

THERMODYNAMICS OF THE SPIN-POLARIZED UNITARY FERMI GAS

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NC State, September 27th, 2018

[LR, Drut, Braun *in preparation*]

[LR, Loheac, Drut, Braun arXiv:1807.04664]

[LR, Porter, Drut, Braun *Phys. Rev. D* 96, 094506, 2017]



Helmholtz Graduate School for Hadron and Ion Research



Center for
Scientific
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ULTRACOLD FERMI GASES: WHY ARE THEY INTERESTING?

(nuclear physics, neutron stars, electrons in metals,
superfluidity, controllable experiments, ...)

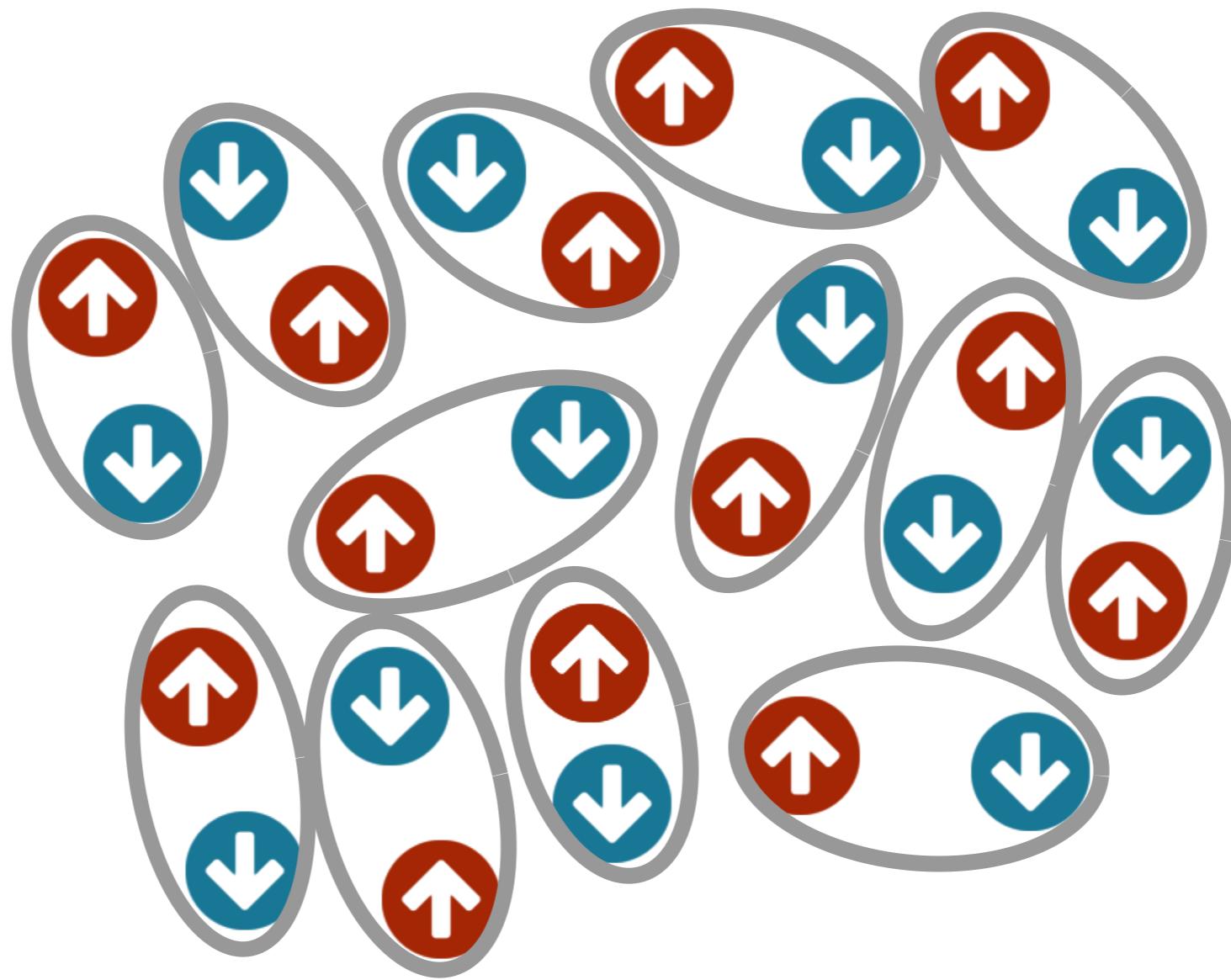
Reviews:

[Ketterle, Zwierlein '08]

[Giorgini, Pitevskii, Stringari '08]

[Bloch, Dalibard, Zwerger '08]

balanced Fermi gas

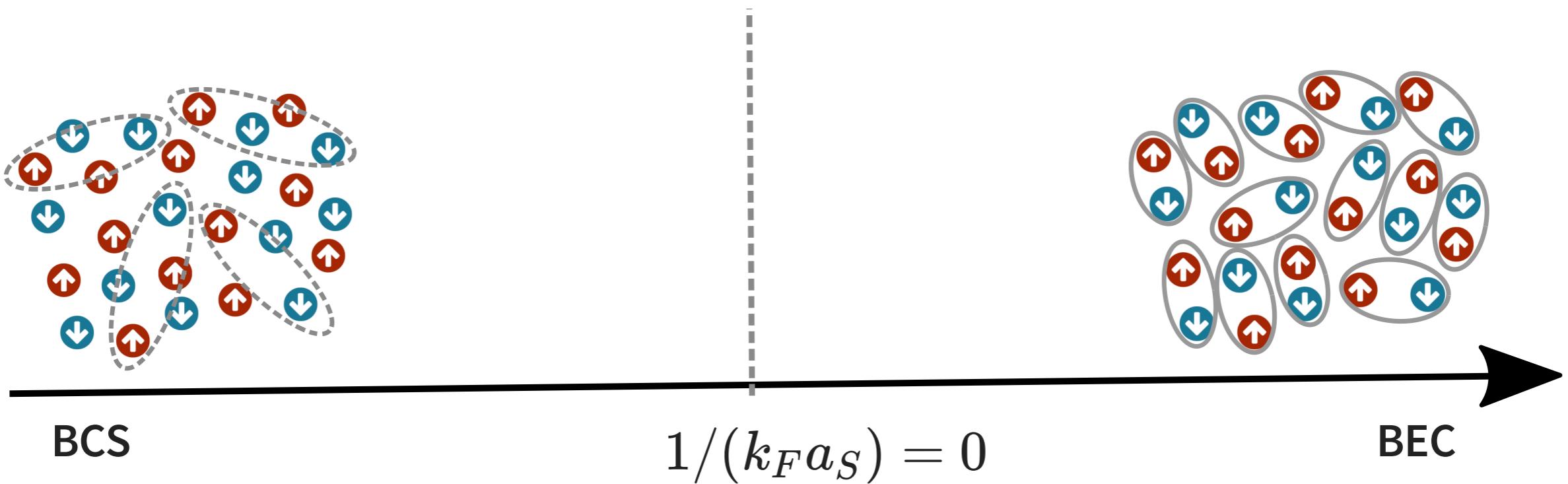


BEC pairing

the unitary Fermi gas

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

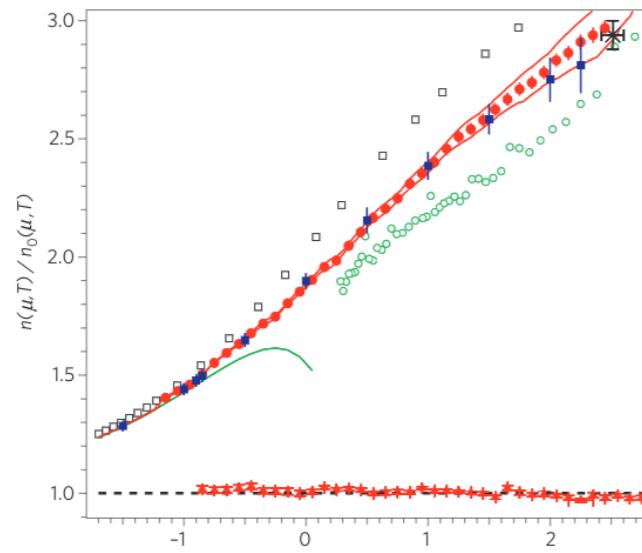
$$a_S \gg n^{-1/3} \gg r_0$$



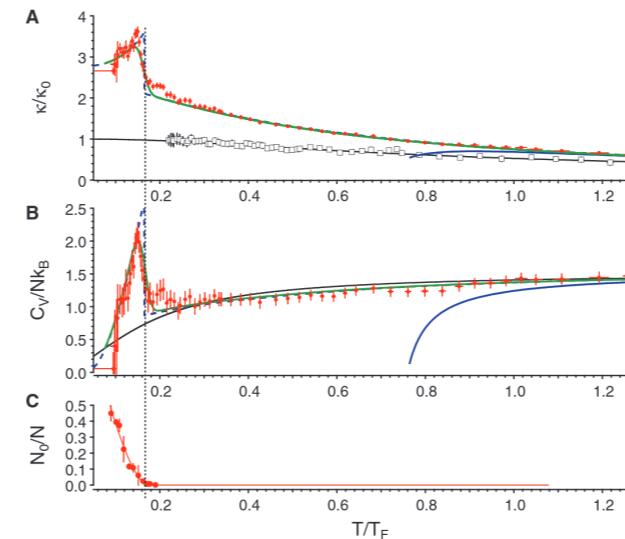
density & temperature are only dimensionful scales in the system

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

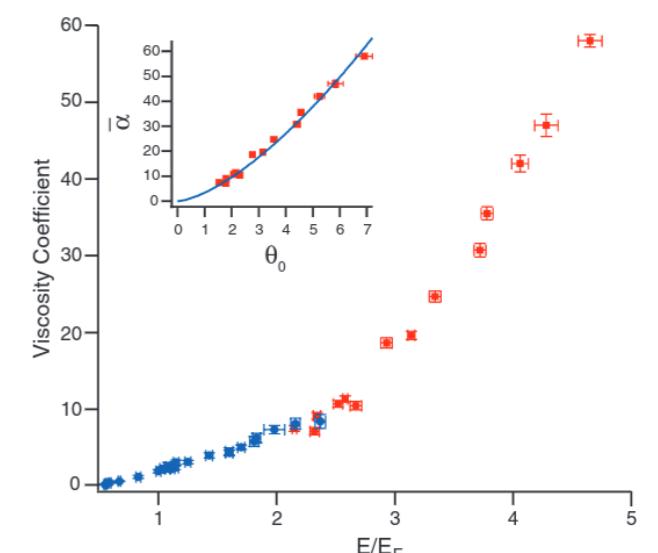
the unitary Fermi gas: many experiments



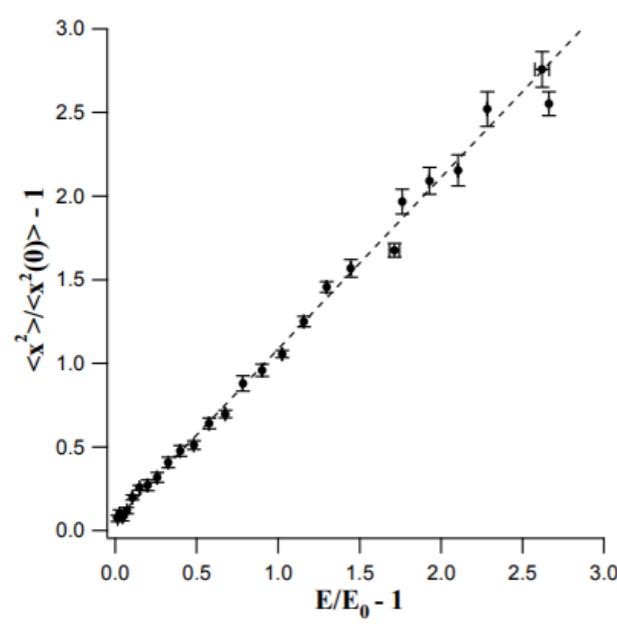
[van Houcke et al. '12]



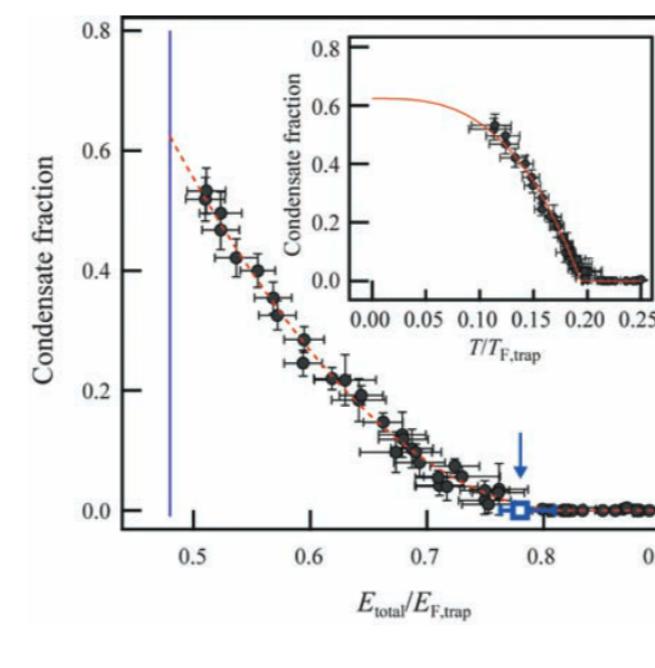
[Ku et al. '12]



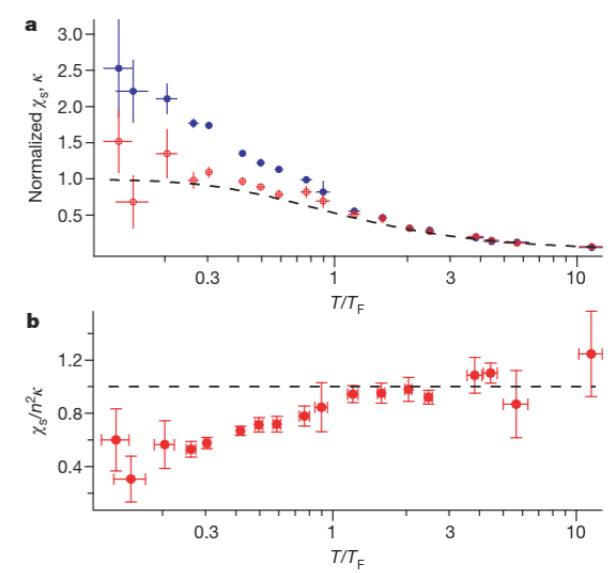
[Cao et al. '11]



[Thomas, Kinast, Turpalov '05]

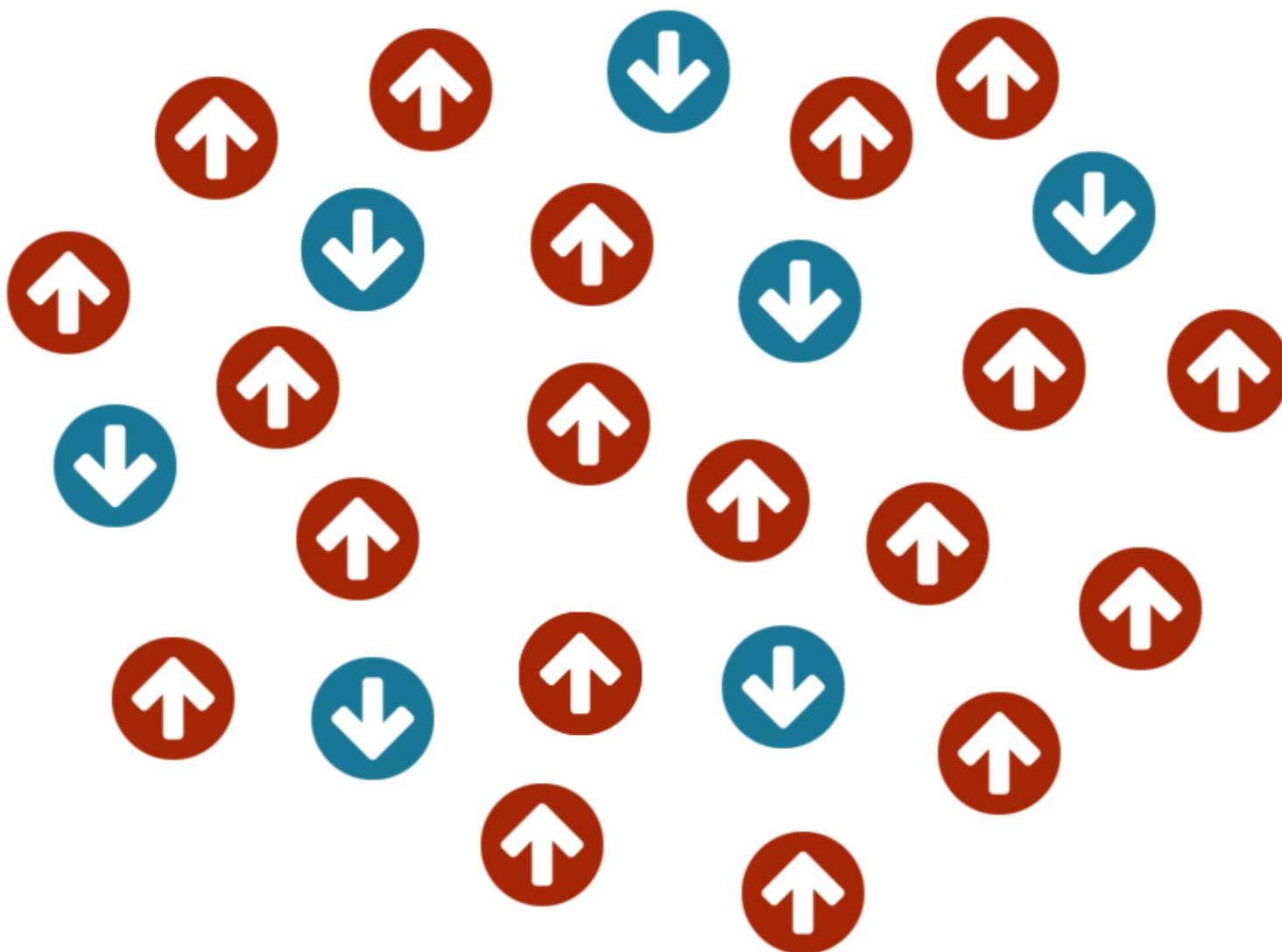


[Horikoshi et al. '10]



[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:

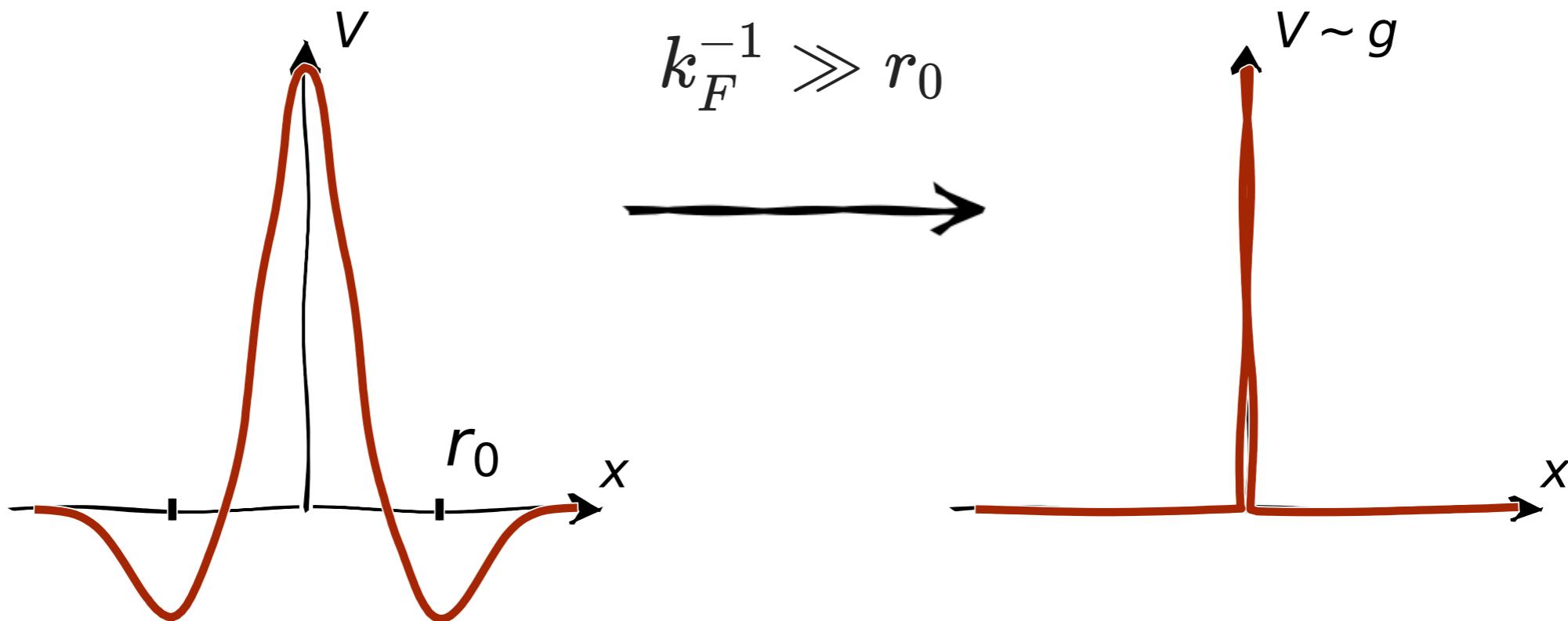
can we get the EOS for polarized systems?

how does T_C change with polarization?

model: contact interaction

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

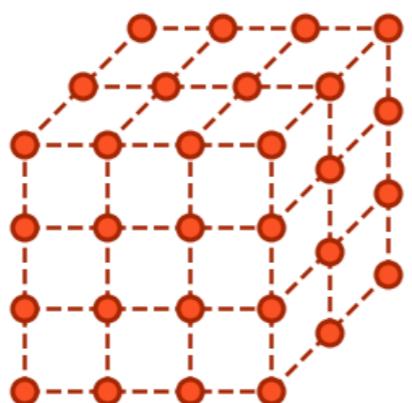
$$+ g \int d^d x \hat{\psi}_\uparrow^\dagger(\vec{x}) \hat{\psi}_\uparrow(\vec{x}) \hat{\psi}_\downarrow^\dagger(\vec{x}) \hat{\psi}_\downarrow(\vec{x})$$



what do we need to compute?

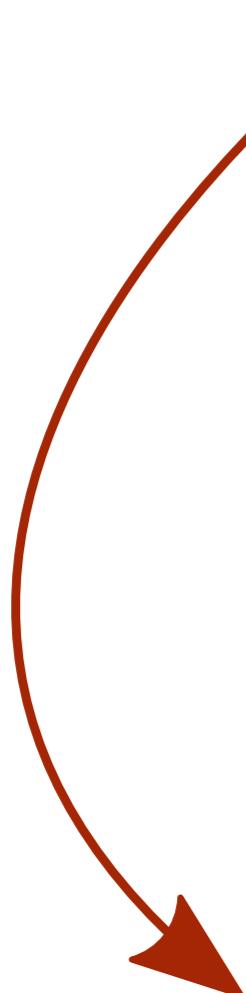
$$\mathcal{Z} = \text{Tr}[e^{-\beta \hat{H}}] = \text{Tr}[e^{-\beta(\hat{T} + \hat{V})}]$$

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



+ Trotter decomposition

+ Hubbard-Stratonovich transformation

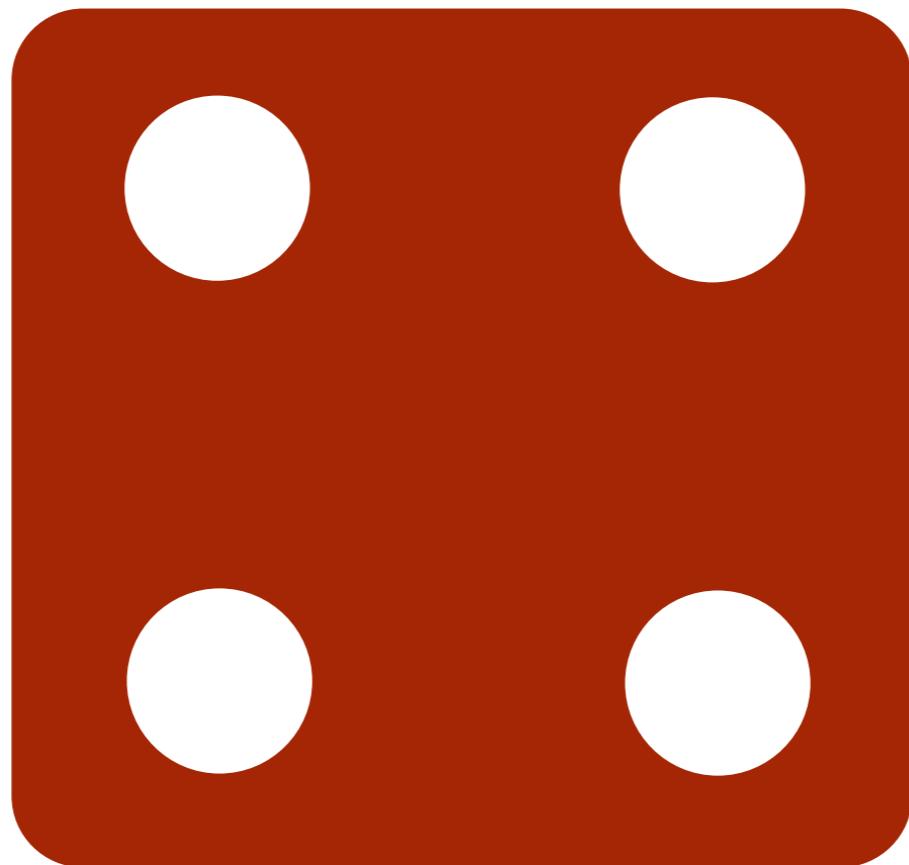


rewrite the problem as a path-integral:

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

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

roll some dice



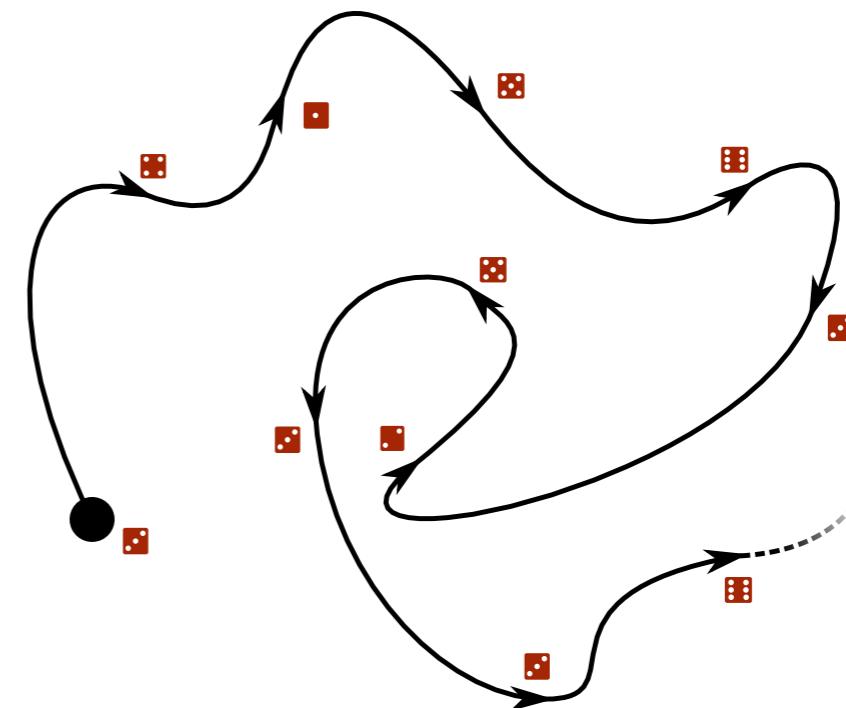
(create random auxiliary field configurations)

Monte Carlo in a nutshell

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

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

- 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

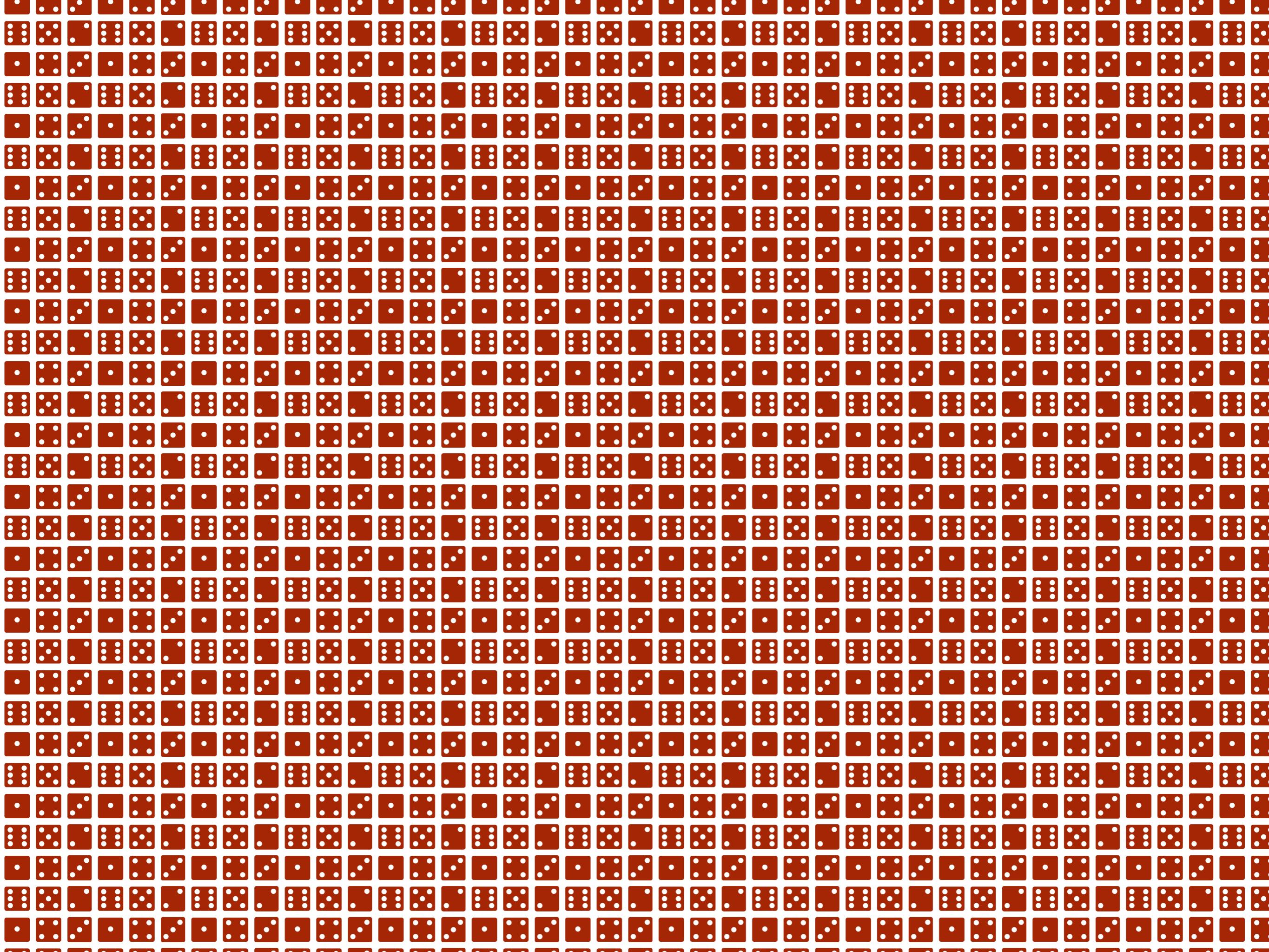


Markov chain typically produced with Metropolis algorithm (accept/reject step)

workhorse of lattice QCD: hybrid Monte Carlo (HMC)

[Duane, Kennedy, Pendleton, Roweth '87]

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



THE SIGN PROBLEM

(computational effort increases exponentially with system size)

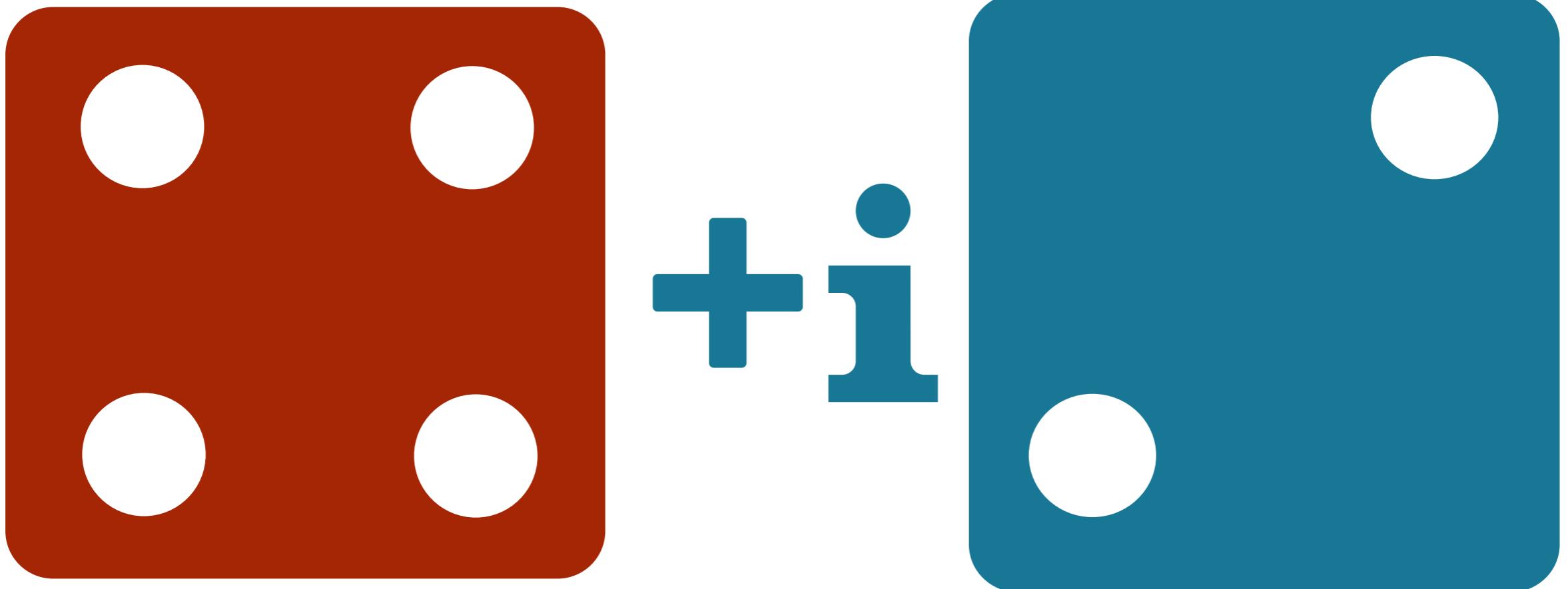
[Troyer, Wiese '05]

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

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

$$\begin{aligned} N_\uparrow &\neq N_\downarrow \\ \mu_\uparrow &\neq \mu_\downarrow \\ m_\uparrow &\neq m_\downarrow \\ g &> 0 \end{aligned}$$

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):

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

fictitious time
(not physical)

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

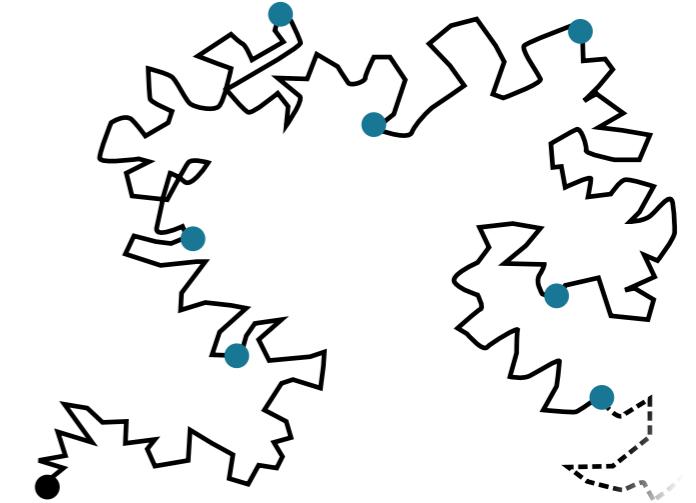
[Parisi, Wu '81; Damgaard,Huffel '87]

[Aarts '09; Seiler '17]

[Loheac, Drut '17; LR, Porter, Drut, Braun '17]

complex Langevin (CL)

use discrete Langevin equations
to produce a Markov chain:



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

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

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

introduce
a "regulator"

[Loheac, Drut '17]

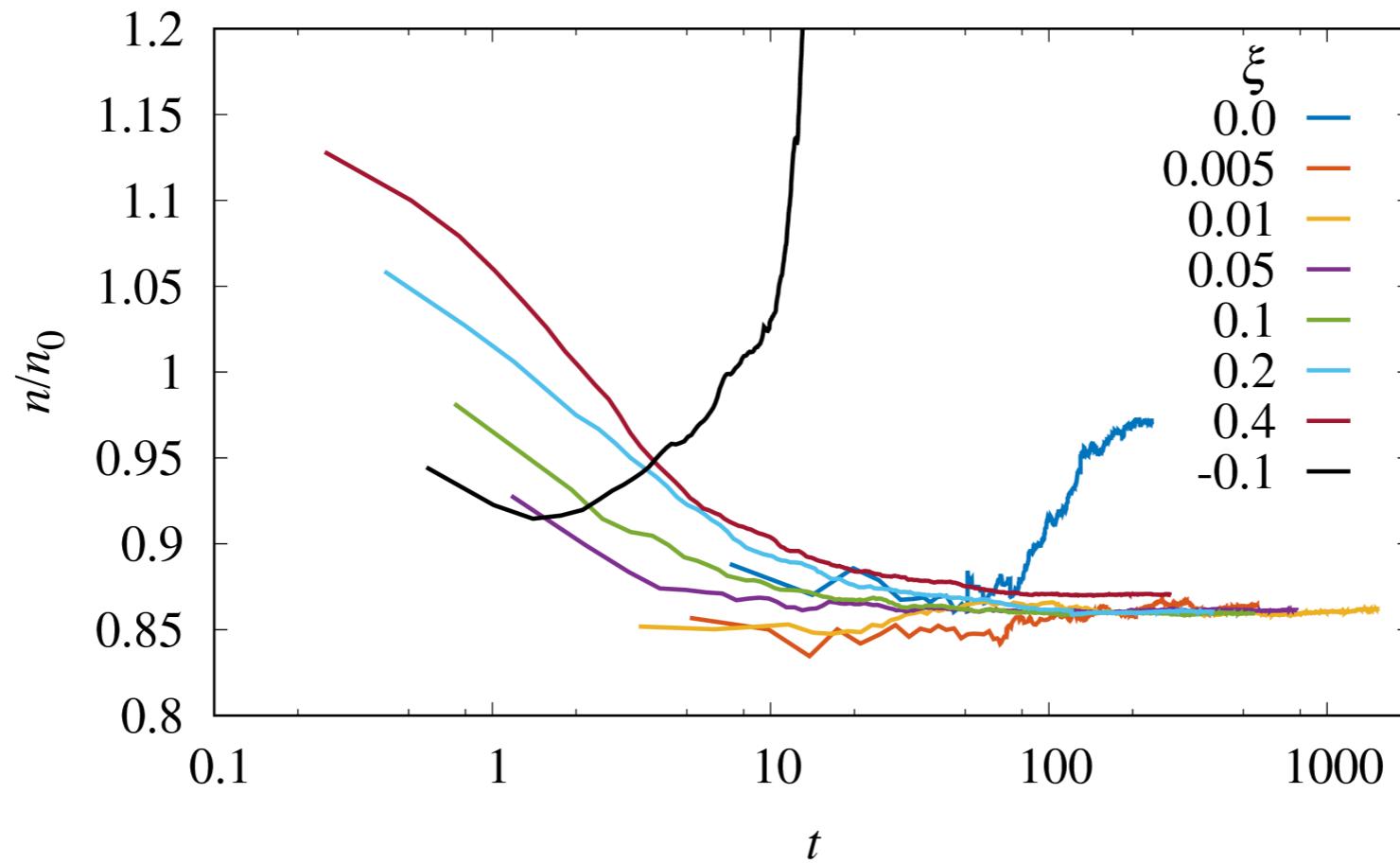
condition: $S[\phi]$ must be bounded from below!

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

effect of the regulator

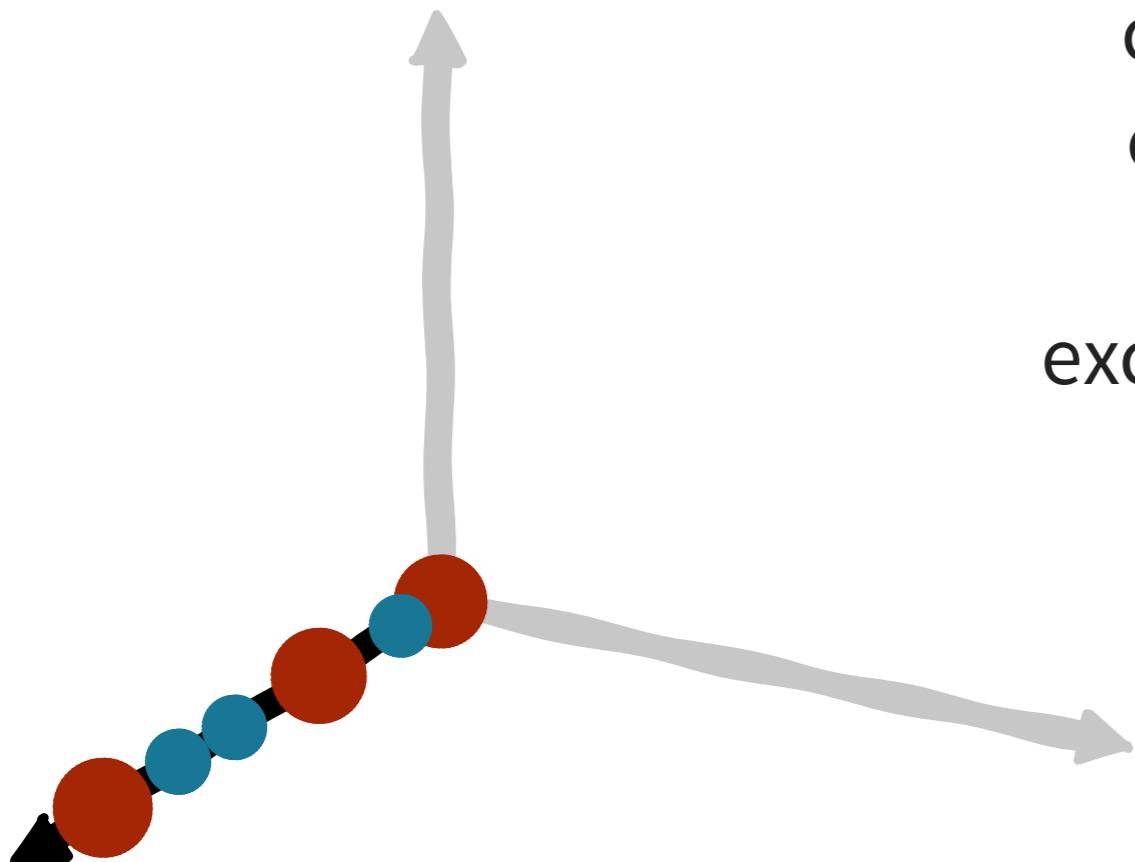
[Loheac,Drut '17]

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

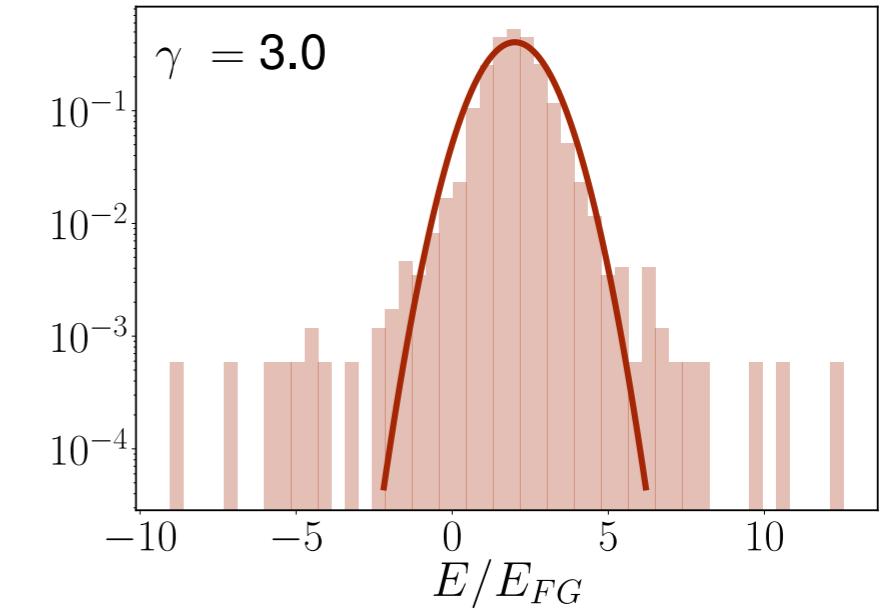
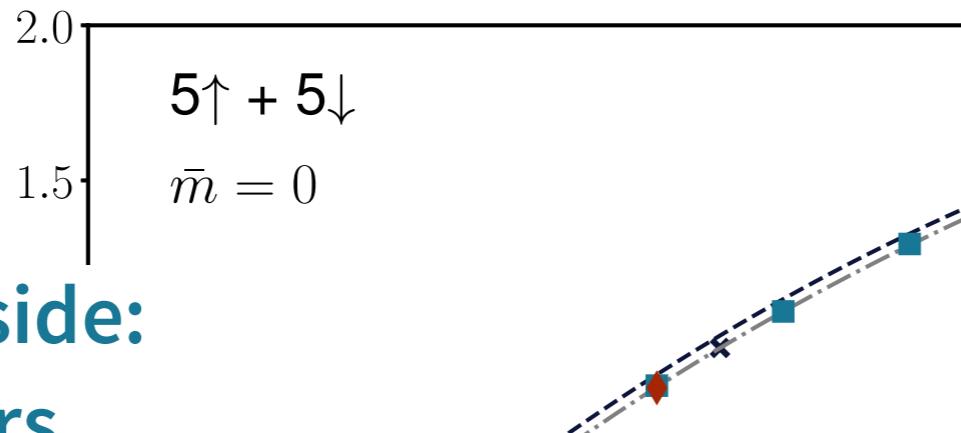
also accessible in experiment

[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]

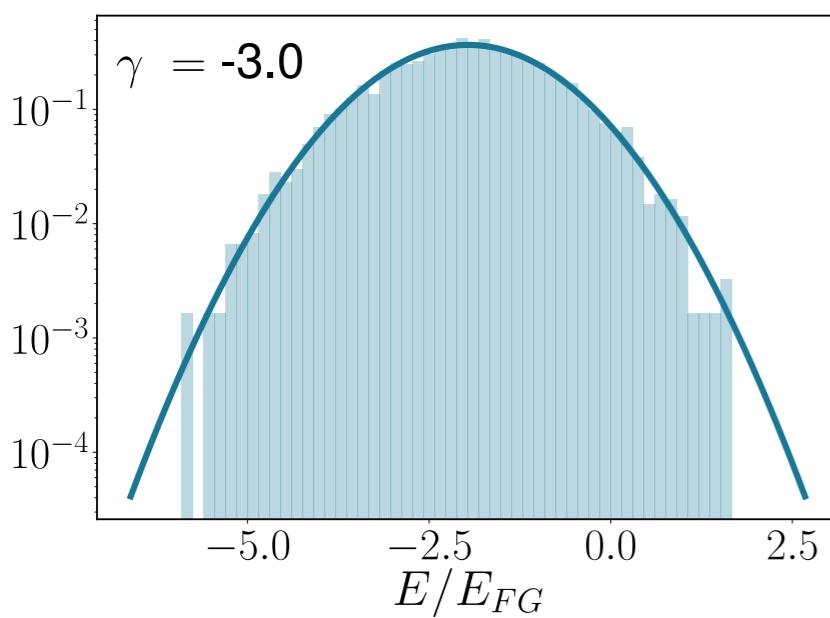
attractive side:
no outliers,
no problems!



repulsive side:
outliers skew
expectation values!

('fat tail' problem)

$$\gamma = g/n$$



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

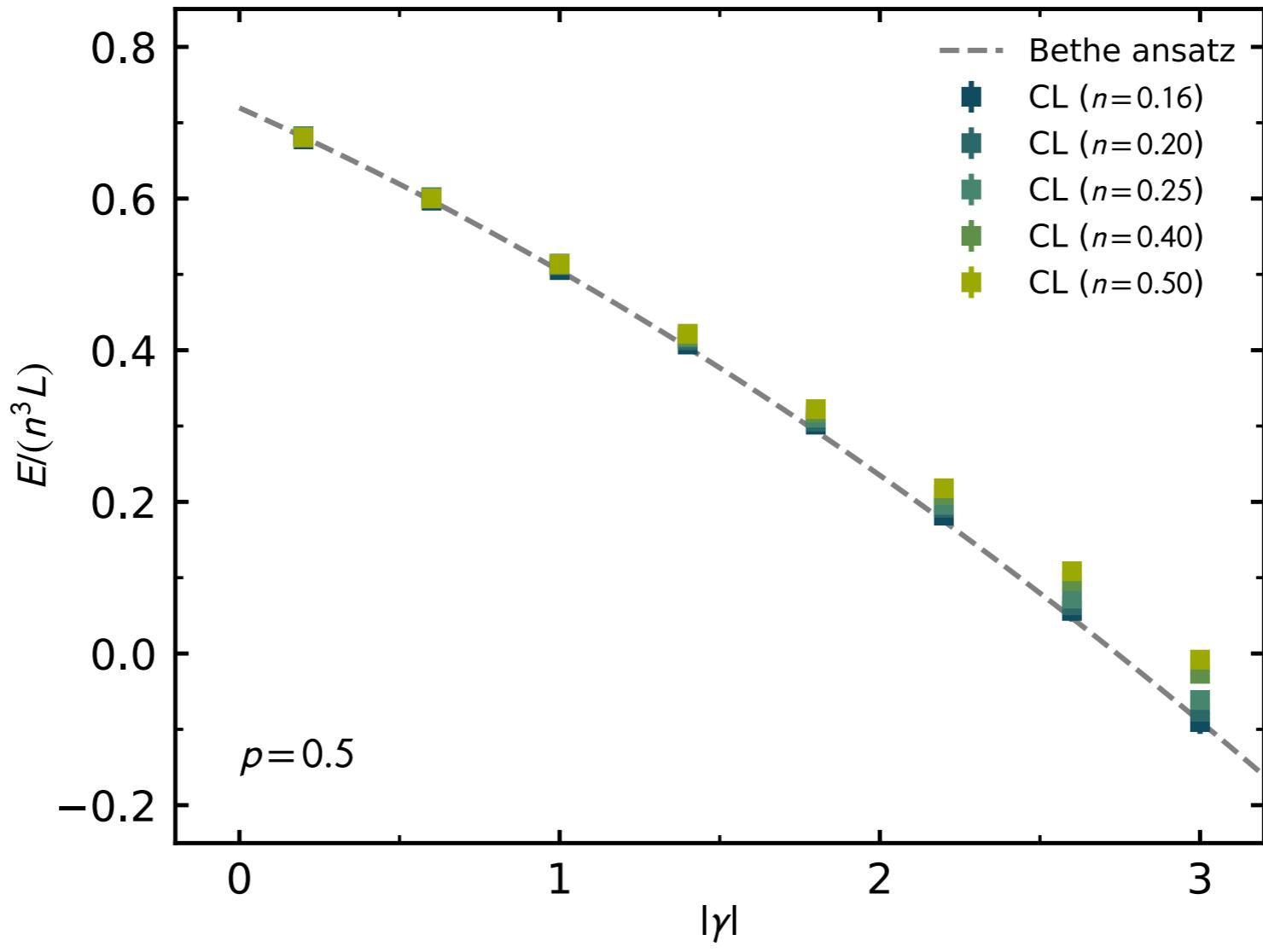
[DFT-RG: Kemler, Pospiech, Braun '17; Kemler '17]

[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)

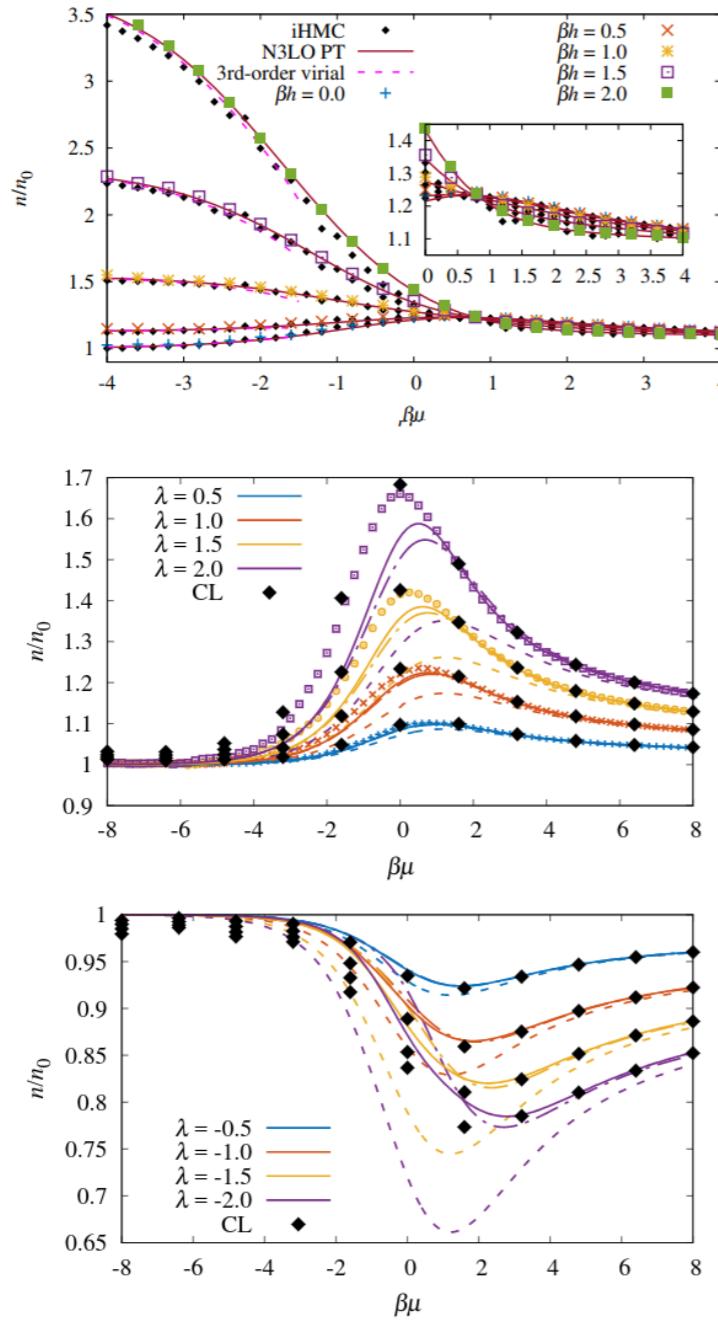


$$\gamma = g/n$$
$$p = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}}$$

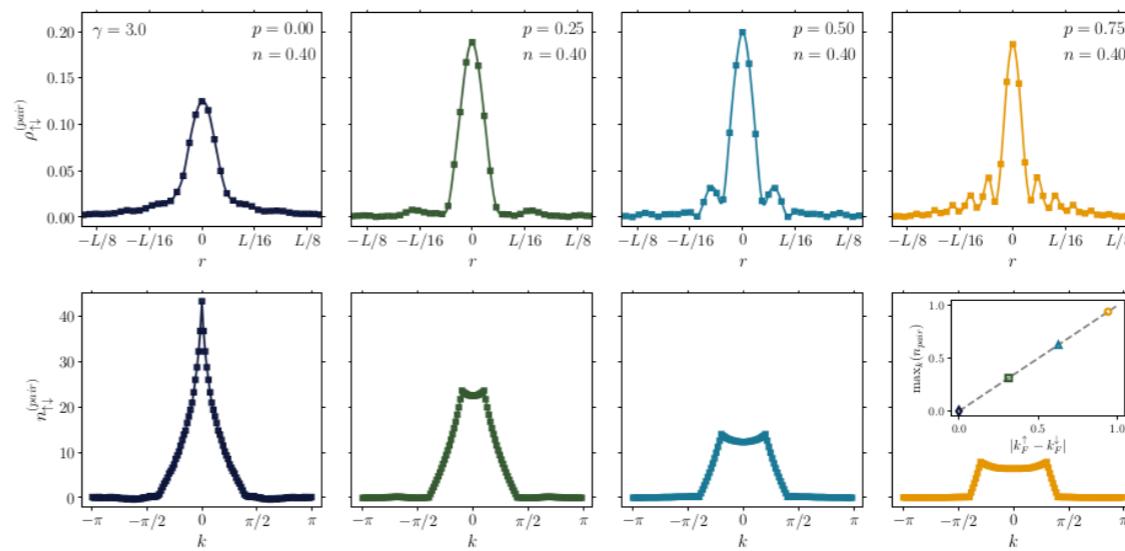
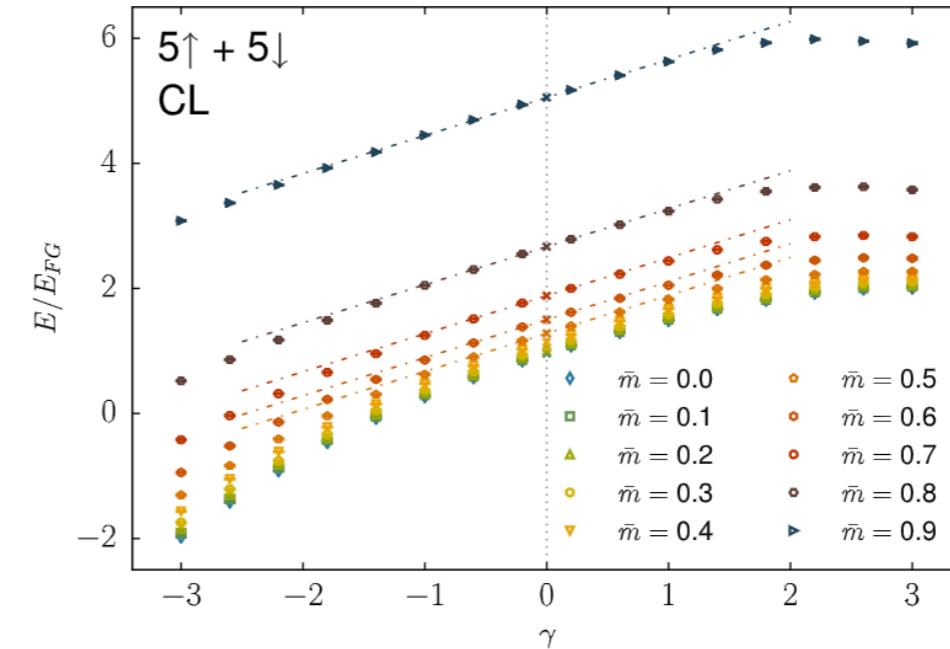
[BA: Iida, Wadati '07; Tracy, Widom '16]

but wait: there's more!

[Loheac,Drut '17]



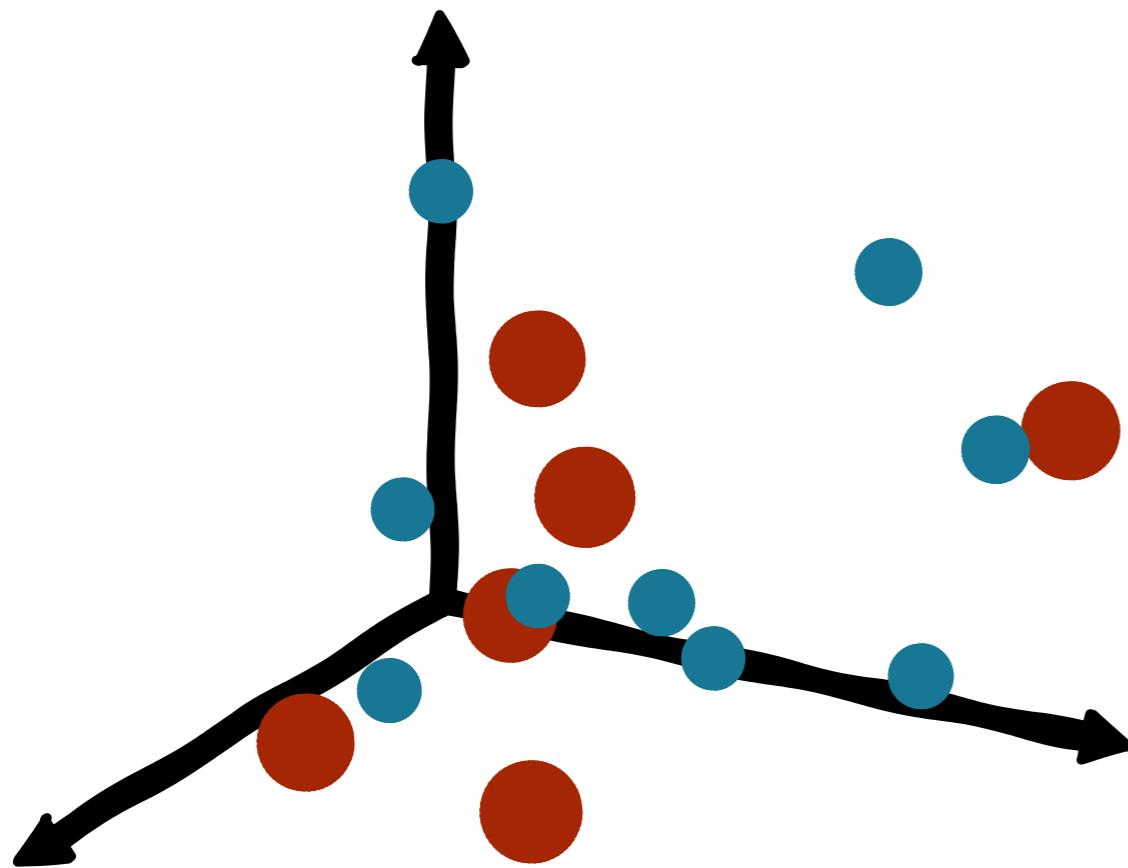
[LR,Porter,Drut,Braun '17]



[Loheac,Braun,Drut '18]

[LR,Drut,Braun *in preparation*]

three dimensional systems at $T > 0$



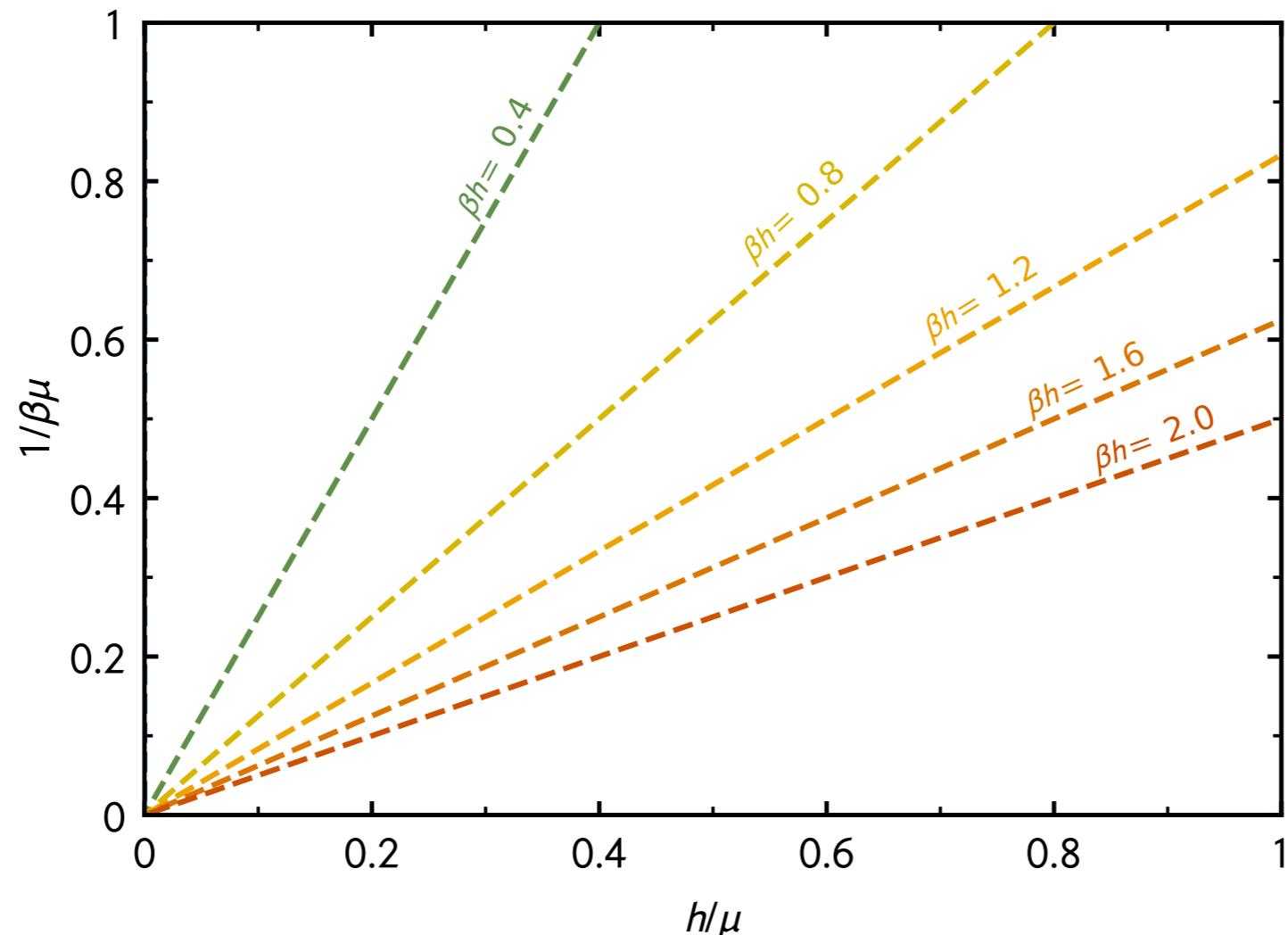
$$\begin{aligned}\mathcal{Z} &= \text{Tr} \left[e^{-\beta(\hat{H}-\mu_{\uparrow}\hat{N}_{\uparrow}-\mu_{\downarrow}\hat{N}_{\downarrow})} \right] \\ &= \text{Tr} \left[e^{-\beta(\hat{H}-\mu\hat{N}-h\hat{M})} \right]\end{aligned}$$

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

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

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

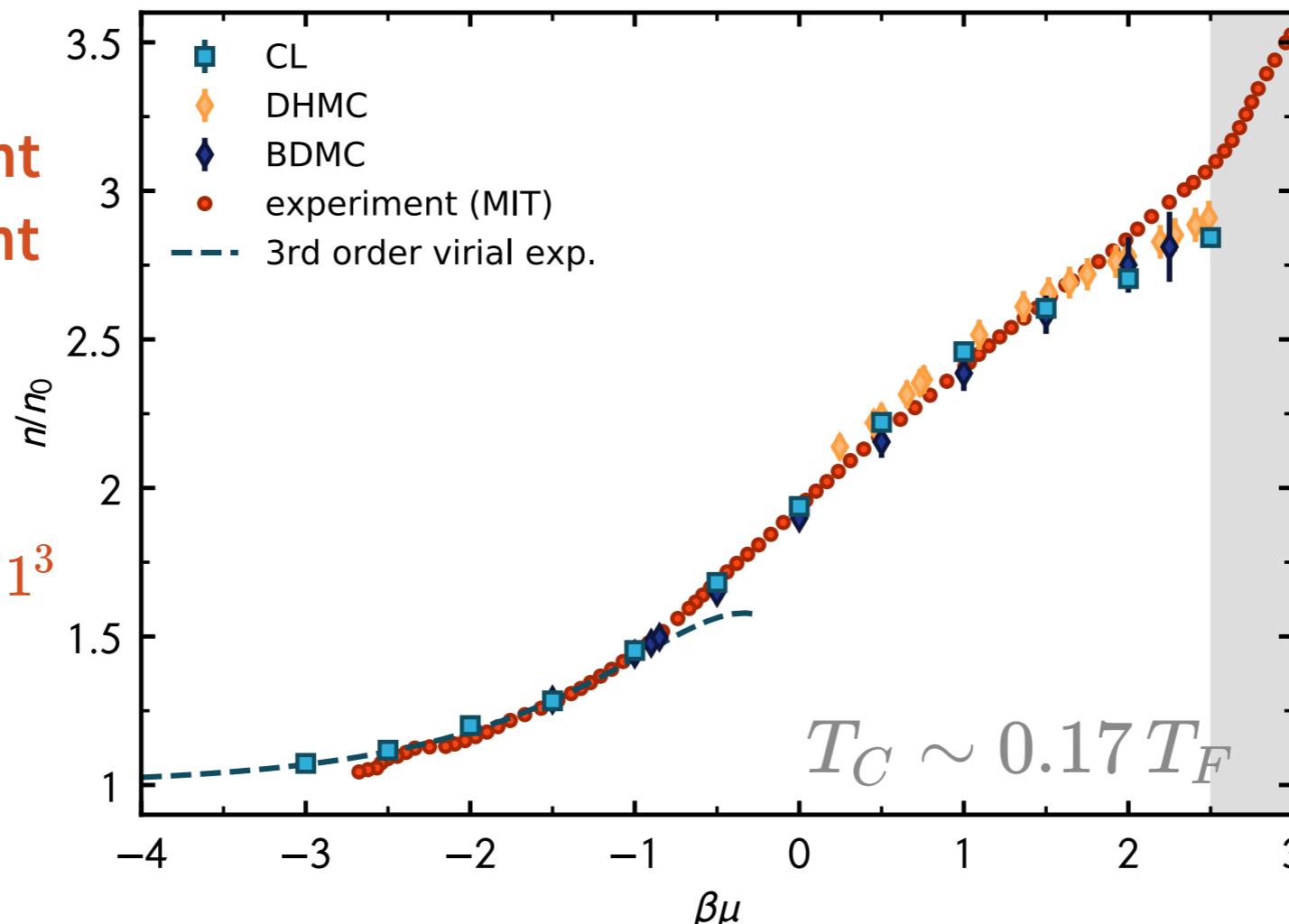
[LR, Loheac, Drut, Braun '18]

[experiment/BDMC: van Houcke et al. '12]

[DHMC: Drut, Lähde, Wlazłowski, 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

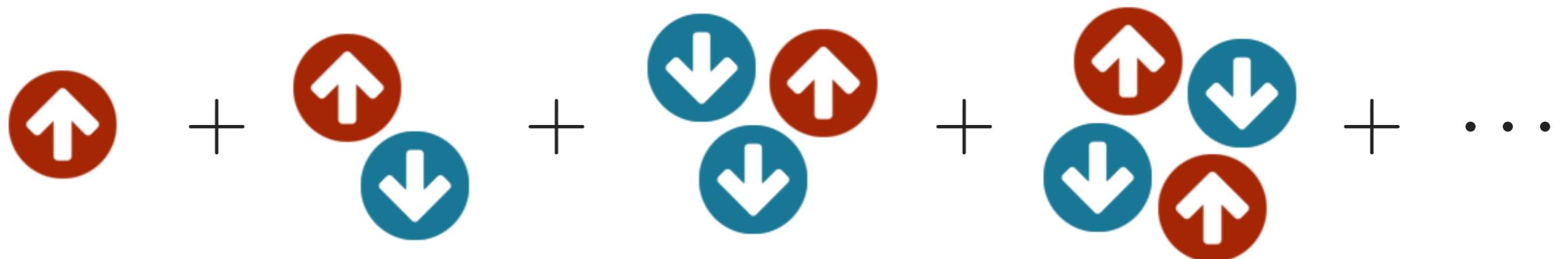
interlude: the virial expansion

dilute gases: few-body correlations dominate

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

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

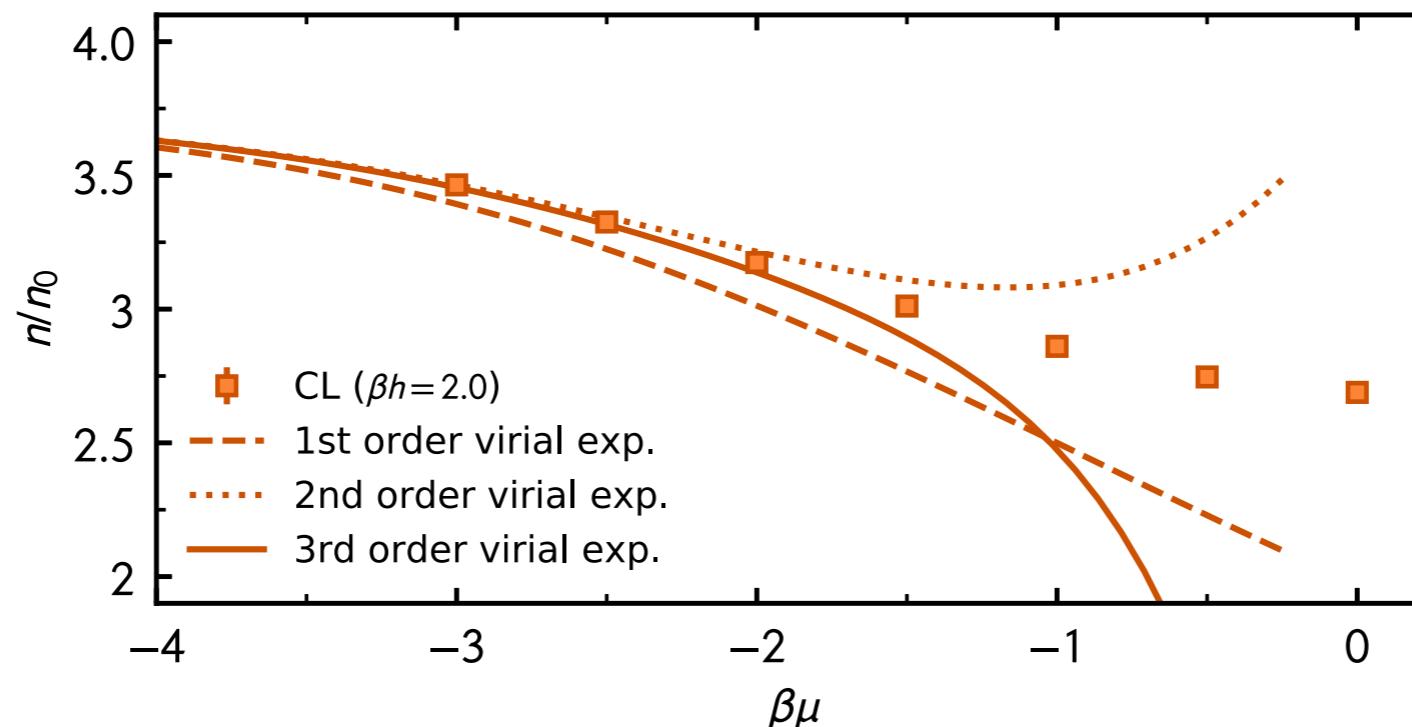
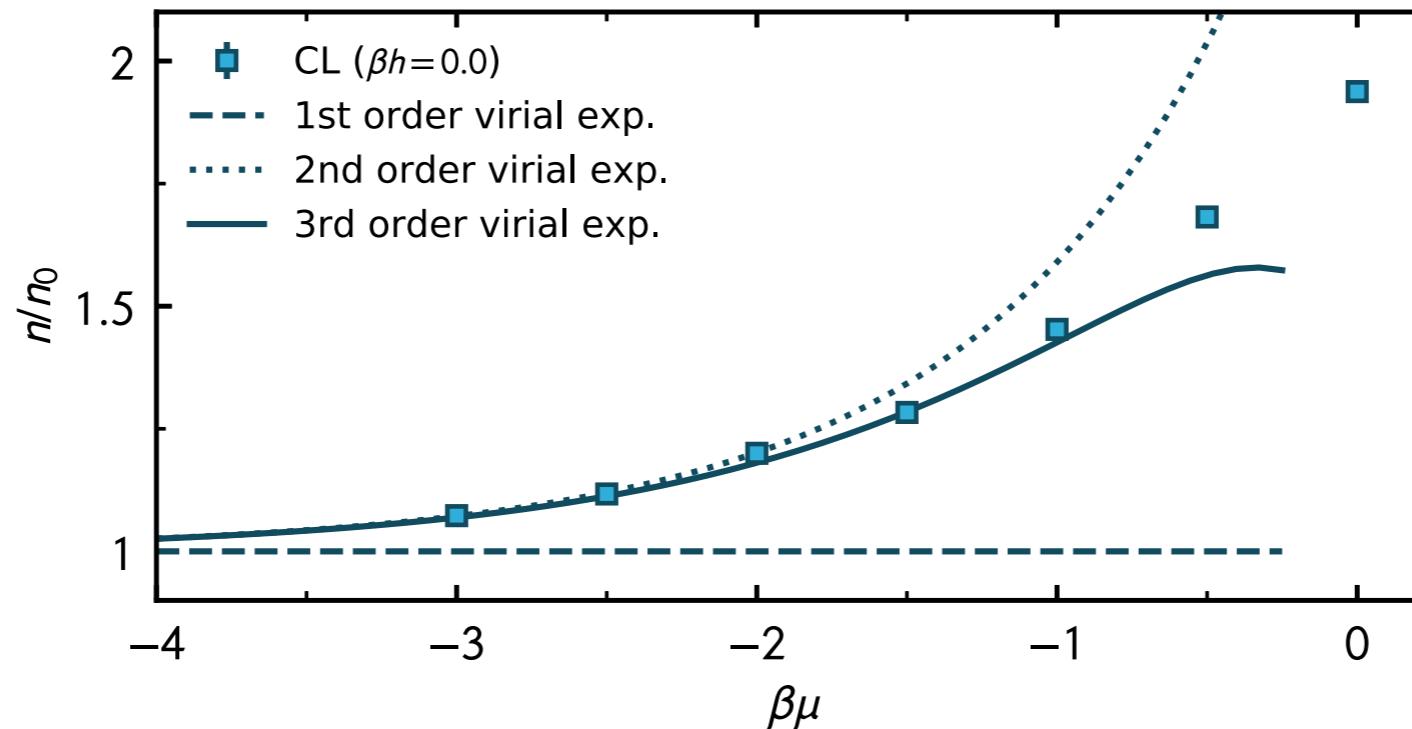
$$\ln \mathcal{Z} = Q_1 \sum_n z^n b_n$$



density EOS (virial regime)

[LR, Loheac, Drut, Braun '18]

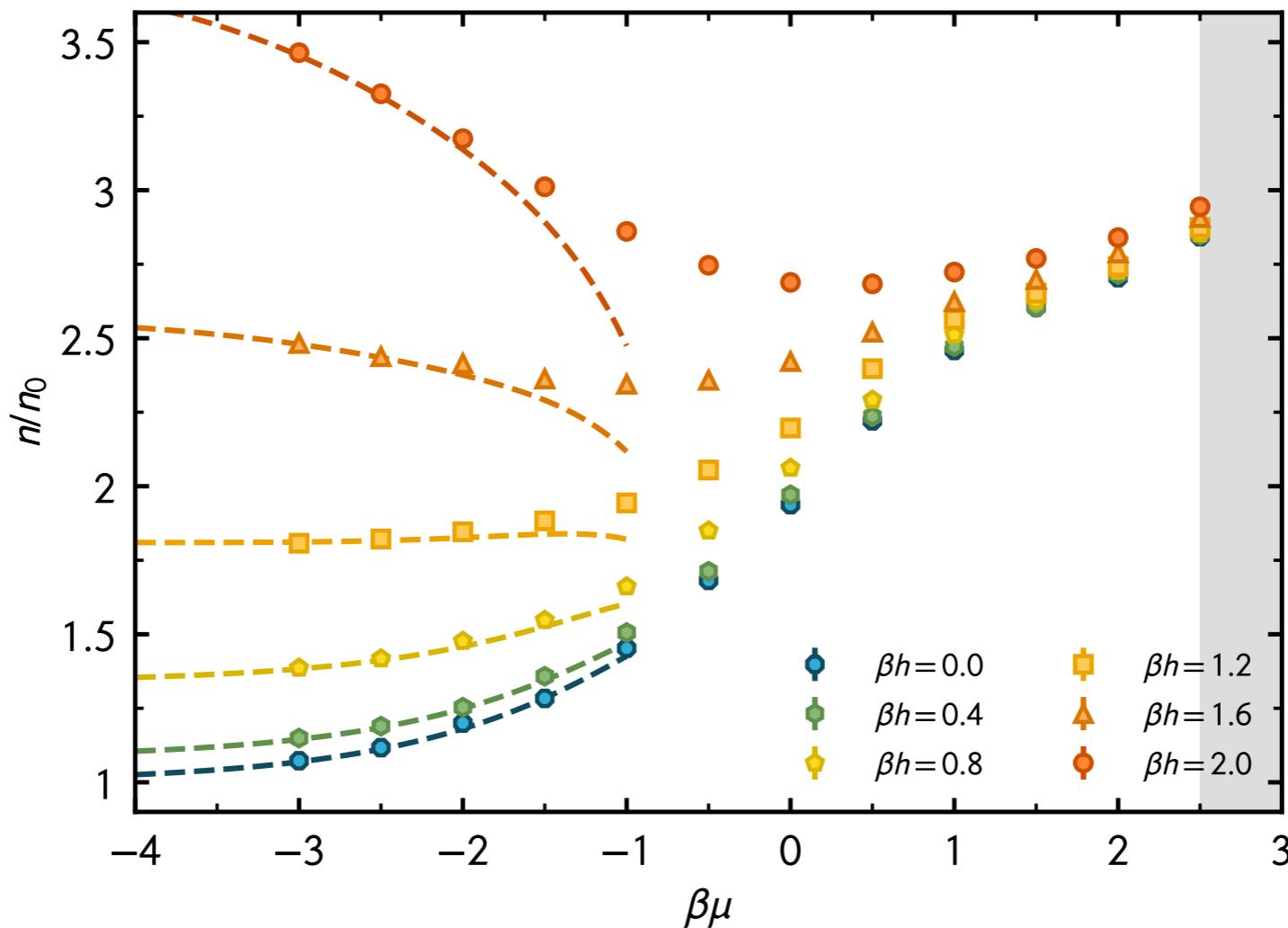
VE approaches
the CL results
order-by-order



VE deviates earlier
for polarized
systems

density EOS at finite polarization

[LR, Loheac, Drut, Braun '18]



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

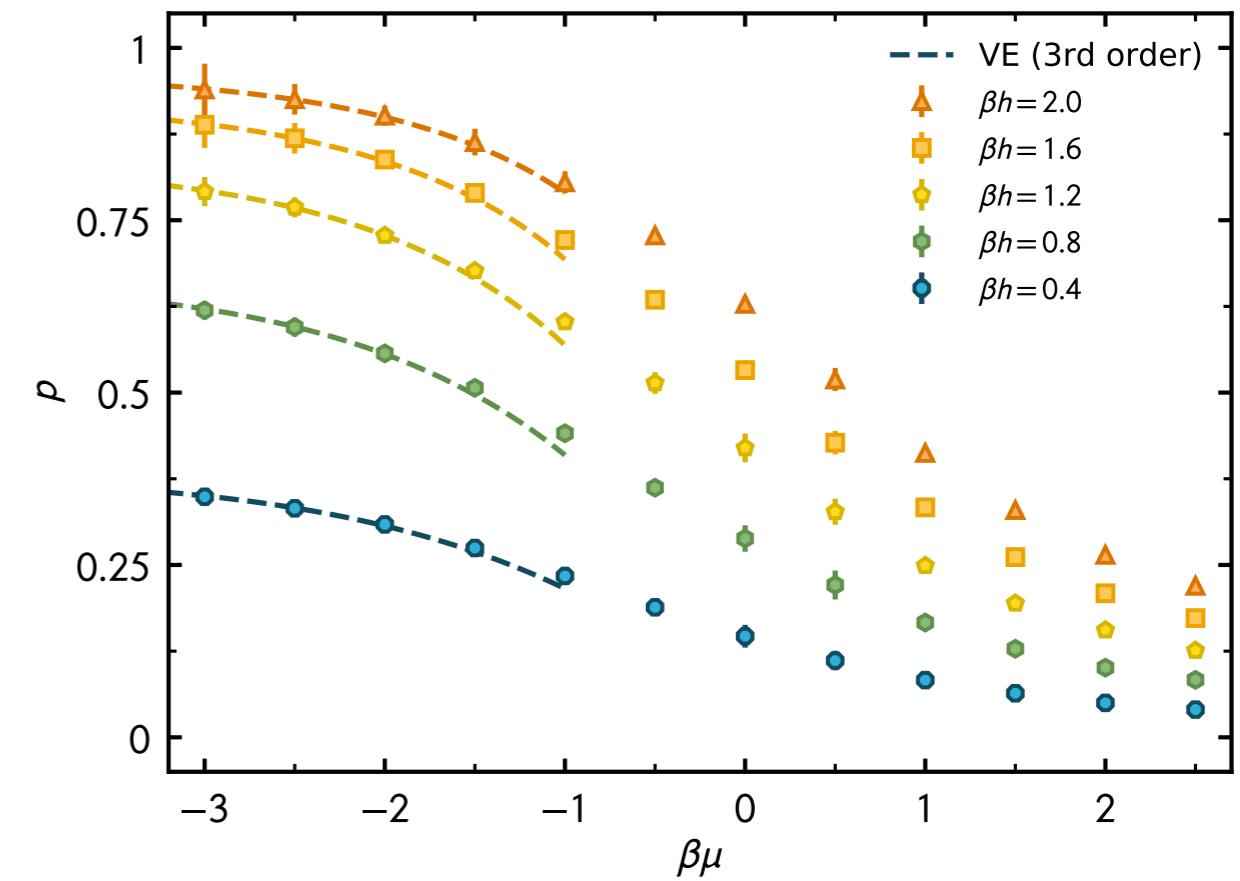
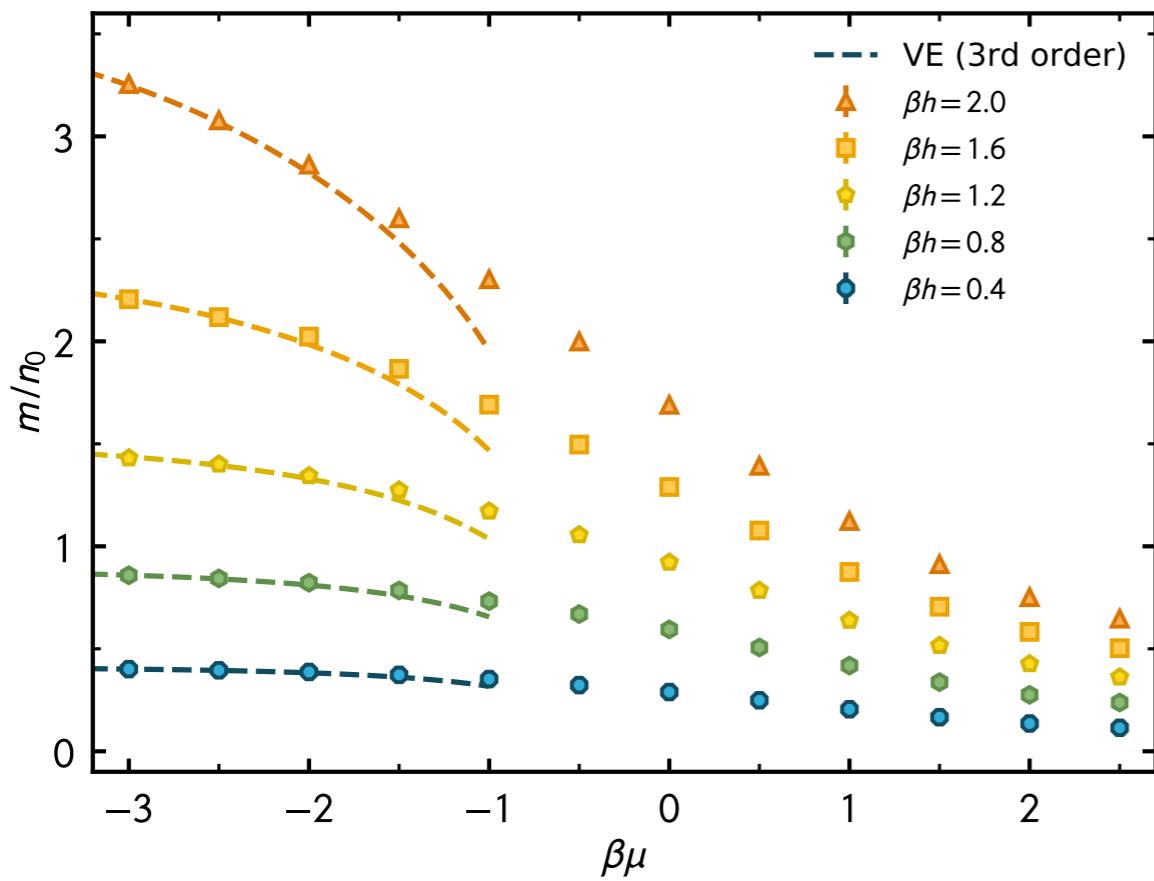
excellent agreement with virial expansion for all polarizations

magnetization & polarization

[LR, Loheac, Drut, Braun '18]

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

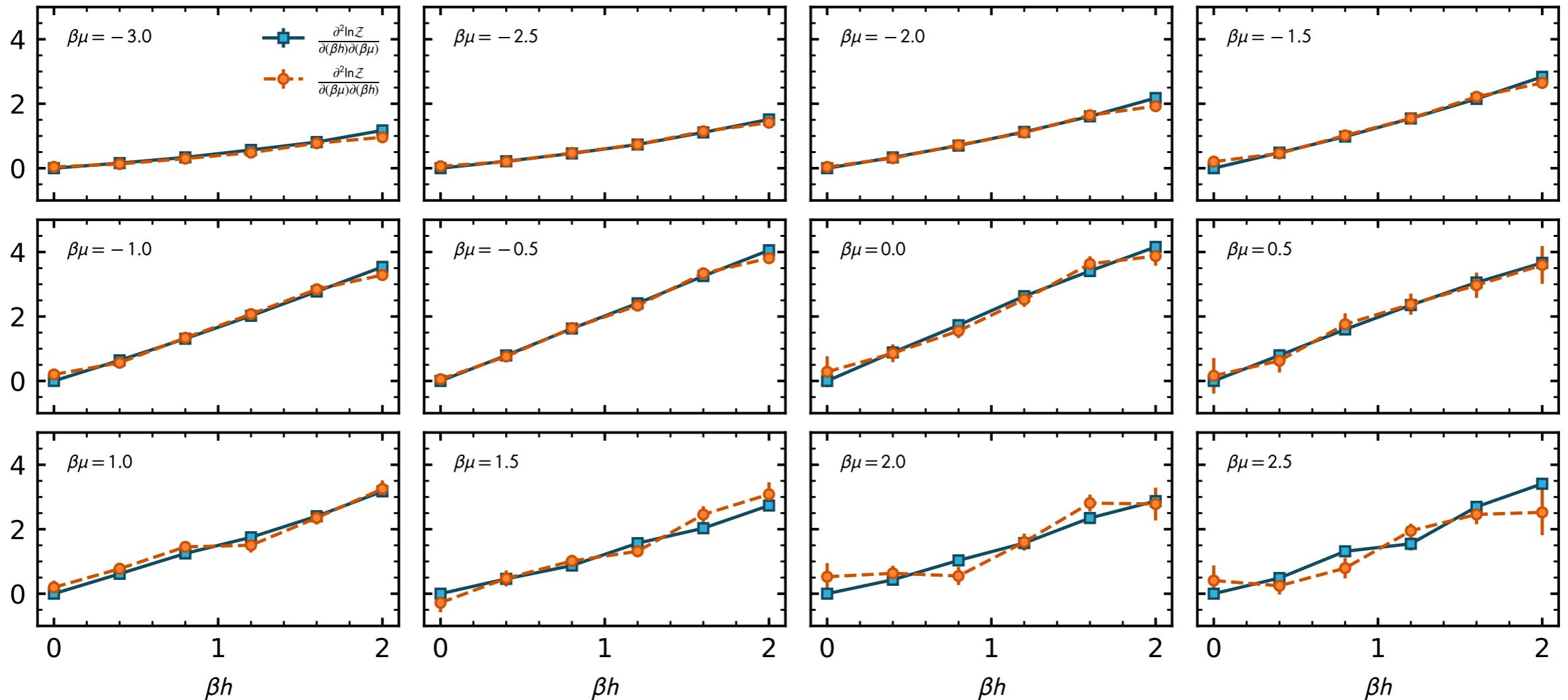
$$p = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}} = \frac{m}{n}$$



Maxwell relations: consistency check

[LR, Loheac, Drut, Braun '18]

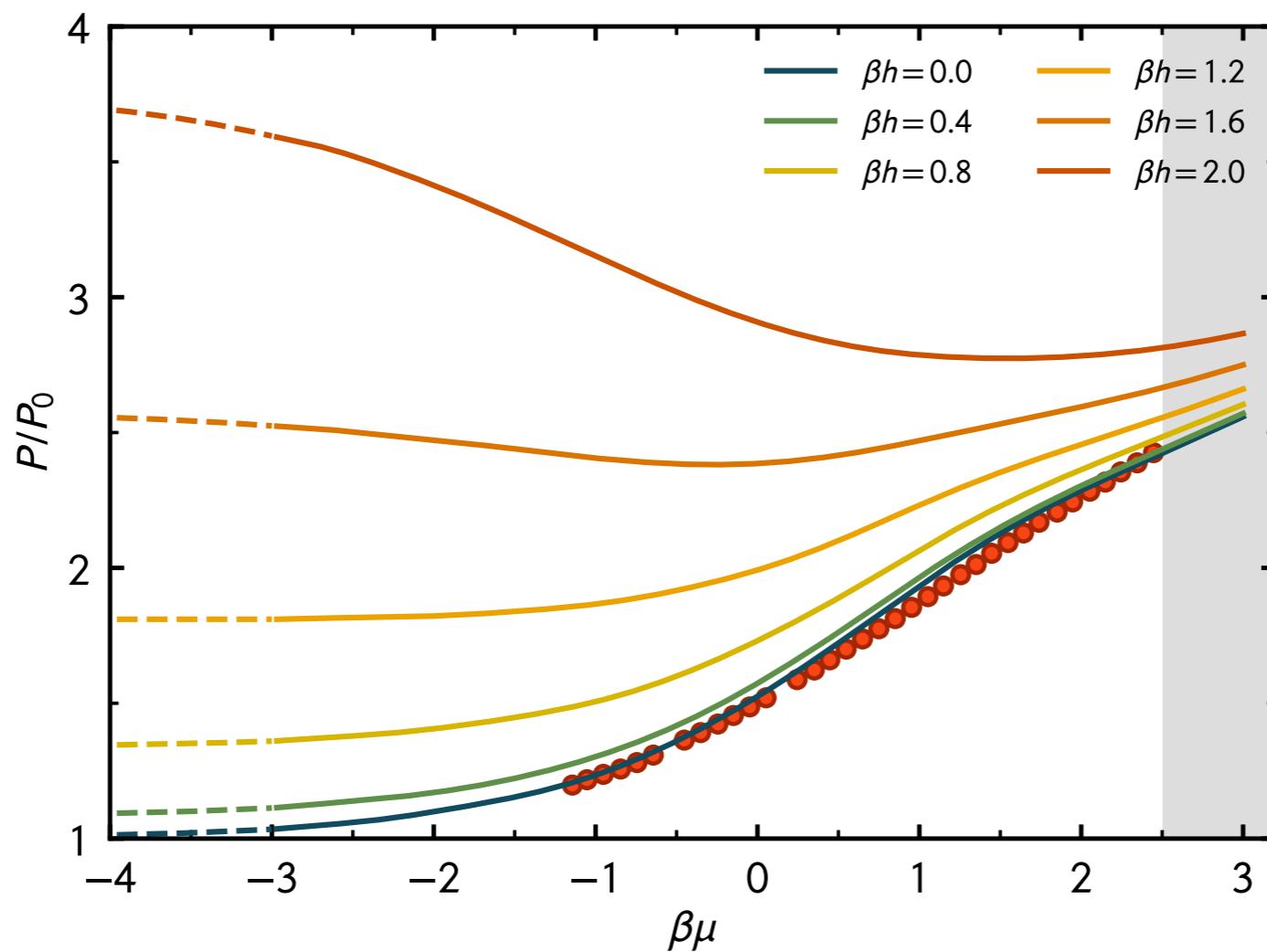
$$\left(\frac{\partial n}{\partial(\beta h)} \right)_{\beta\mu} \stackrel{!}{=} \left(\frac{\partial m}{\partial(\beta\mu)} \right)_{\beta h}$$



pressure equation of state

[LR, Loheac, Drut, Braun '18]

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

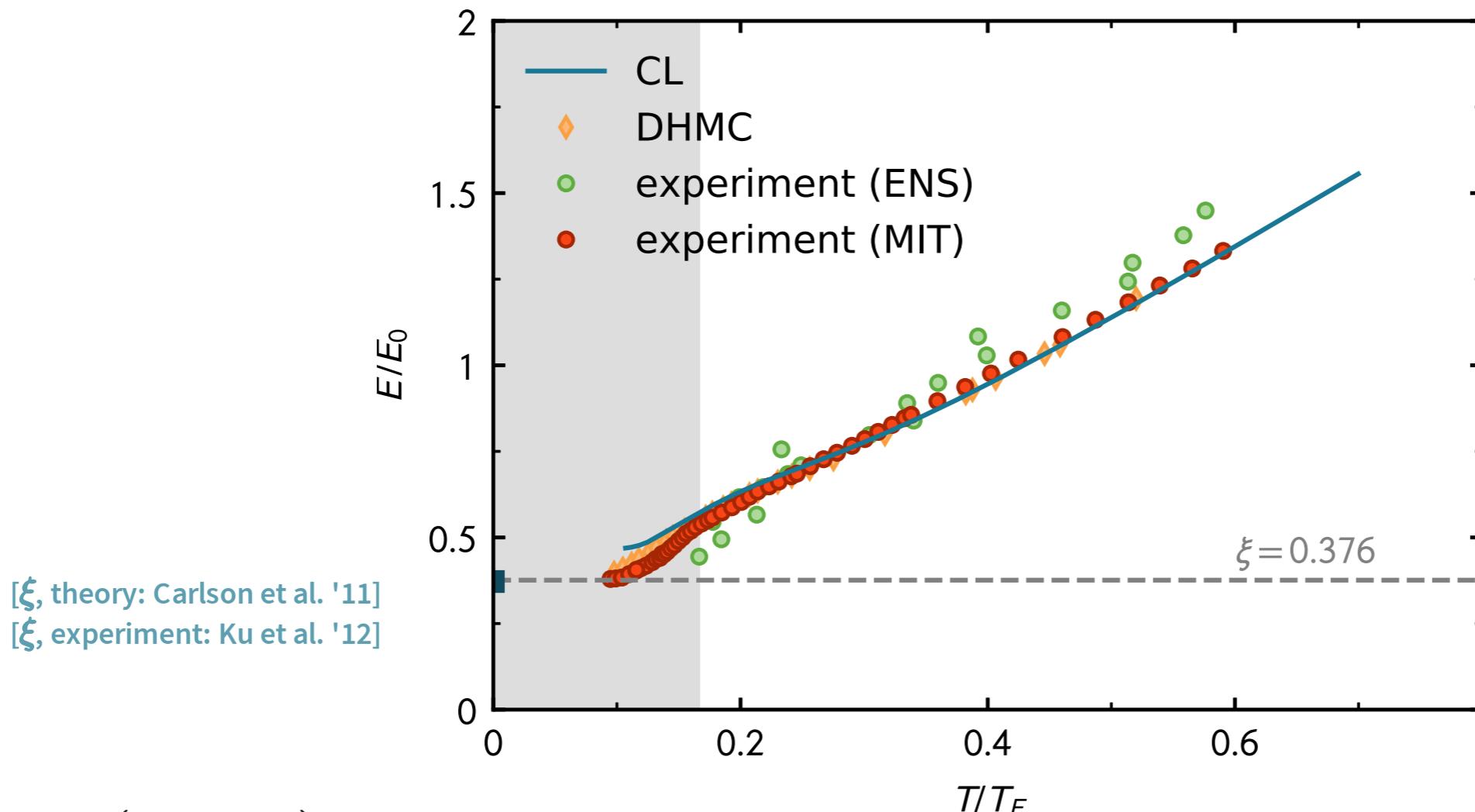


[experiment: Ku et al. '12]

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]

$[\xi, \text{theory: Carlson et al. '11}]$

$[\xi, \text{experiment: Ku et al. '12}]$

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

[universality: Ho '04]

[experiment: Ku et al. '12; Nascimbène et al. '12]

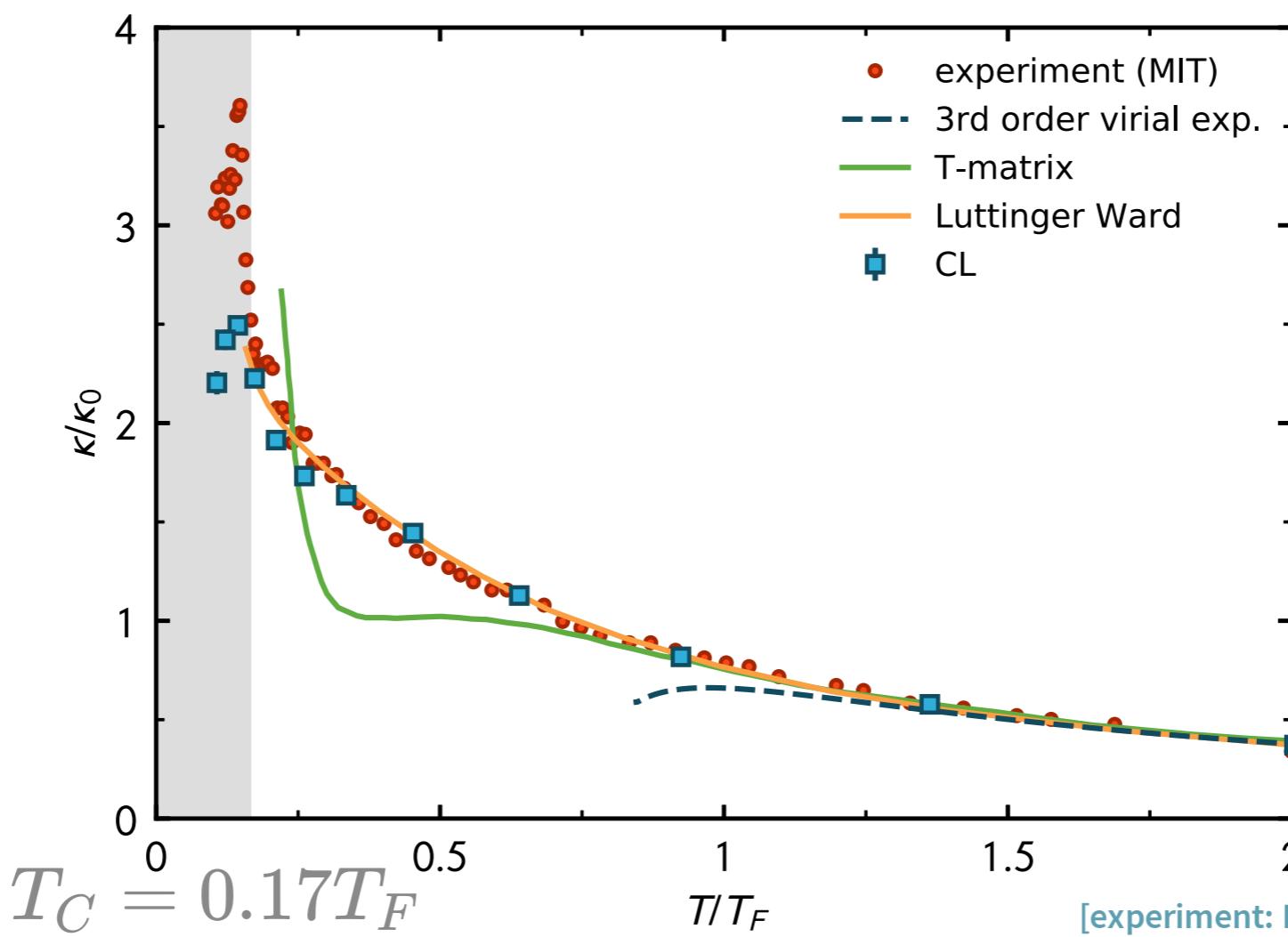
[DHMC: Drut et al. '12]

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



features of curve
recovered with CL

quantitative
disagreement
at low
temperatures

[experiment: Ku et al. '12]

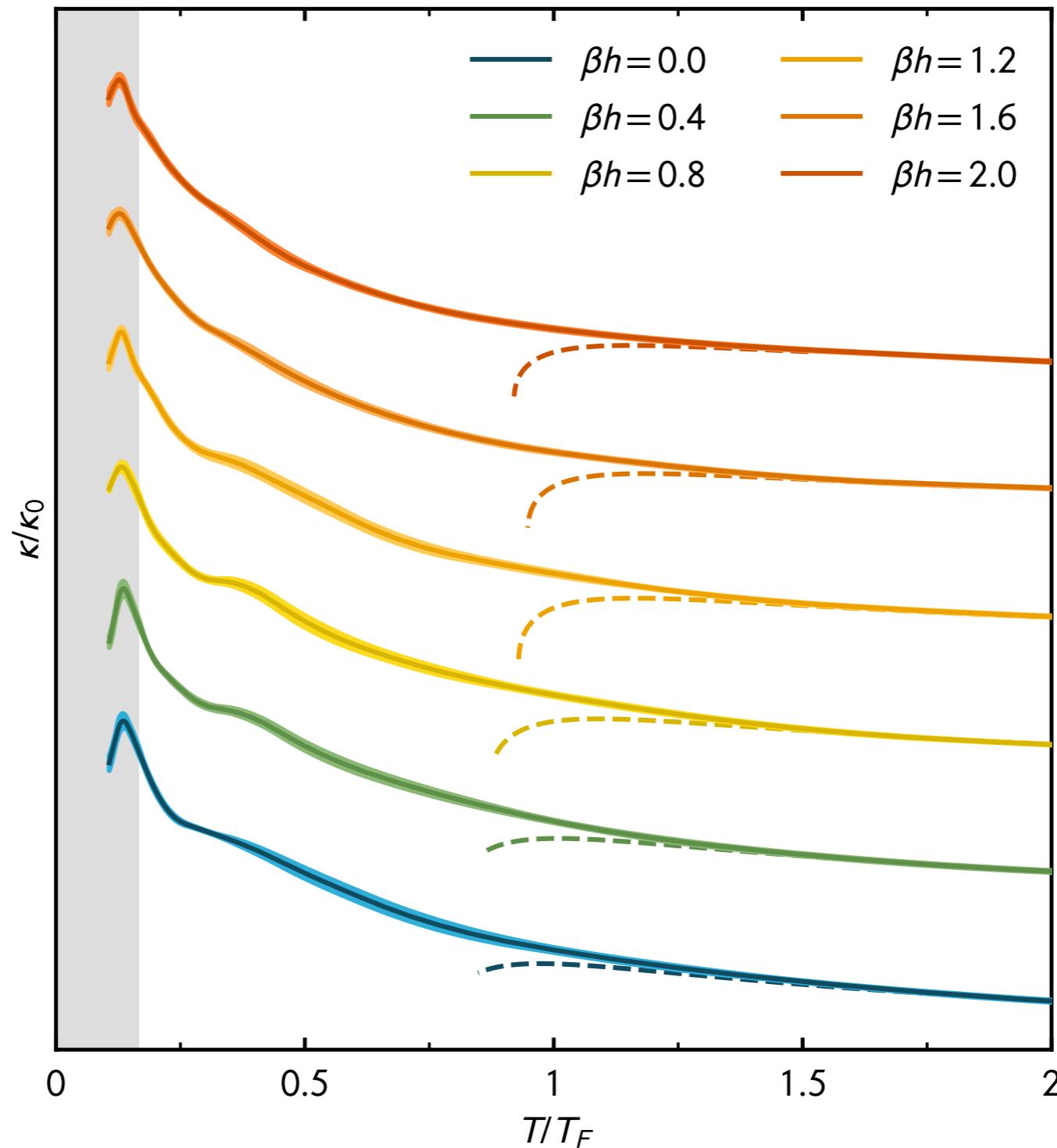
[Luttinger-Ward: Enns, Haussmann '12]

[T-matrix: Pantel et al. '14]

compressibility for polarized systems

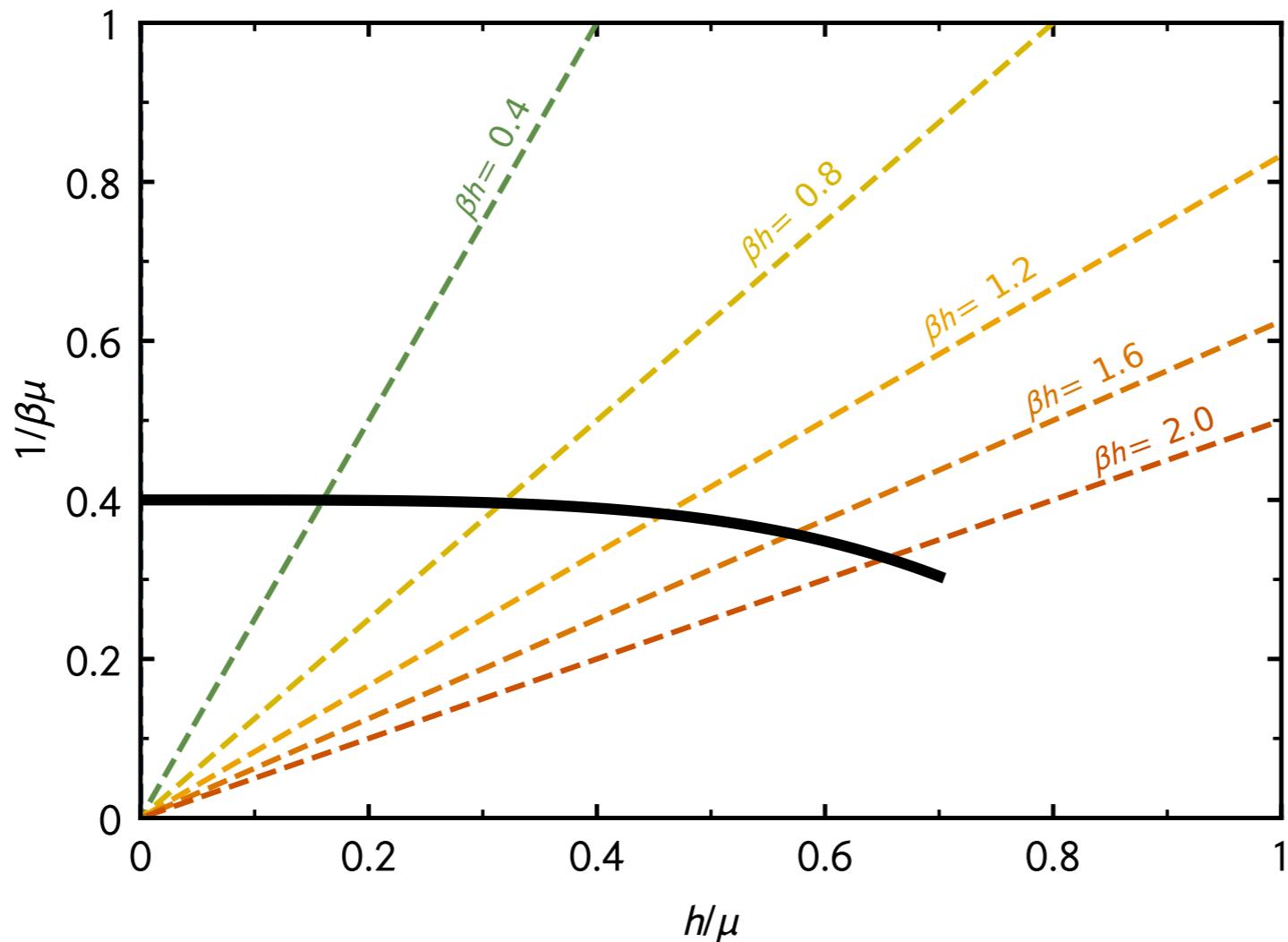
[LR, Loheac, Drut, Braun '18]

weak dependence
of the critical
temperature on
polarization
indicated



challenging to
extract precise T_C

UFG phase diagram (sketch)



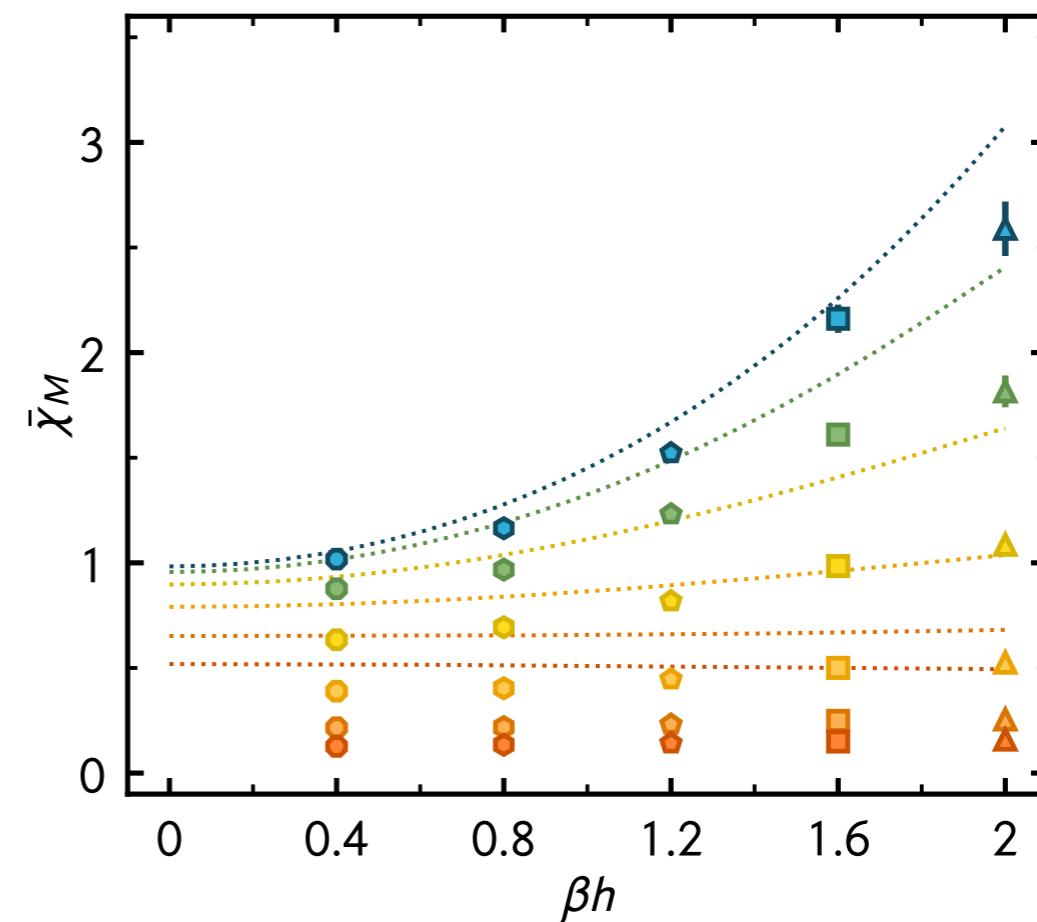
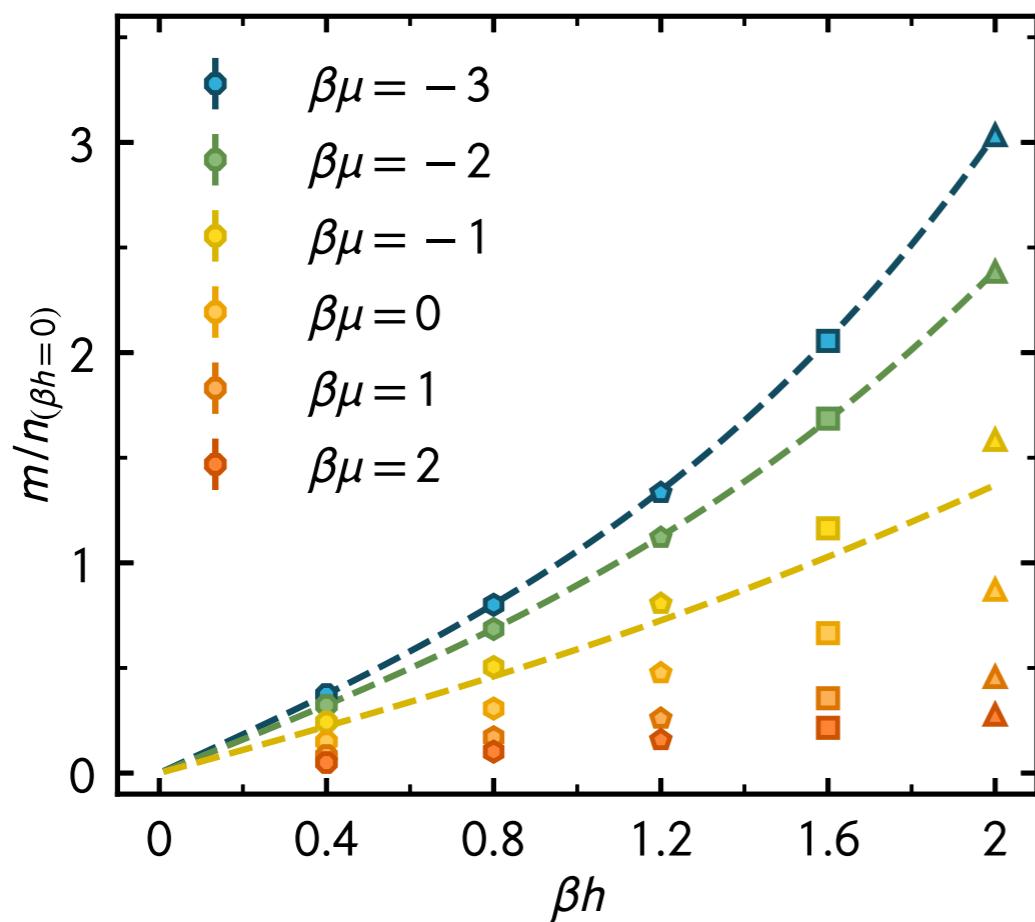
$$\mu = \frac{\mu_{\uparrow} + \mu_{\downarrow}}{2}$$

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

spin susceptibility

[LR, Loheac, Drut, Braun '18]

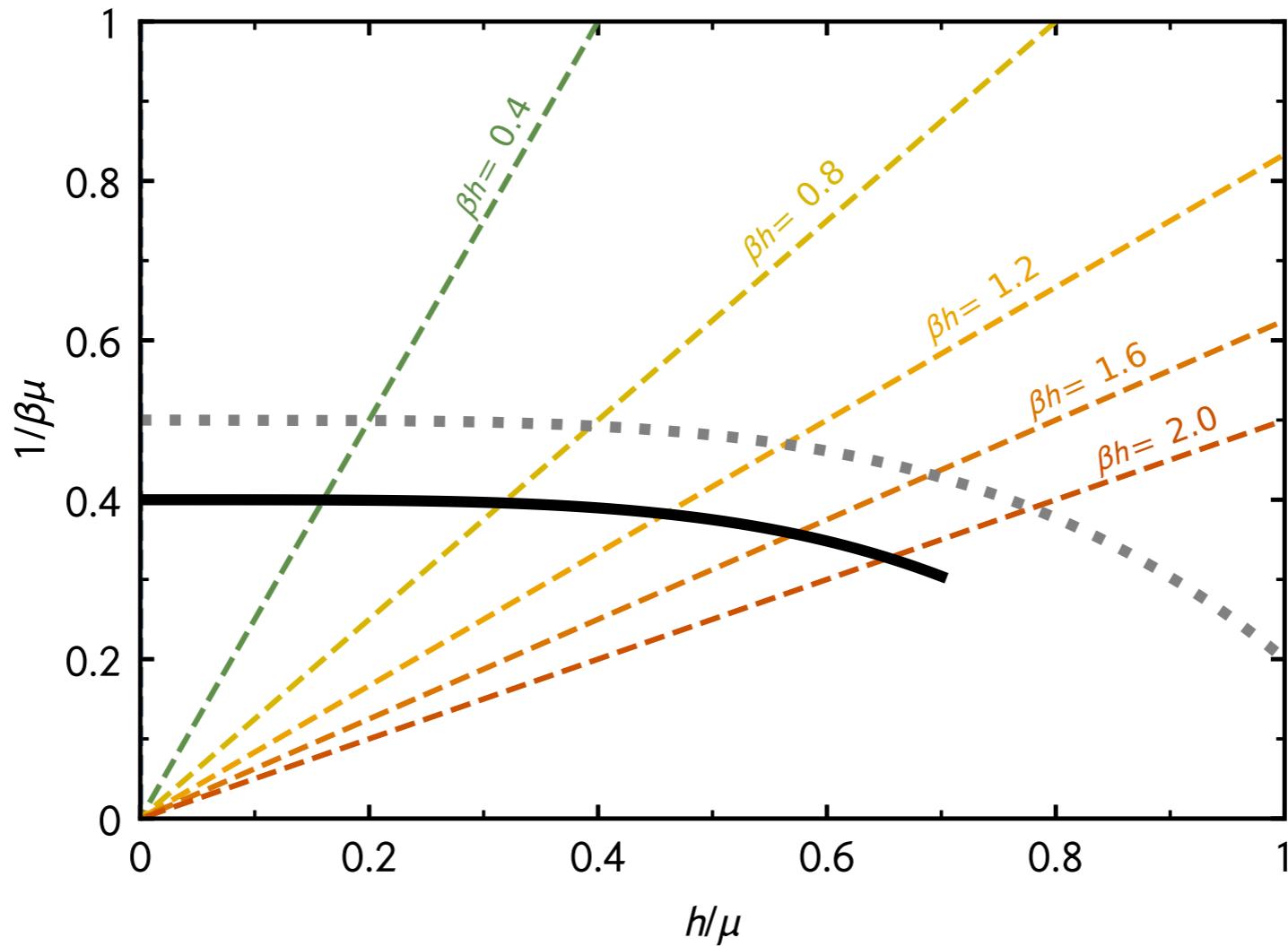
$$\chi = \left(\frac{\partial m}{\partial h} \right)_{T,V,\mu}$$



Pauli susceptibility field independent at low field and T

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

UFG phase diagram (sketch)



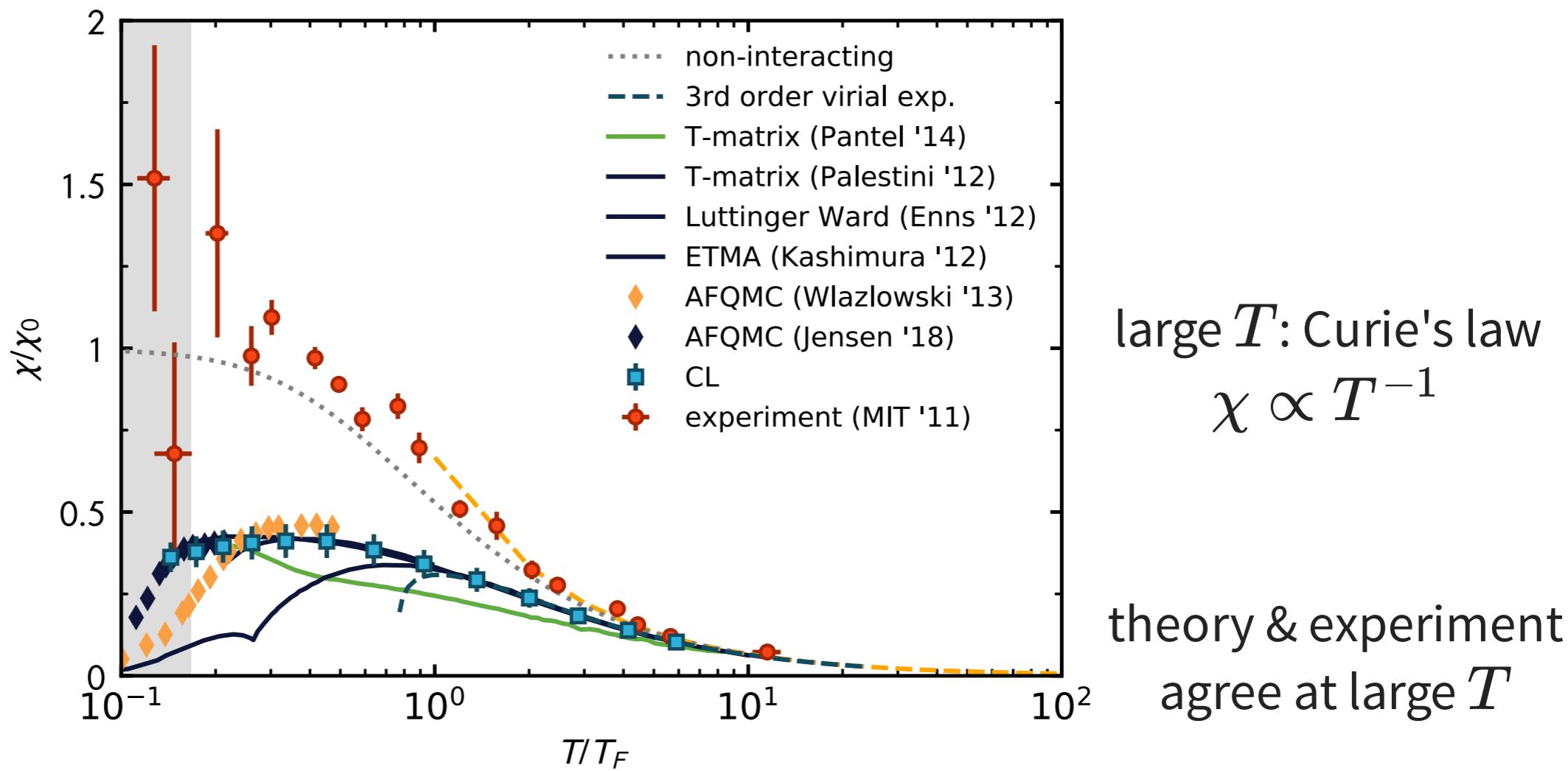
$$\mu = \frac{\mu_{\uparrow} + \mu_{\downarrow}}{2}$$

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

magnetic susceptibility (unpolarized)

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

low T :
discrepancy
between
experiment and
theory



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

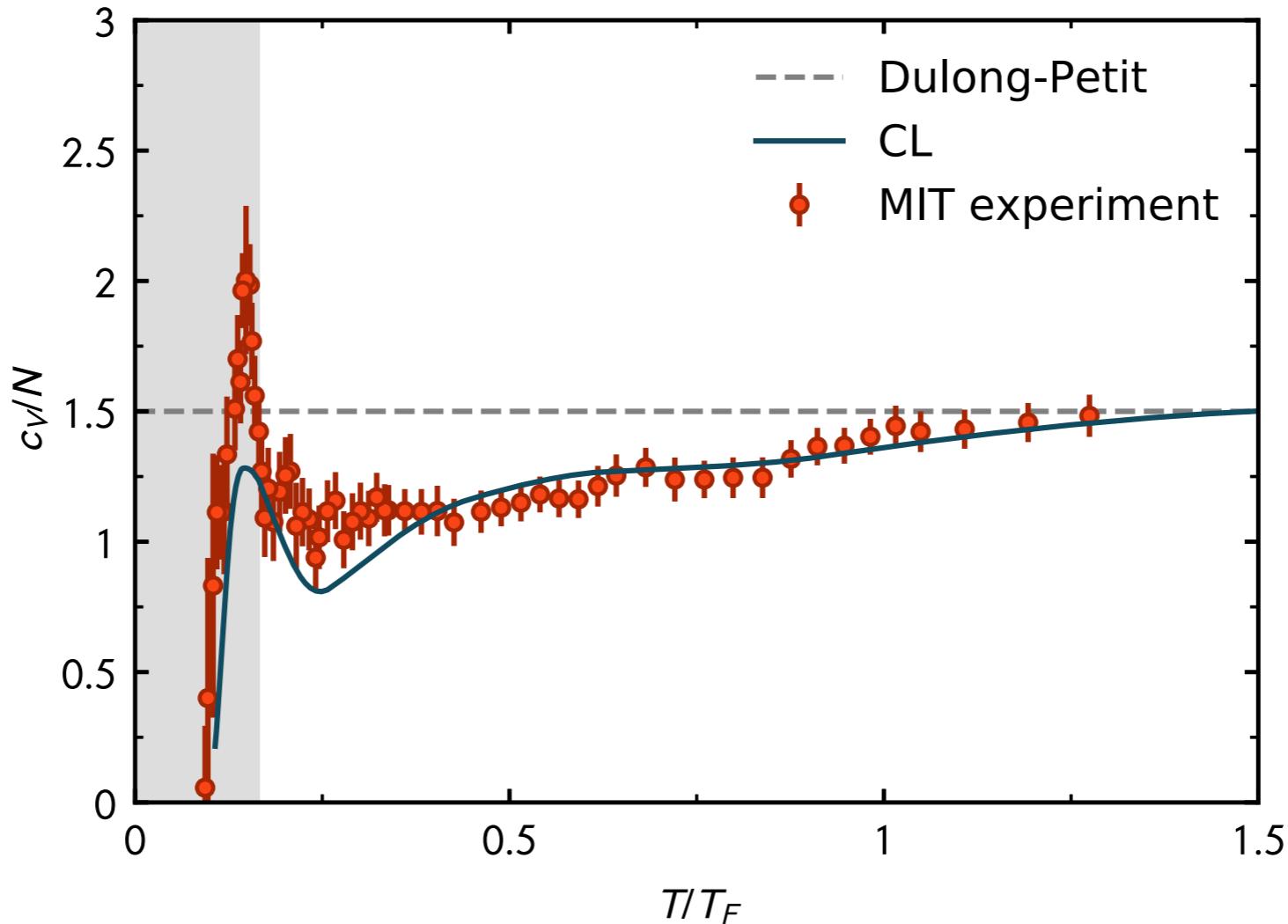
search for **inhomogeneous phases** in 2D/3D

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

specific heat

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

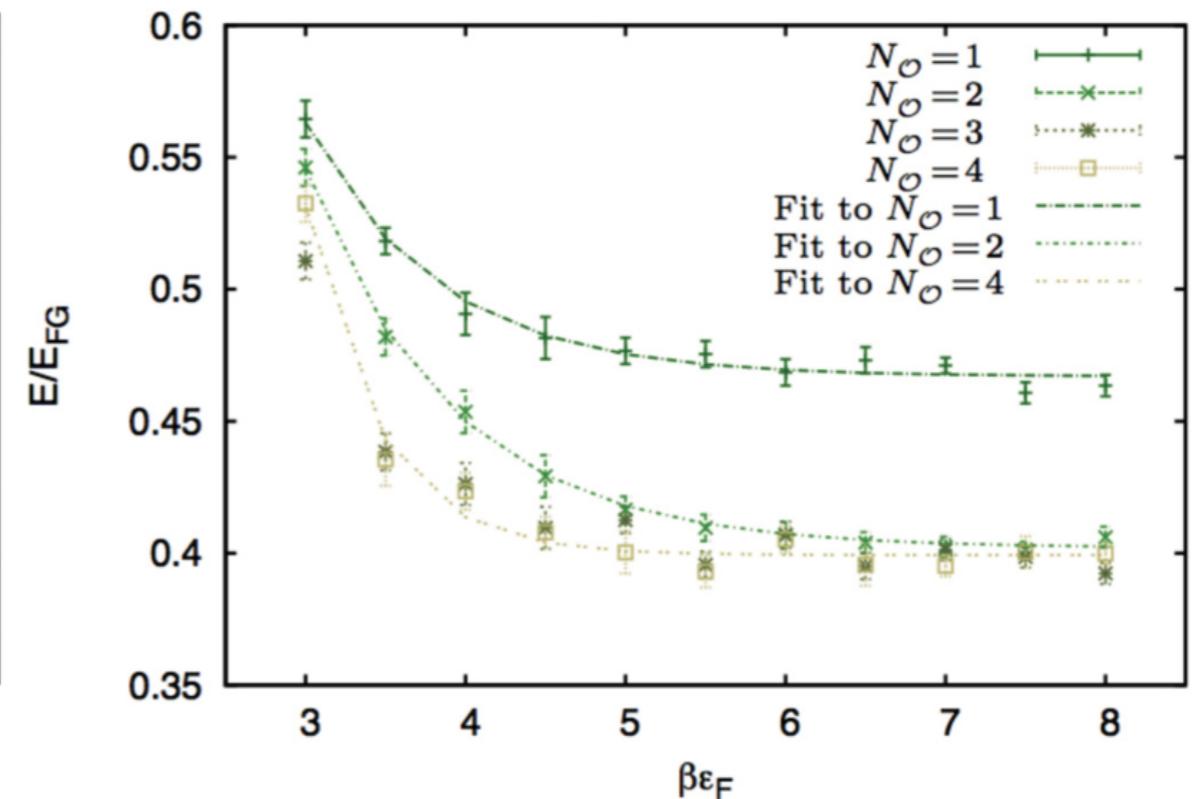
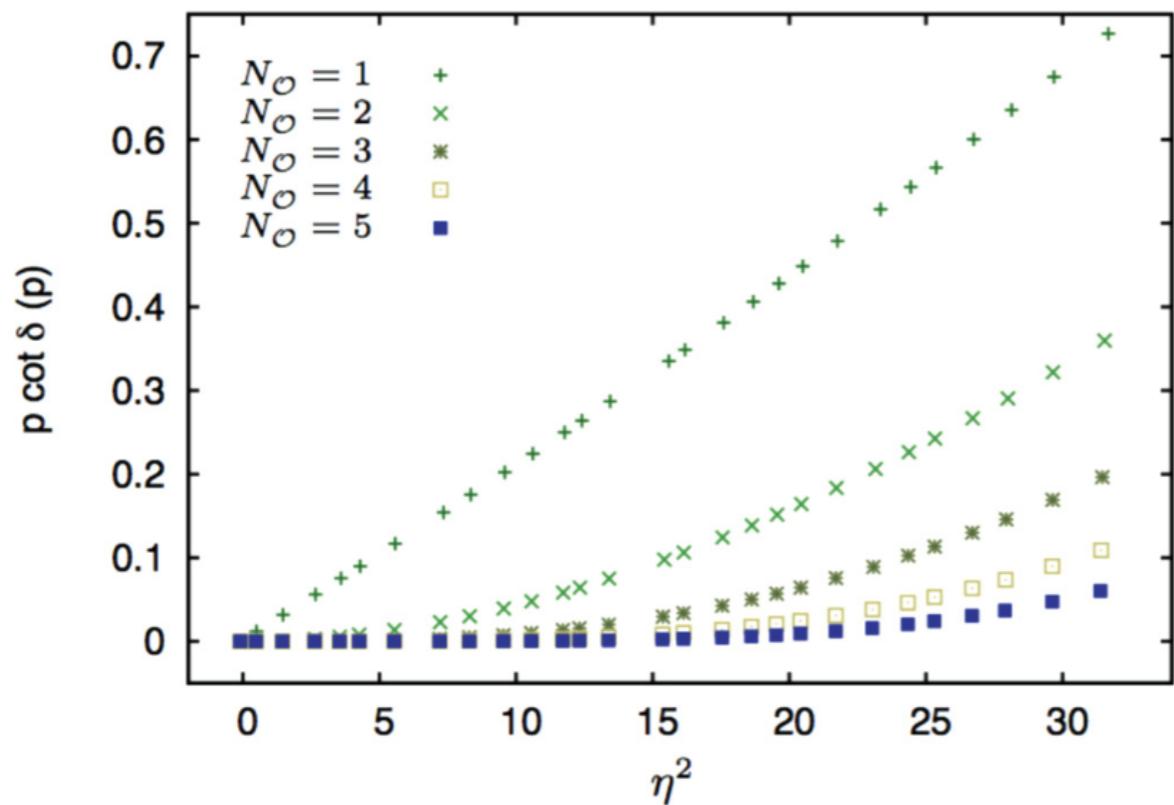
$$\frac{C_V}{N} = \left(\frac{\partial E}{\partial T} \right)_{N,V} = \frac{3}{2} \left(\frac{T}{T_F} \right)^{-1} \left(\frac{p}{p_0} - \frac{\kappa_0}{\kappa} \right)$$



improved lattice operators

[Drut '12]

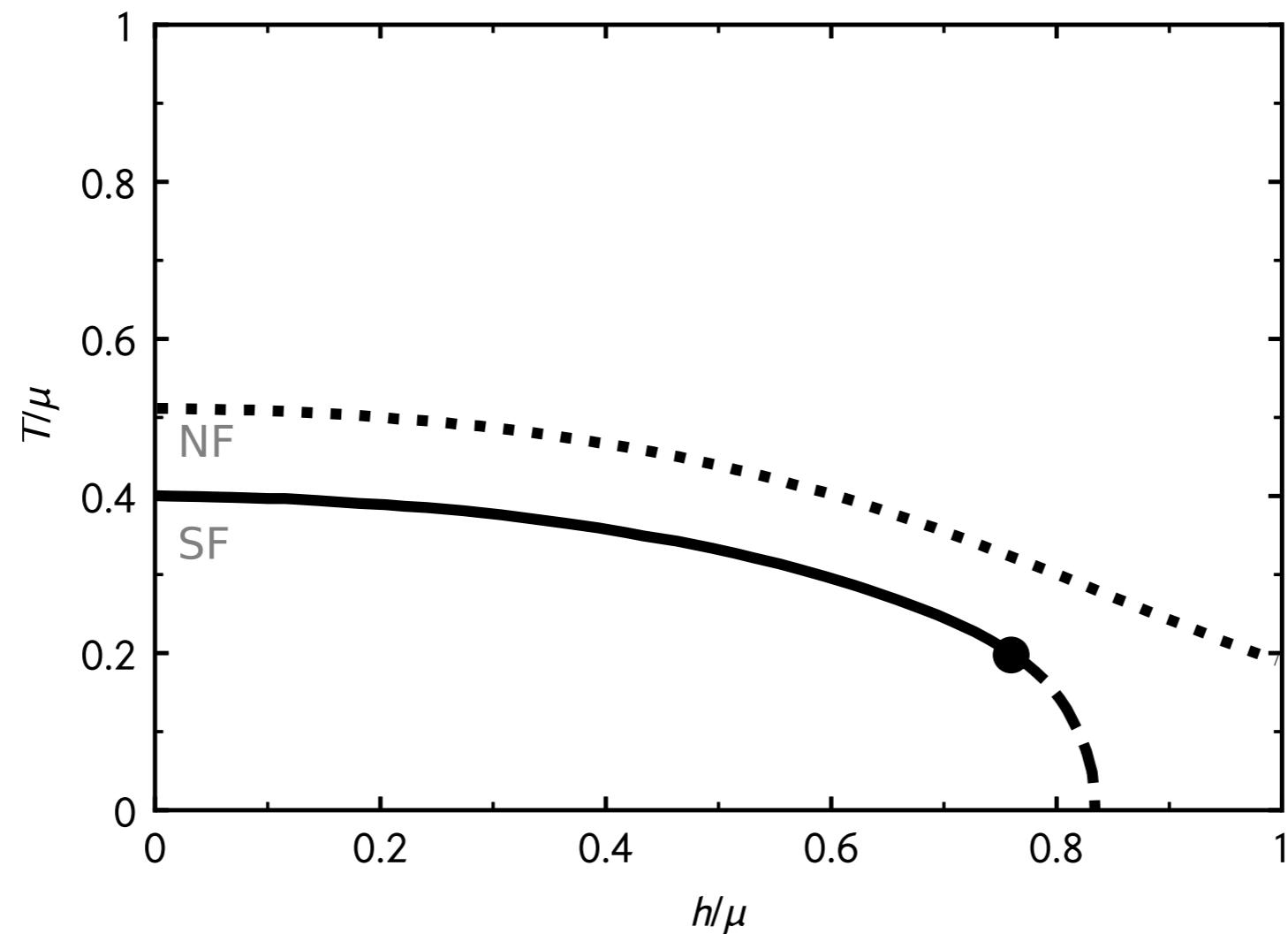
$$p \cot \delta(p) = -\frac{1}{a} + \frac{1}{2} r_{eff} p^2 + \mathcal{O}(p^4)$$



scattering is tuned to reproduce unitarity at finite momenta

[see also: Endres et al. 11']

UFG phase diagram - functional renormalization group (fRG)



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

[Boettcher et al. '14]