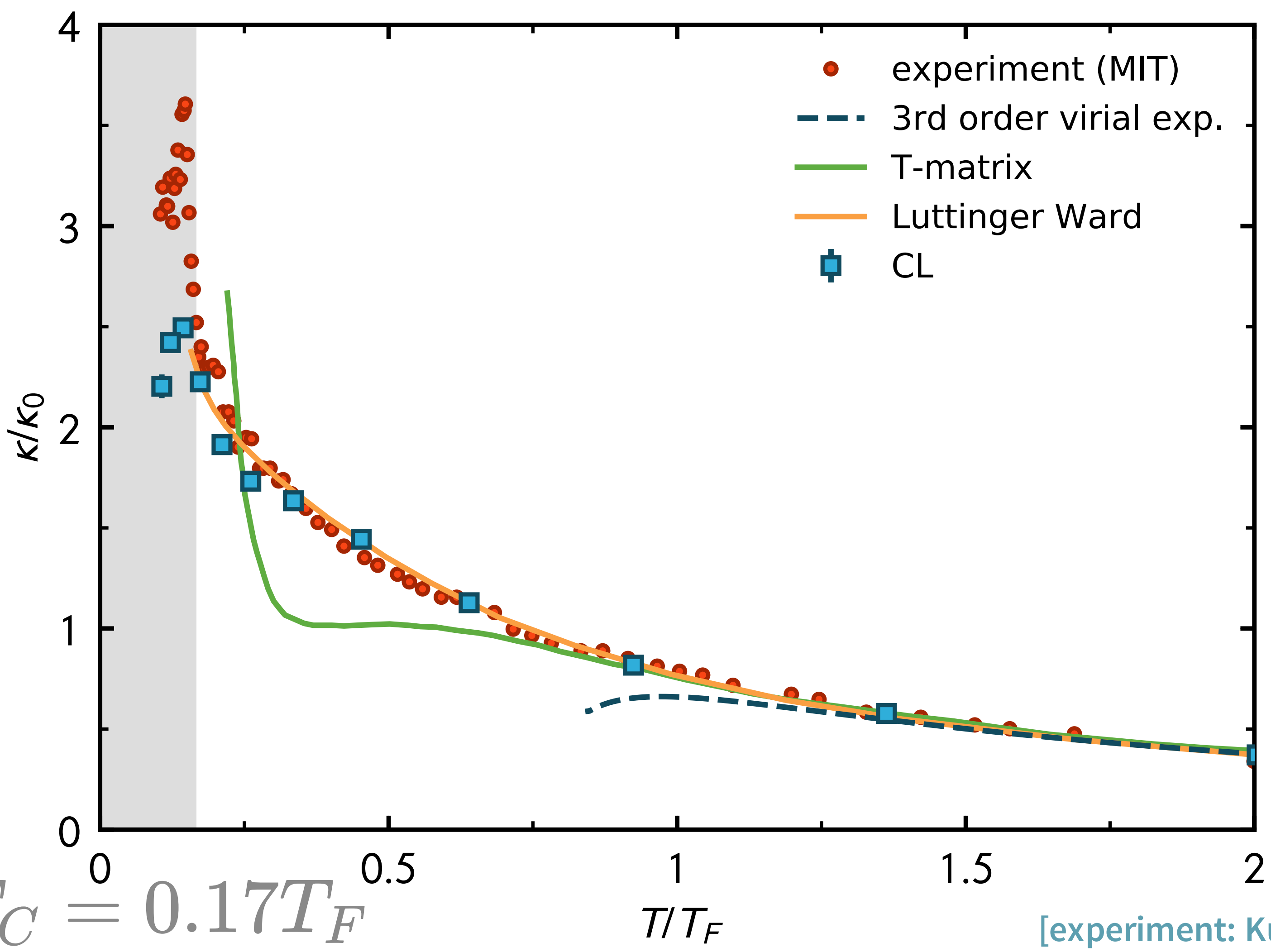
[universality: Ho '04]
[experiment: Ku et al. '12; Nascimbène et al. '12]
[DHMC: Drut et al. '12]

compressibility (unpolarized)

[LR, Loheac, Drut, Braun '18]

$$\kappa = \frac{1}{n}\left(\frac{\partial n}{\partial P}\right)_{T,V,h} = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_{T,V,h}$$

sudden increase of κ indicates superfluid phase transition



$T_C = 0.17 T_F$

features of curve recovered with CL

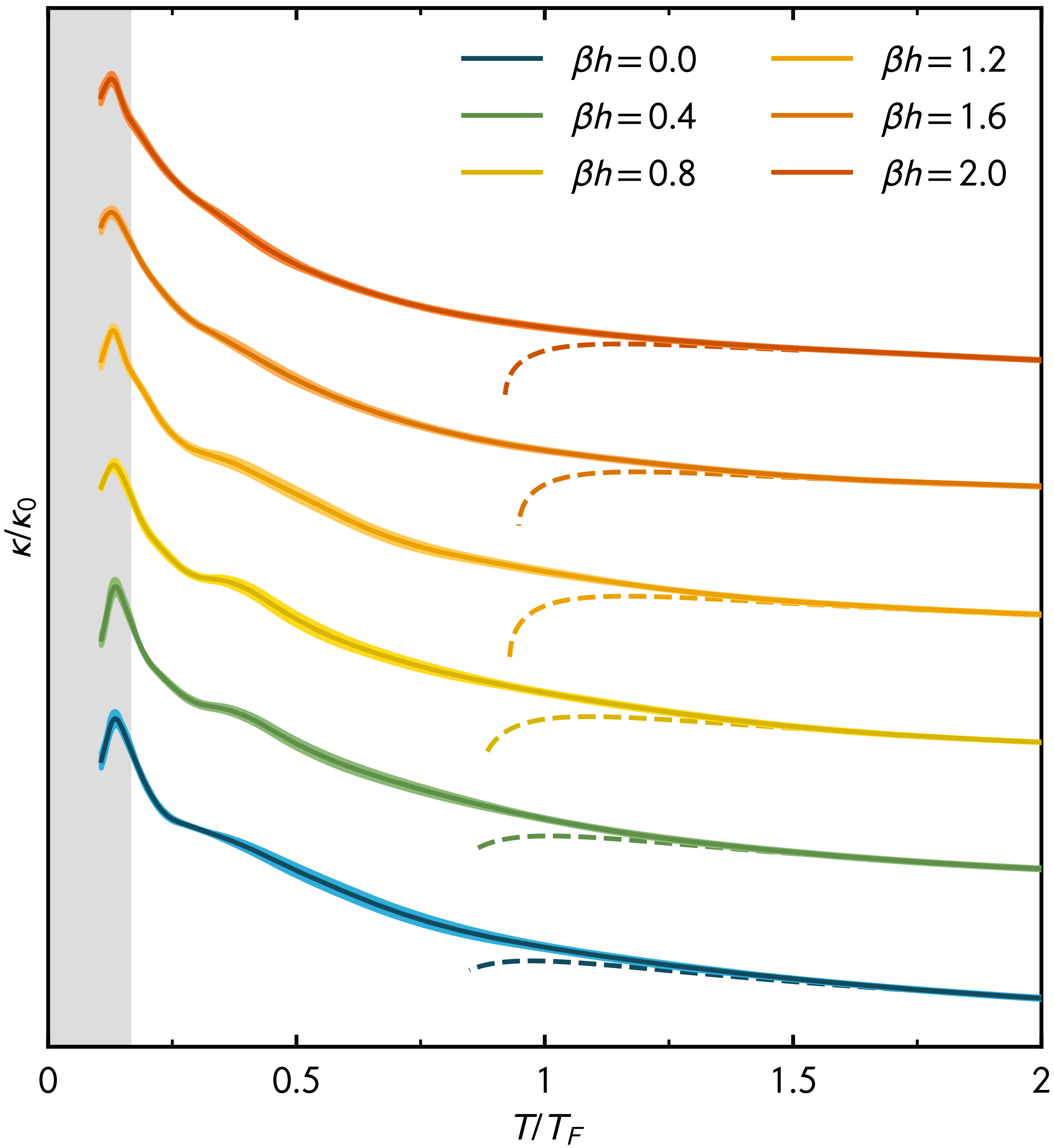
quantitative disagreement at low temperatures

[experiment: Ku et al. '12]
[Luttinger-Ward: Enns,Haussmann '12]
[T-matrix: Pantel et al. '14]

compressibility for polarized systems

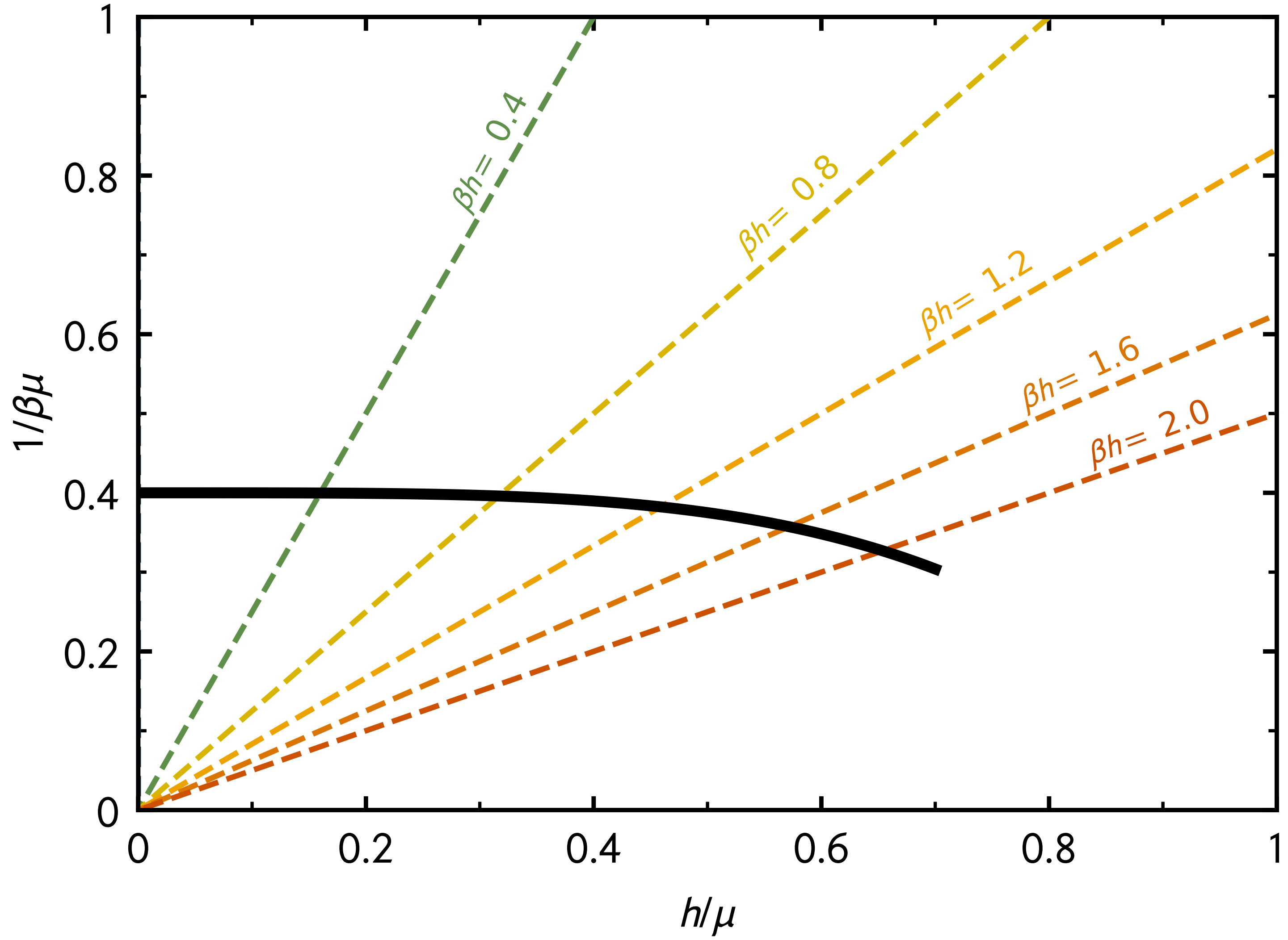
[LR, Loheac, Drut, Braun '18]

weak dependence of the critical temperature on polarization indicated



challenging to extract precise T_C

UFG phase diagram (sketch)

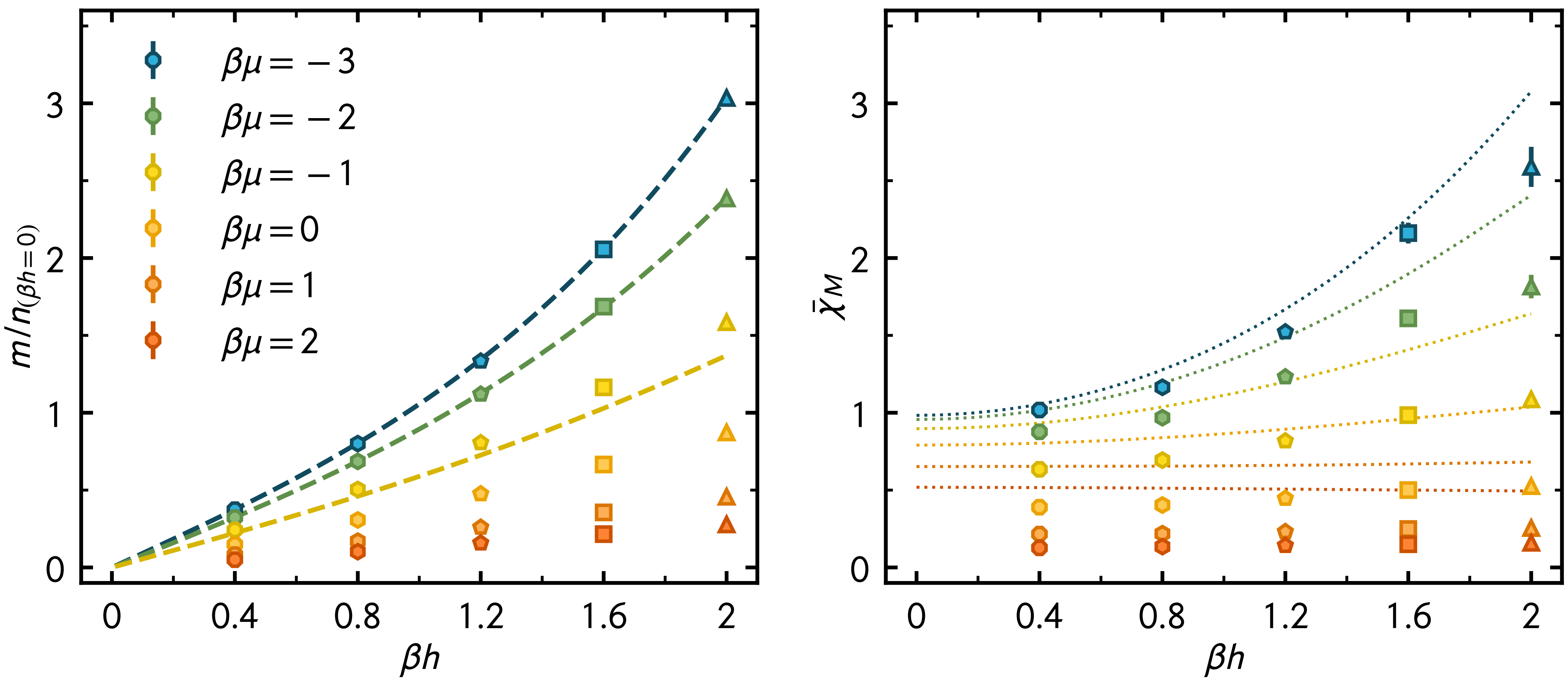


$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$
$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

spin susceptibility

[LR, Loheac, Drut, Braun '18]

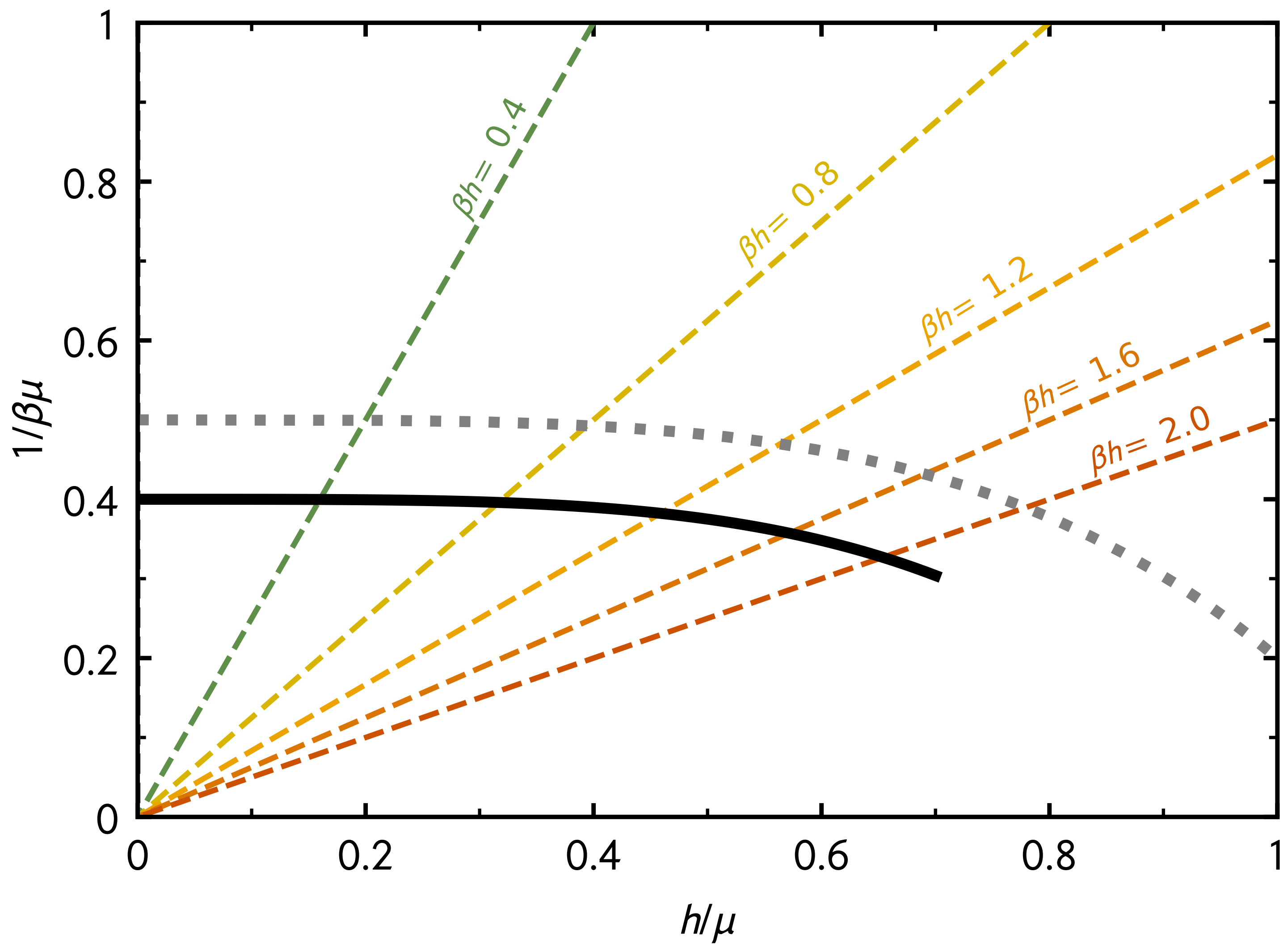
$$\chi = \left(\frac{\partial m}{\partial h}\right)_{T,V,\mu}$$



Pauli susceptibility field independent at low field and T

UFG: dependence on βh very similar to FG, but rescaled

UFG phase diagram (sketch)

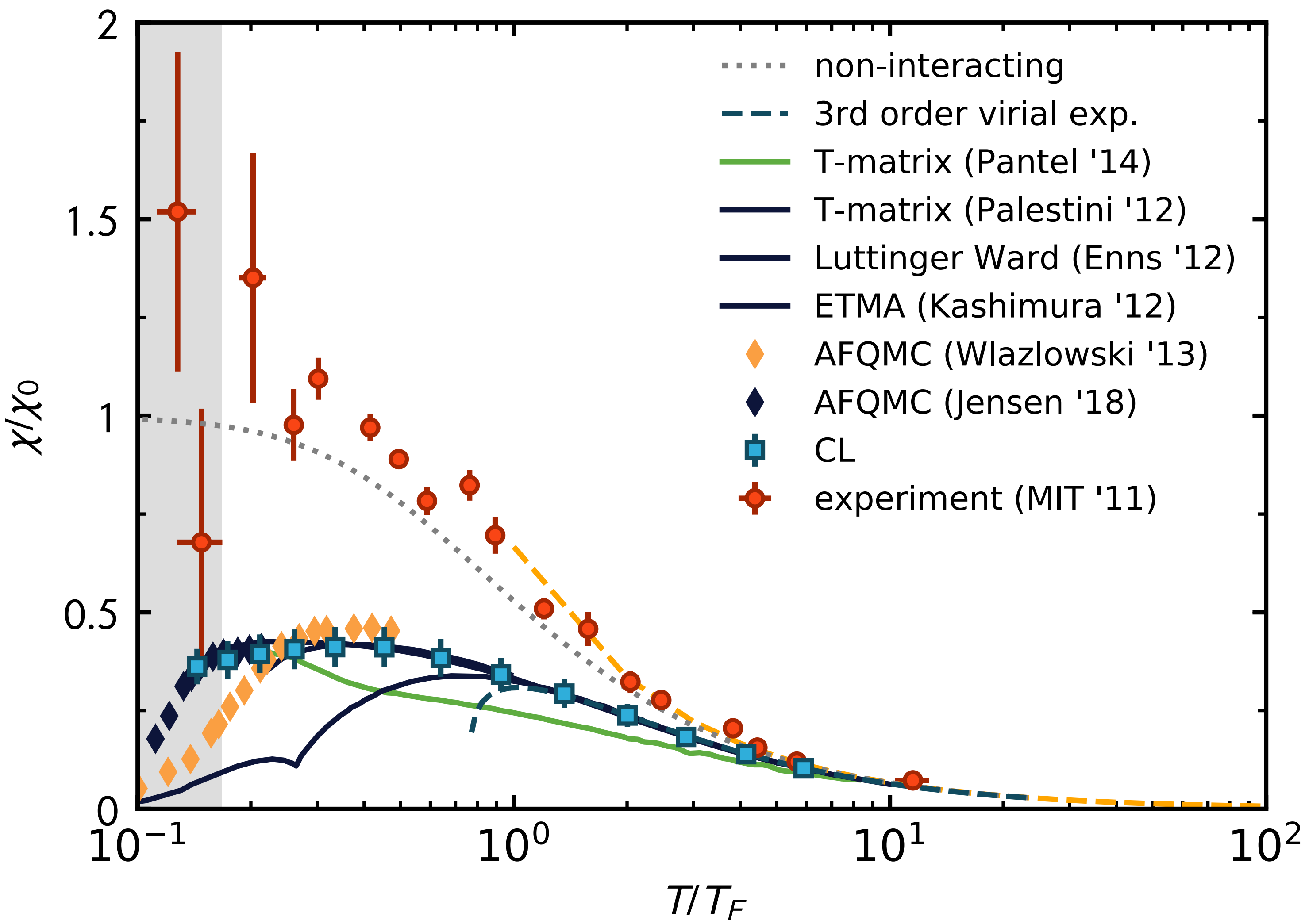


$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$
$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun *in preparation*]

low T: discrepancy between experiment and theory



large T: Curie's law

$$\chi \propto T^{-1}$$

theory & experiment agree at large T

Pseudogap:
suppression of χ at $T > T_C$

[recent review: Jensen et al. '18]

CL: pseudogap possible
T^* and T_C seem to be very close

RECAP

spin polarized Fermi gases are hard to treat:
accessible with the **complex Langevin** method

complex Langevin **compares well with other methods** wherever possible

EOS, magnetic properties & response accessible for the UFG at $T > 0$ and finite polarization **in ab initio fashion**

WHAT'S NEXT?

investigation of **pair correlations for the UFG**

effect of **mass imbalance**
on pairing behavior

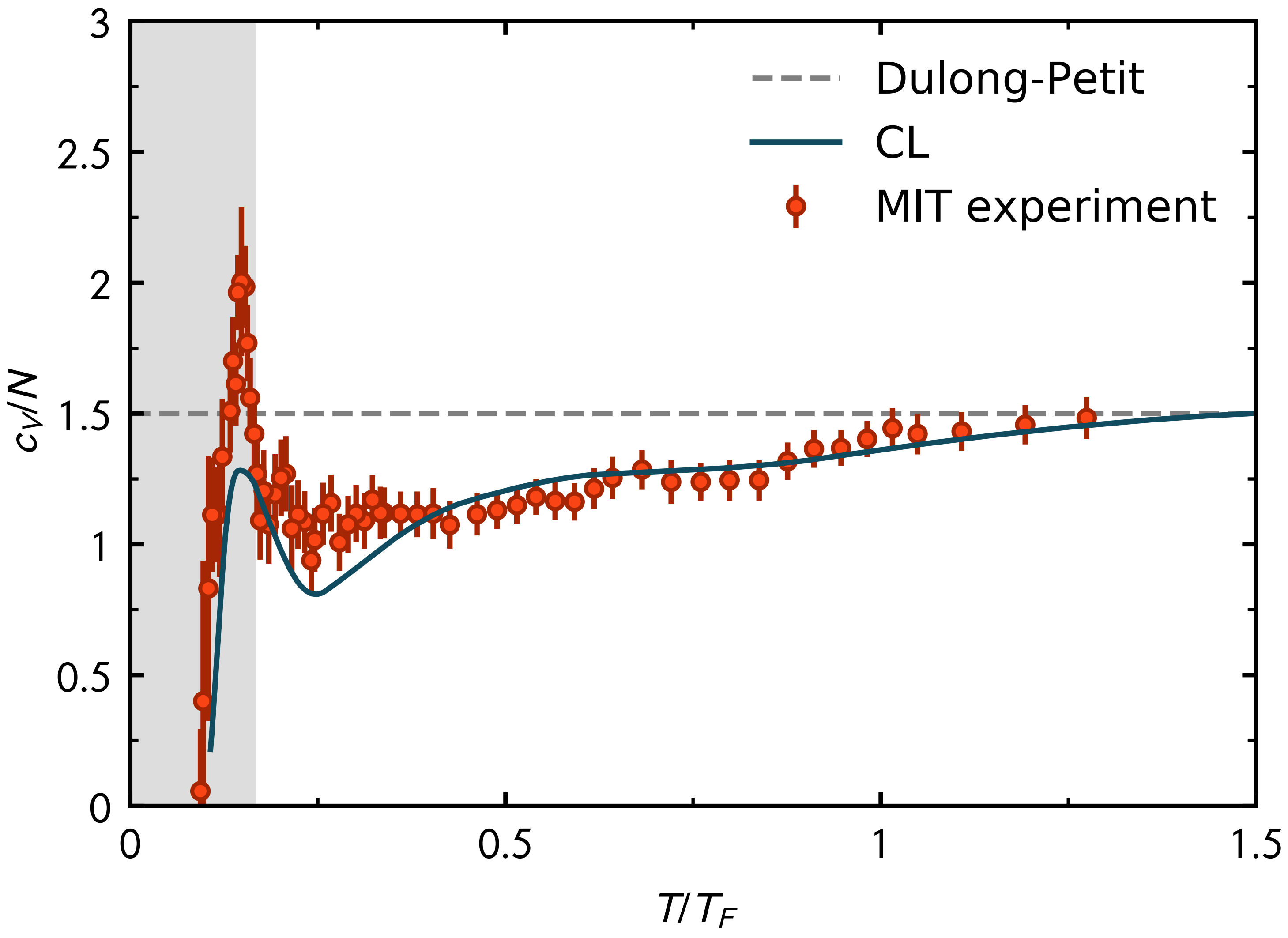
search for **inhomogeneous phases** in 2D/3D

**ab initio phase diagram for
mass- and spin-imbalanced Fermi gases**

specific heat

[LR, Loheac, Drut, Braun *in preparation*]

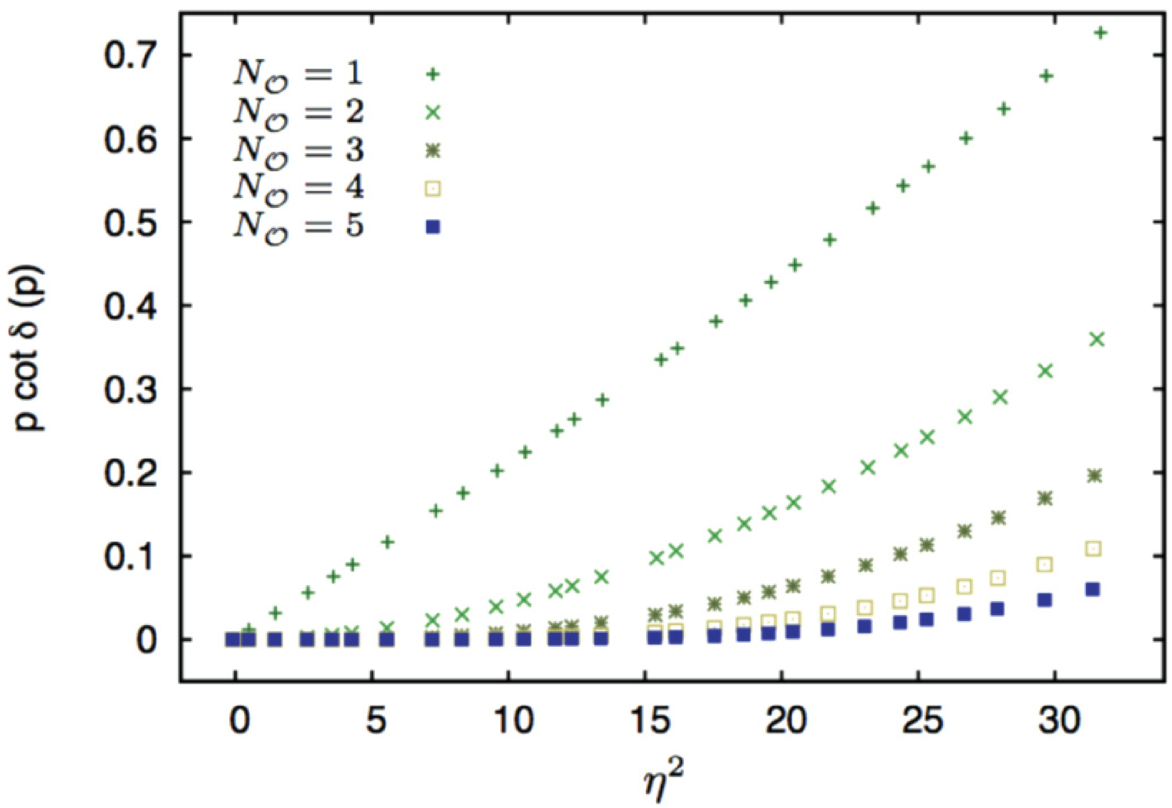
$$\frac{C_V}{N} = \left(\frac{\partial E}{\partial T}\right)_{N,V} = \frac{3}{2}\left(\frac{T}{T_F}\right)^{-1}\left(\frac{p}{p_0} - \frac{\kappa_0}{\kappa}\right)$$

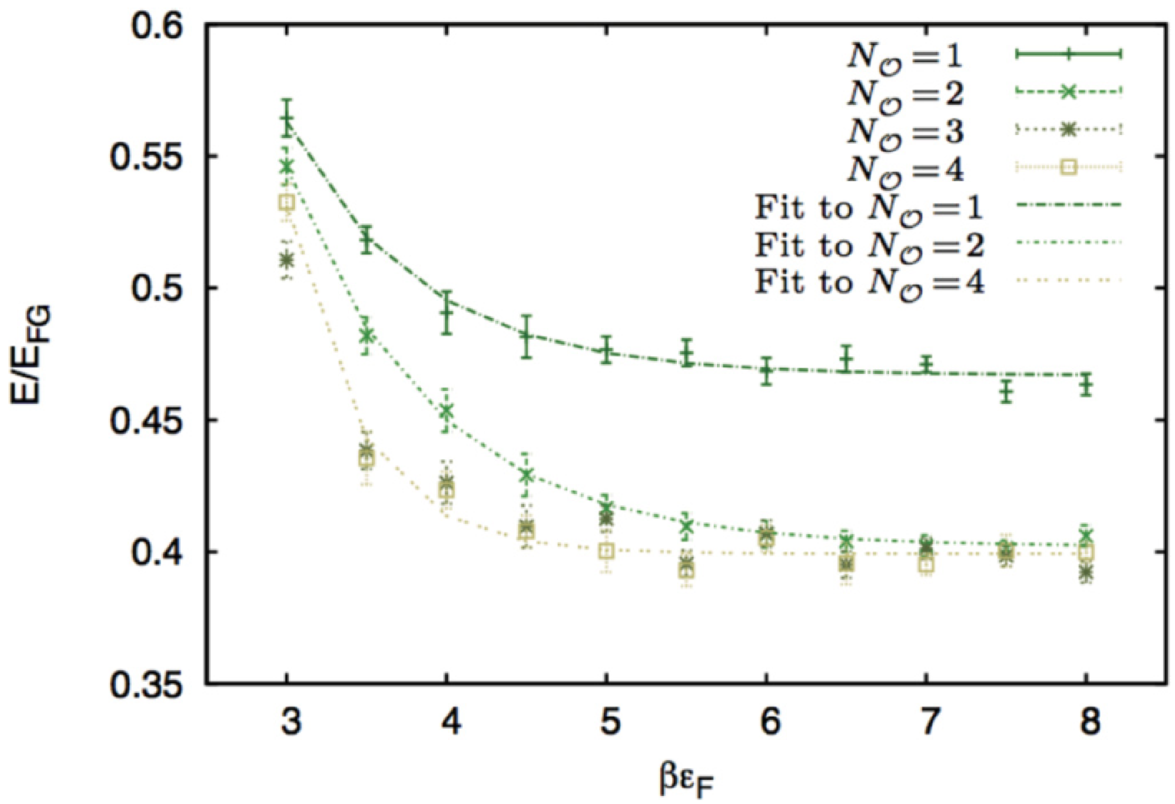


improved lattice operators

[Drut '12]

$$p \cot \delta(p) = -\frac{1}{a} + \frac{1}{2} r_{eff} p^2 + \mathcal{O}(p^4)$$

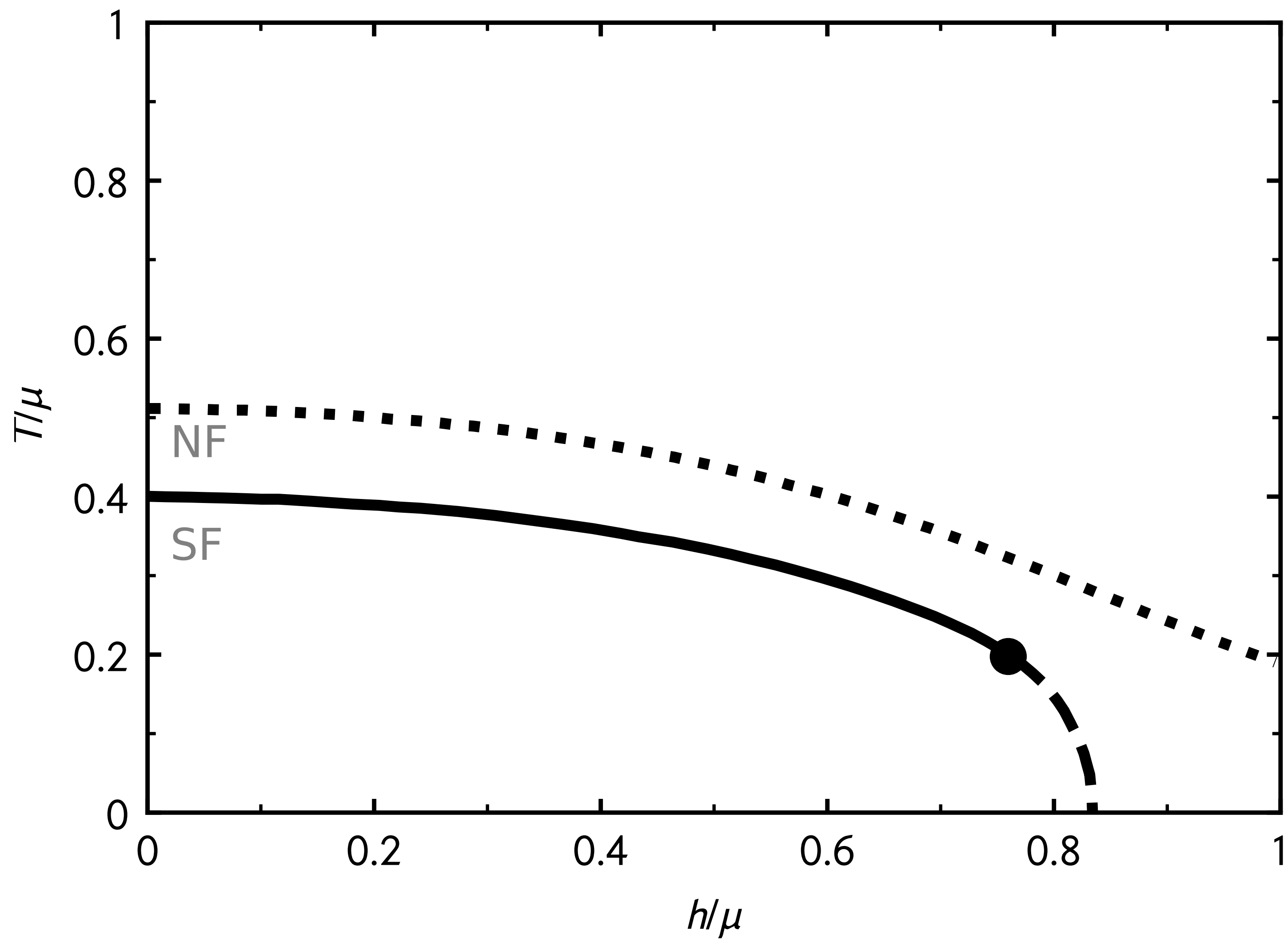




scattering is tuned to reproduce unitarity at finite momenta

[see also: Endres et al. 11']

UFG phase diagram (fRG)



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

[Boettcher et al. '14]