ULTRACOLD FERMIONS AWAY FROM BALANCED SYSTEMS

Lukas Rammelmüller, TU Darmstadt
Hirschegg, January 2018

[LR, Drut, Braun *in preparation*]
[LR, Porter, Drut, Braun *Phys. Rev. D* 96, 094506, 2017]
[LR, Porter, Braun, Drut *Phys. Rev. A* 96, 033635, 2017]

THE PLAN

1) Motivation: what do we want to do and why is it interesting?

2) Method: how to get numbers?

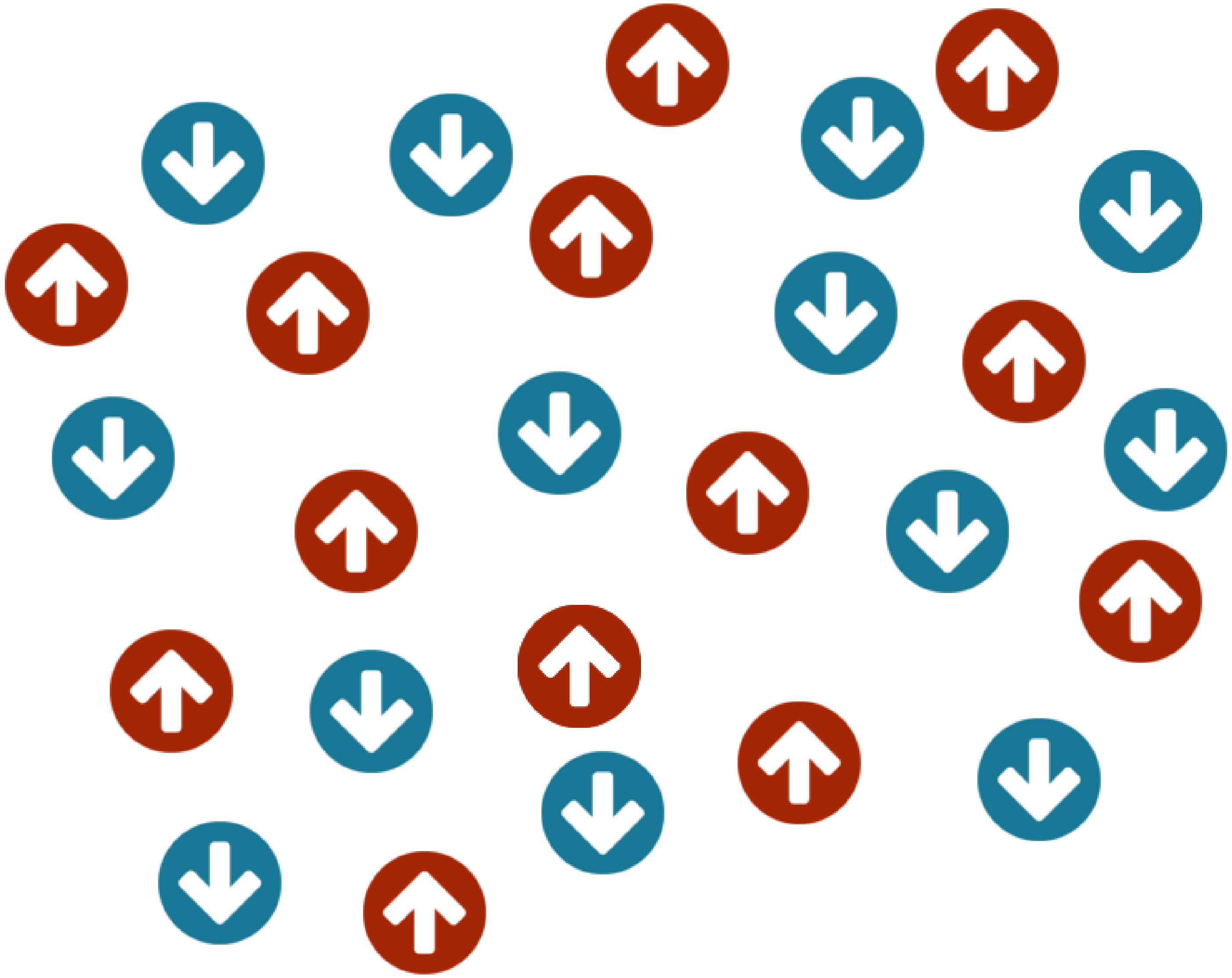
3) Results: 1D & 3D Fermi gases

ULTRACOLD FERMI GASES:
WHY ARE THEY INTERESTING?

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

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

balanced Fermi gas



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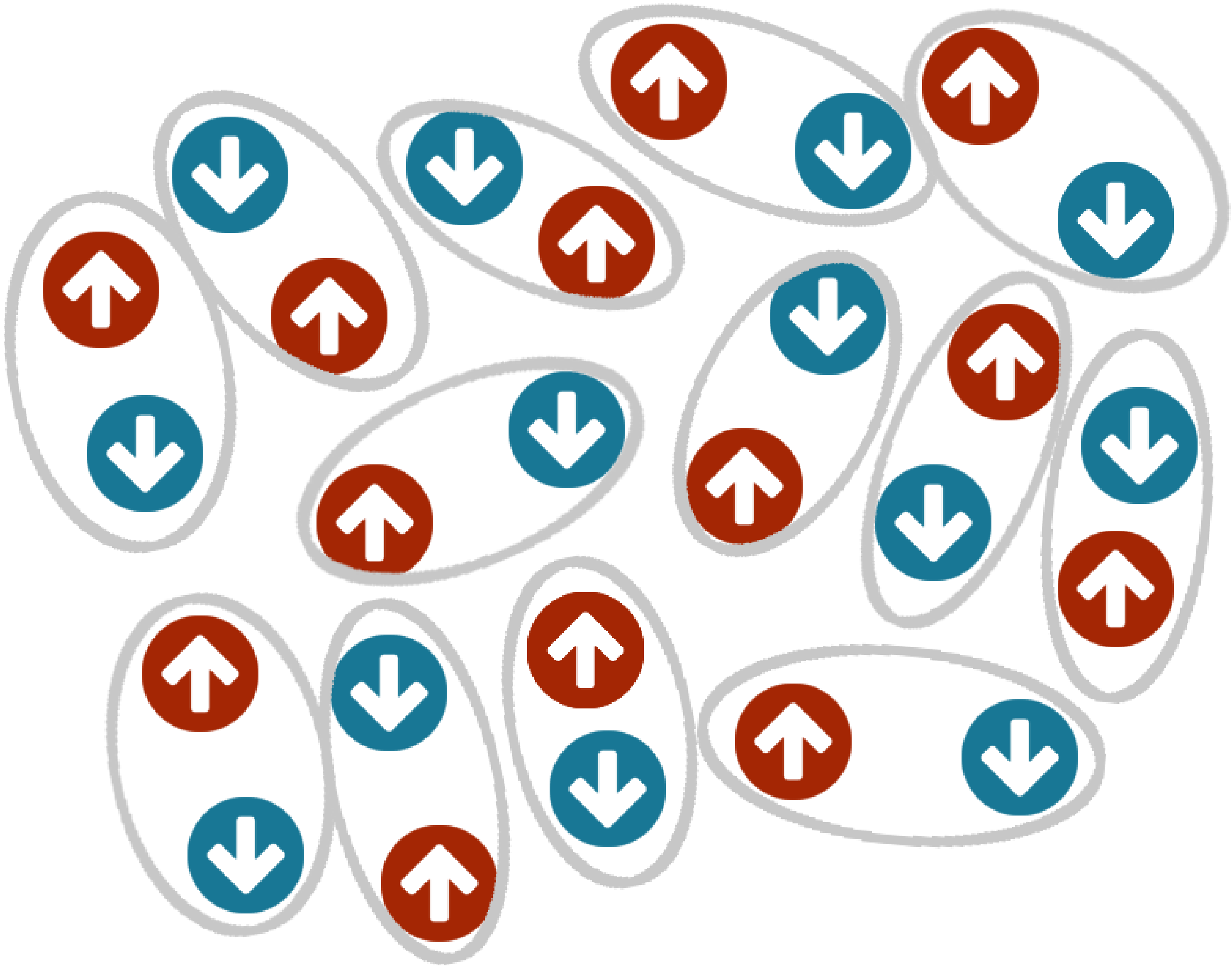
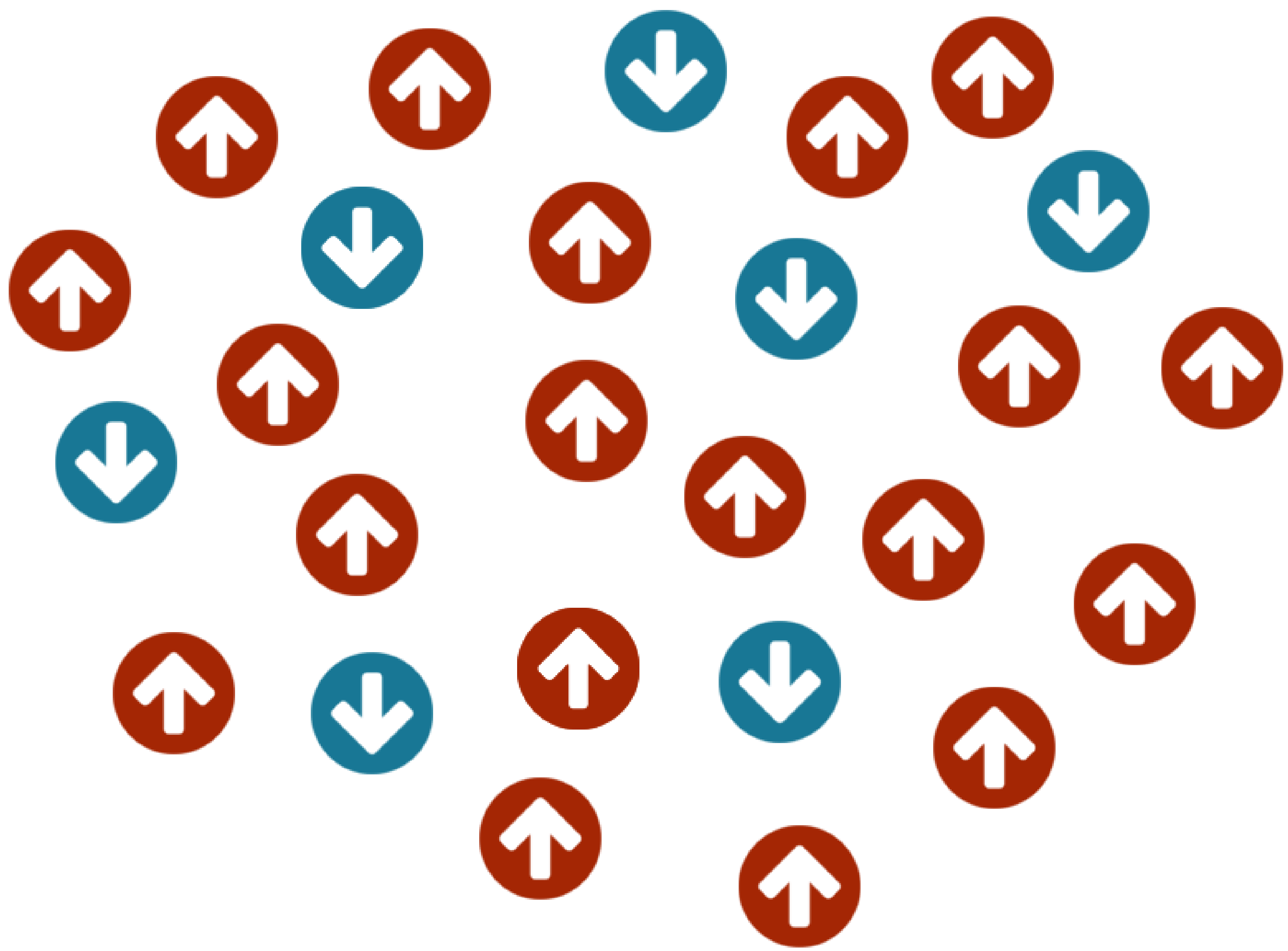
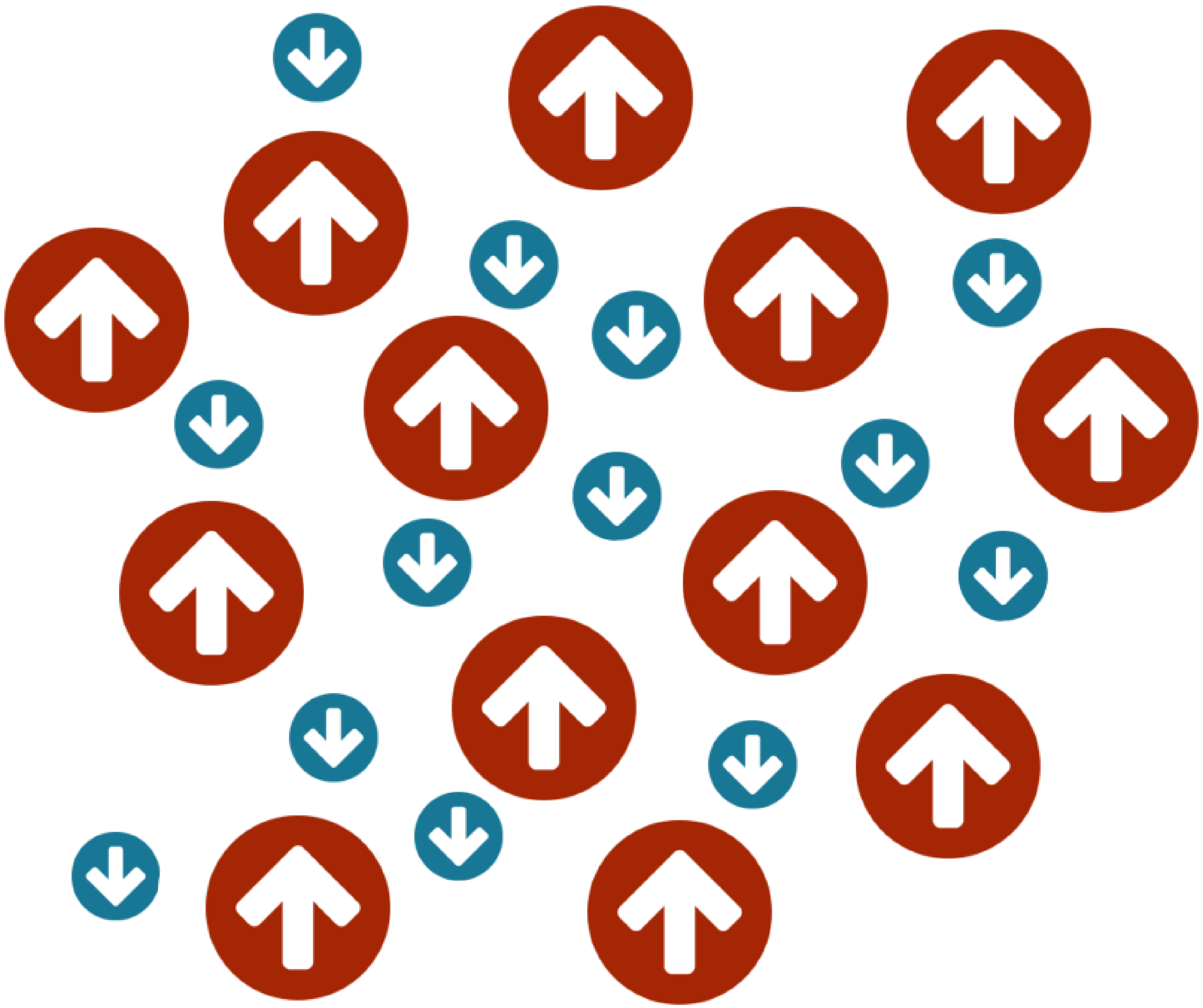


spin polarization



mass imbalance



KEY QUESTIONS

- what happens to the ground-state at finite polarization?
(are there inhomogeneous/supersolid phases?)

- how does the critical temperature for superfluidity change with polarization?

- what happens in systems with particles of different mass?

Model: contact interaction

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

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

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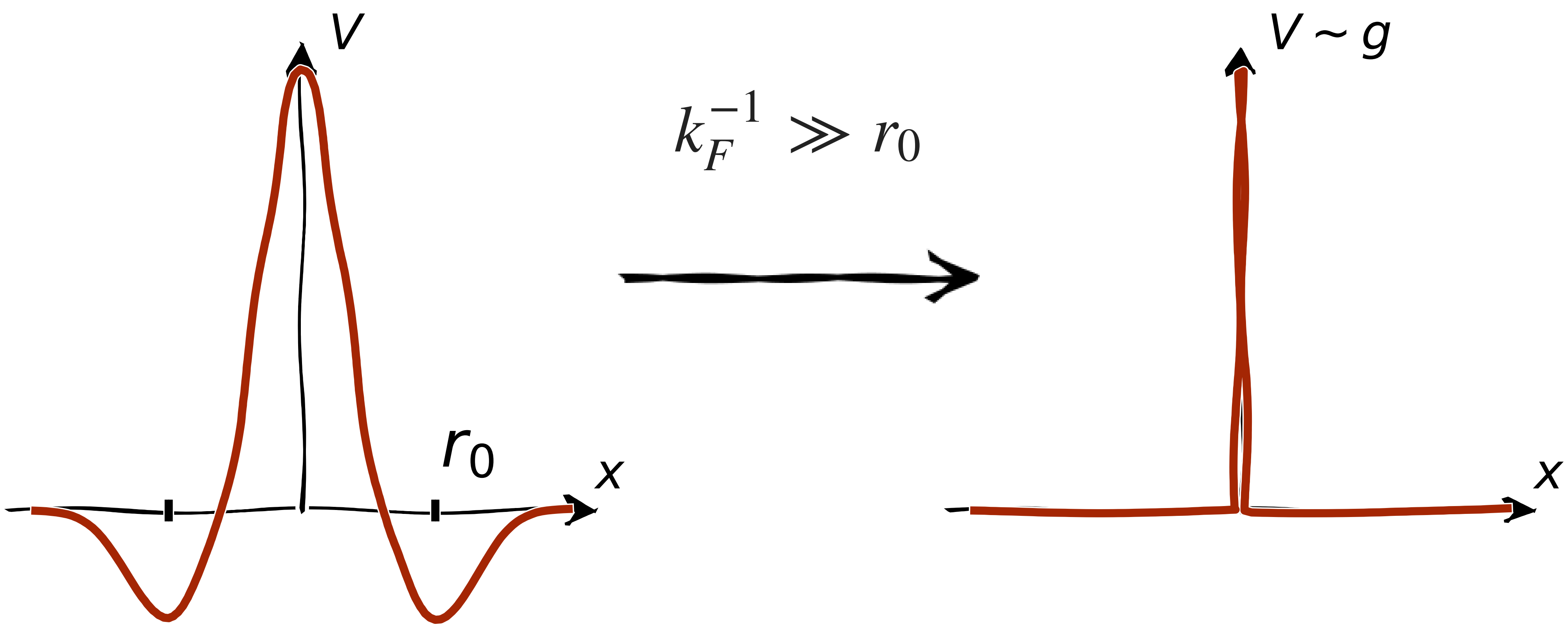

bcs theory
molecular dynamics
matrix product states
diagrammatic monte carlo
bethe ansatz
peps
hmc
machine learning
perturbation theory
gfqmc
density functional theory
quantum monte carlo
dmc
dmft
vmc
ihmc
functional renormalization group
lda
afqmc
tensor networks
fciqmc
mean field
dmrg
langevin dynamics
rpa
pigs
lattice gauge theories
exact diagonalization
coupled cluster

*not exhaustive

What do we need to compute?

(the only technical slide, promise!)

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

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

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Rewrite the problem as a path-integral:

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

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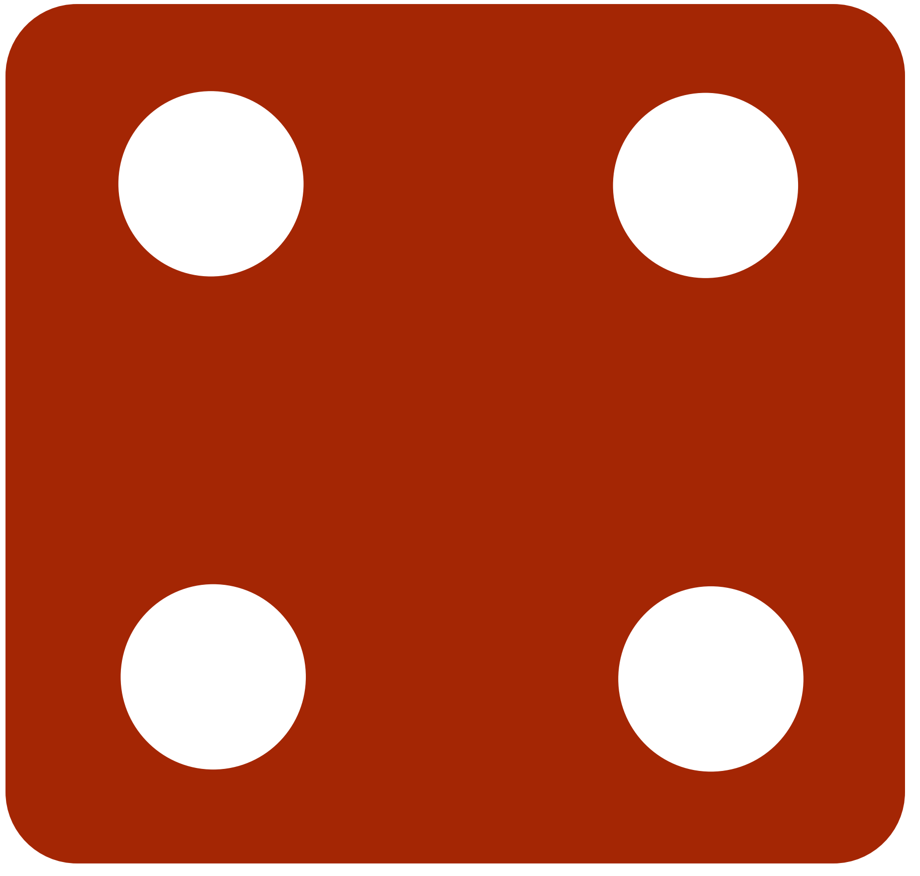
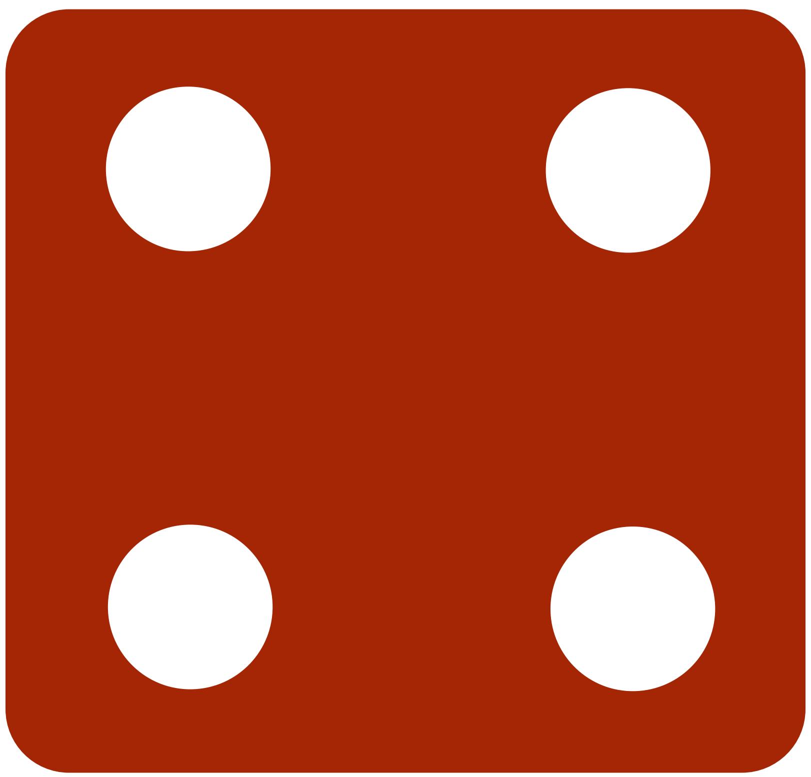
"all" that is left to do: evaluate high-dimensional integral

roll some dice



(create random auxiliary field configurations)

Quantum Monte Carlo (QMC)



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

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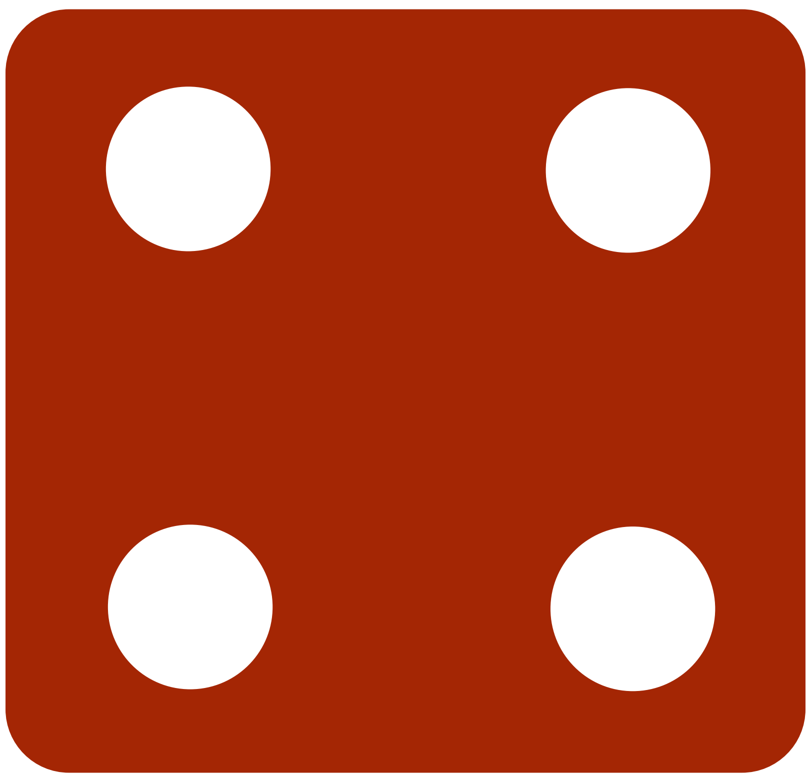

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i. produce a random sample of the auxiliary field ϕ

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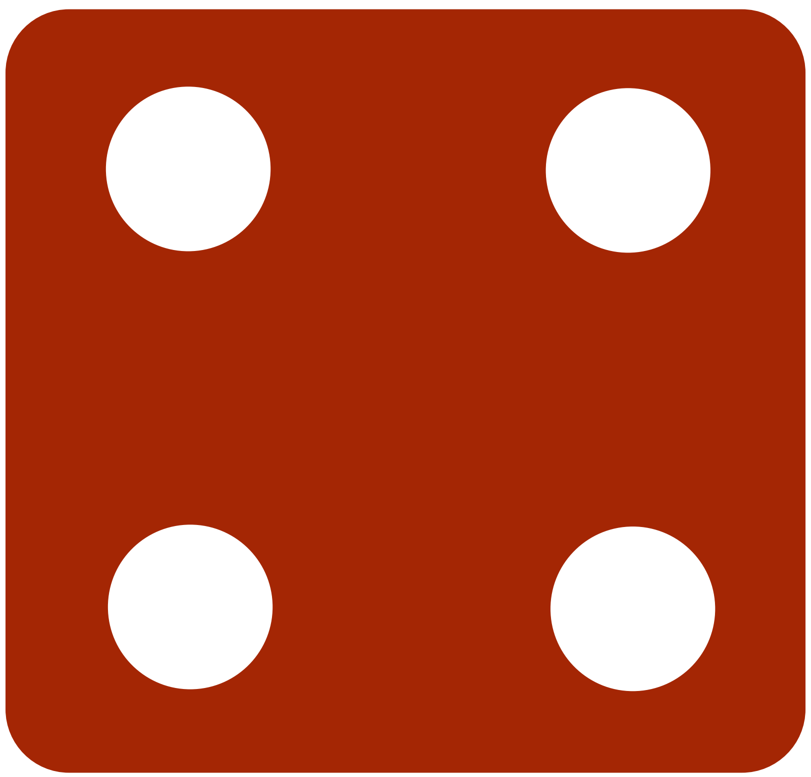

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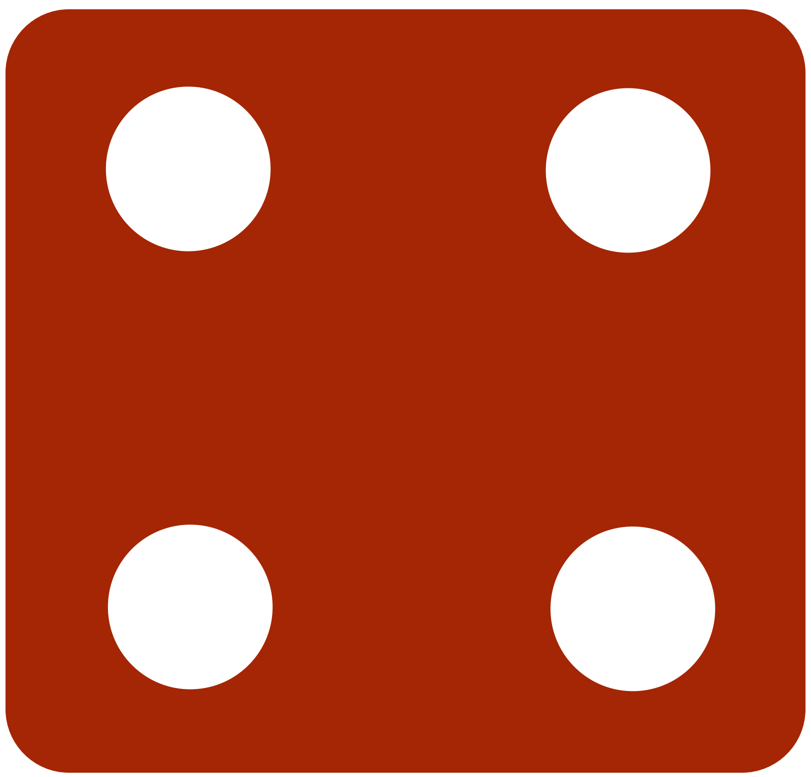

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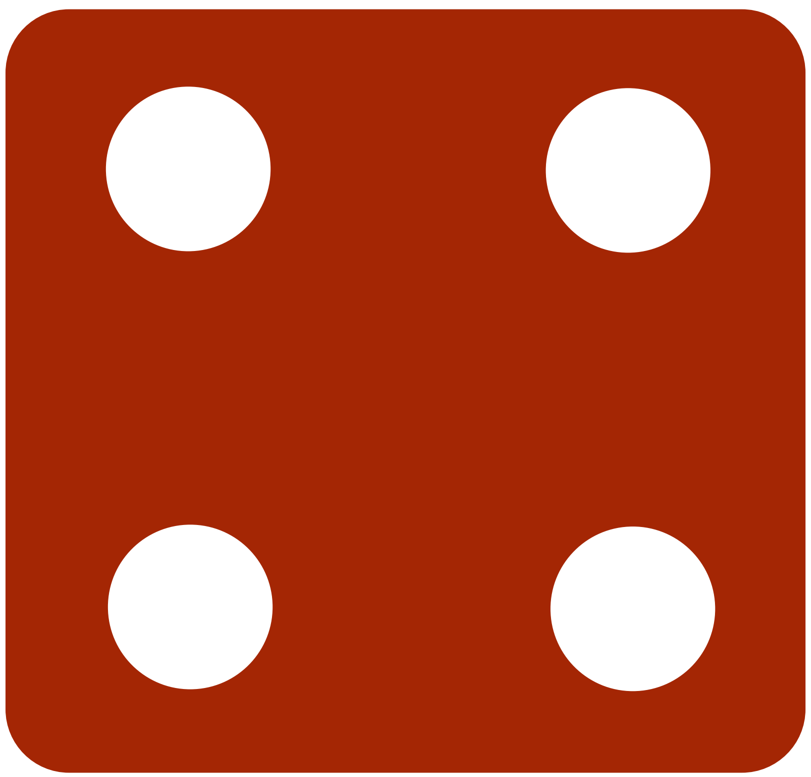

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ii. evaluate the integrand with that value

iii. save result & repeat

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

Statistical uncertainties

$$\sigma \propto \left(\sqrt{\text{\# of (uncorrelated) samples}}\right)^{-1}$$

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EXAMPLE: COIN FLIPS

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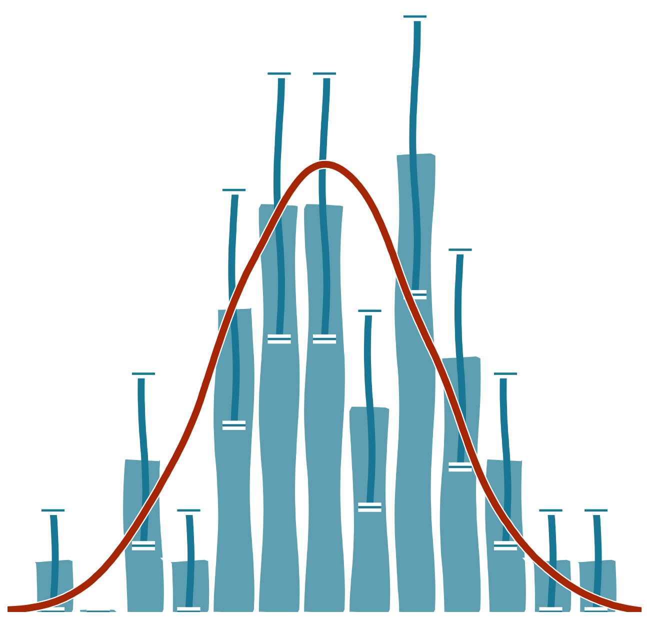

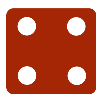 × 50

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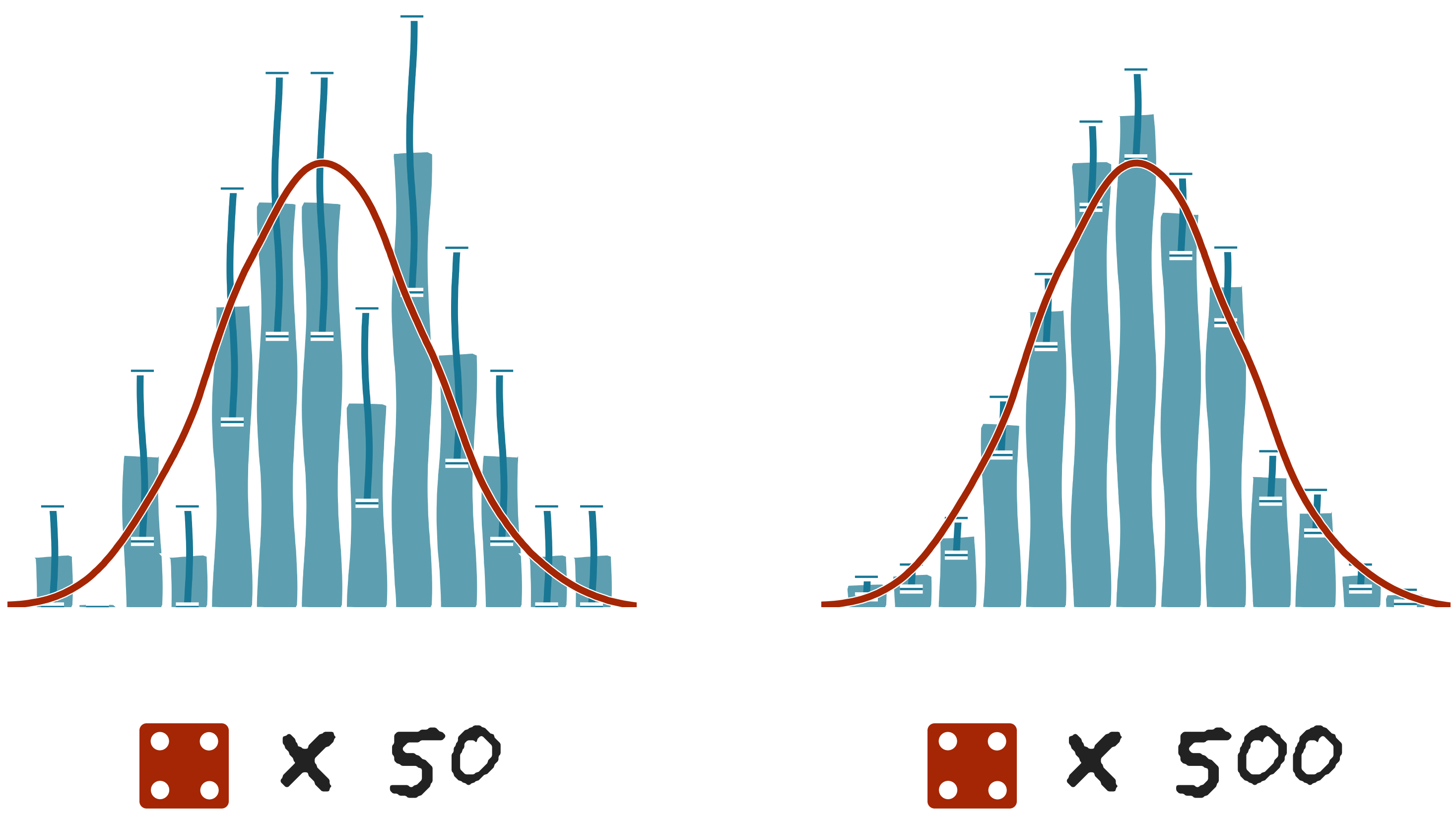

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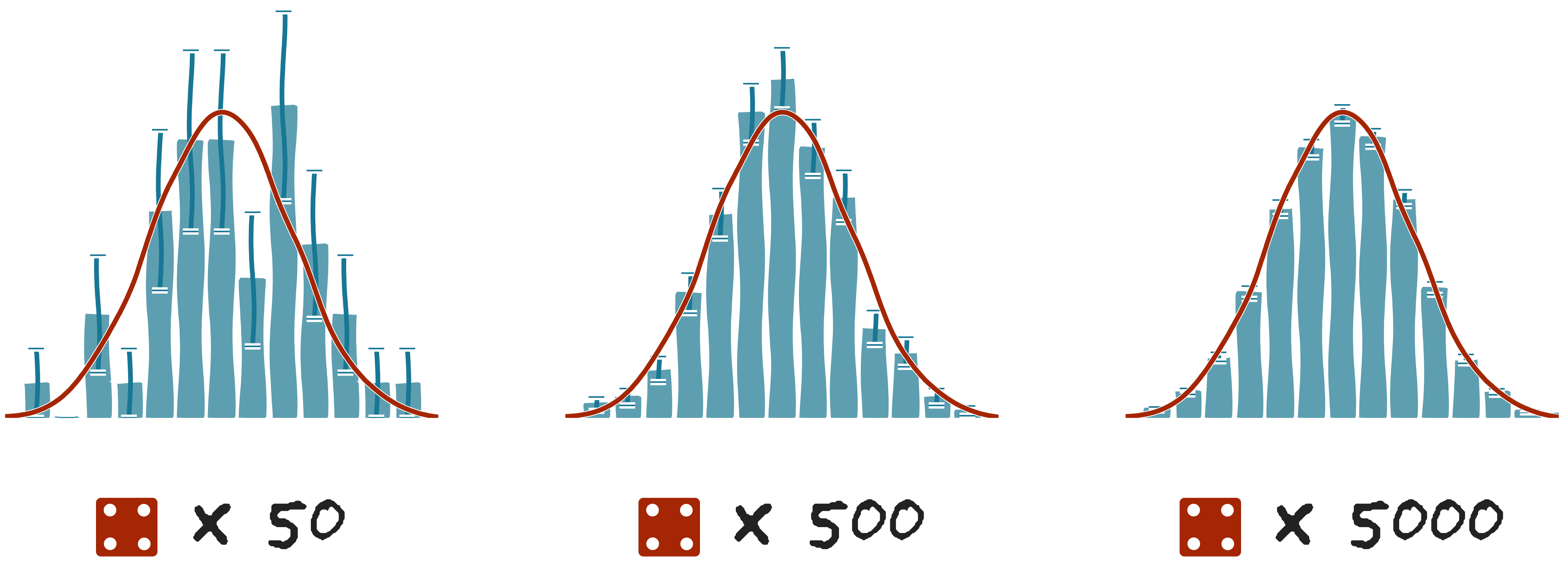

THE SIGN PROBLEM

(computational effort increases exponentially with system size)

[Troyer, Wiese '05]

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

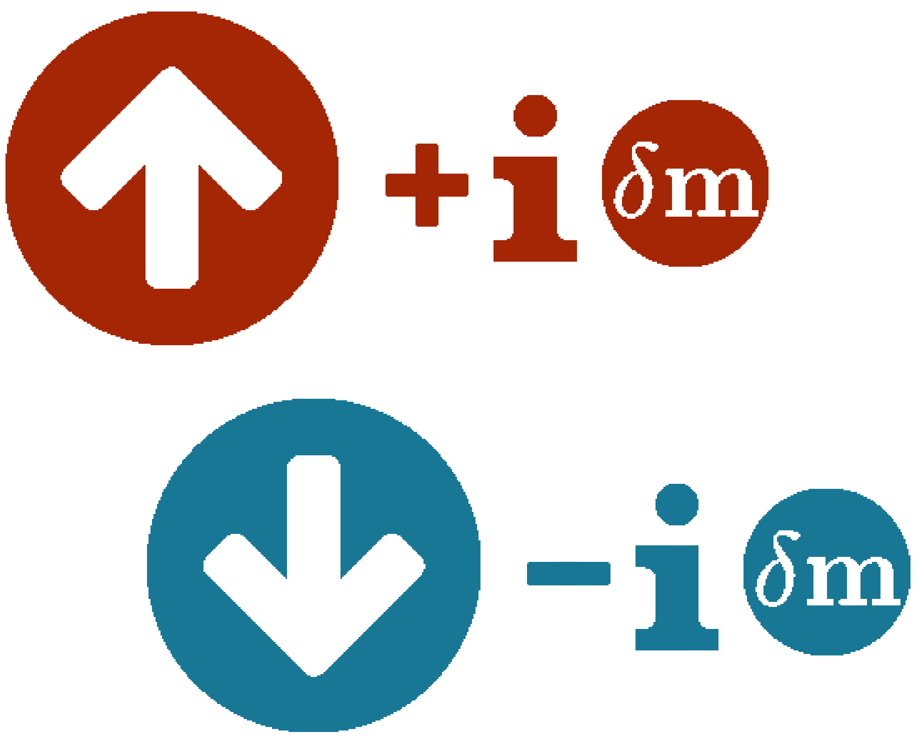
probability measure **not positive (semi-)definite** if:

$N_\uparrow \neq N_\downarrow$

$m_\uparrow \neq m_\downarrow$

$g > 0$

Option I: imaginary mass-imbalance (iHMC)



mases have an imaginary part and are **complex conjugate** to each other

[de Forcrand, Philipsen '02]
[Braun+ '13]
[Roscher, Braun, Chen, Drut '13]
[Braun, Drut, Roscher '15]
[Loheac, Braun, Drut, Roscher '15]

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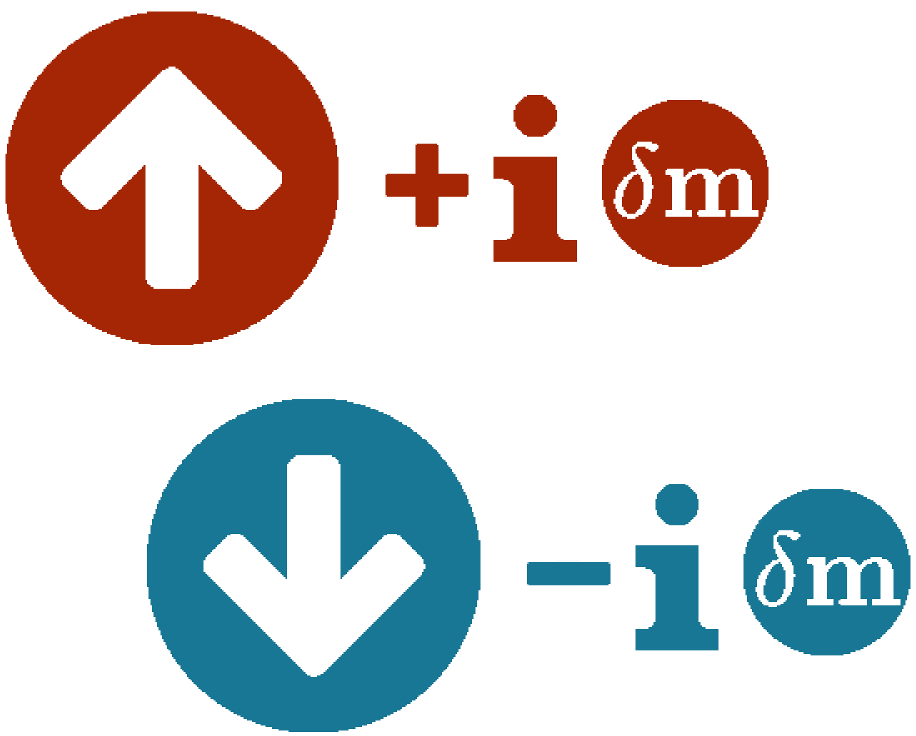

mases have an imaginary part and are **complex conjugate** to each other

probability measure non-negative:

$$\det M_\phi^\uparrow \, \det M_\phi^\downarrow \quad \to \quad |\det M_\phi|^2$$

analytic continuation: $i\bar{m} \;\to\; \bar{m}$
to obtain results for real imbalances

same idea works for
spin-imbalanced systems at finite T
(complex chemical potentials)

[de Forcrand, Philipsen '02]
[Braun+ '13]
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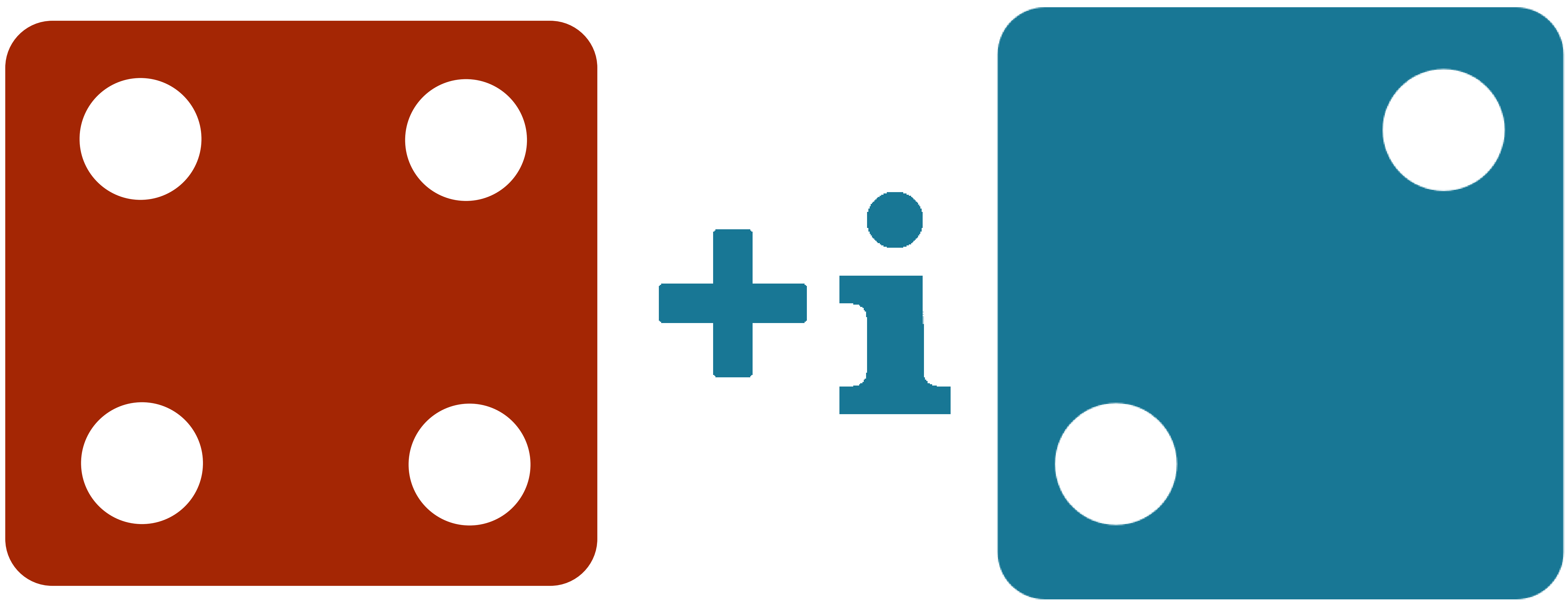
Option II: roll dice with imaginary sides (CL)



(complexified auxiliary fields)

COMPLEX LANGEVIN: OVERVIEW

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):

$$\frac{\partial \phi}{\partial t} = -\frac{\partial S[\phi]}{\partial \phi} + \eta(t)$$

[Parisi, Wu '81]
[Aarts '09; Seiler '17]
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problem: $S[\phi]$ must be bounded from below!

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

[Parisi, Wu '81]
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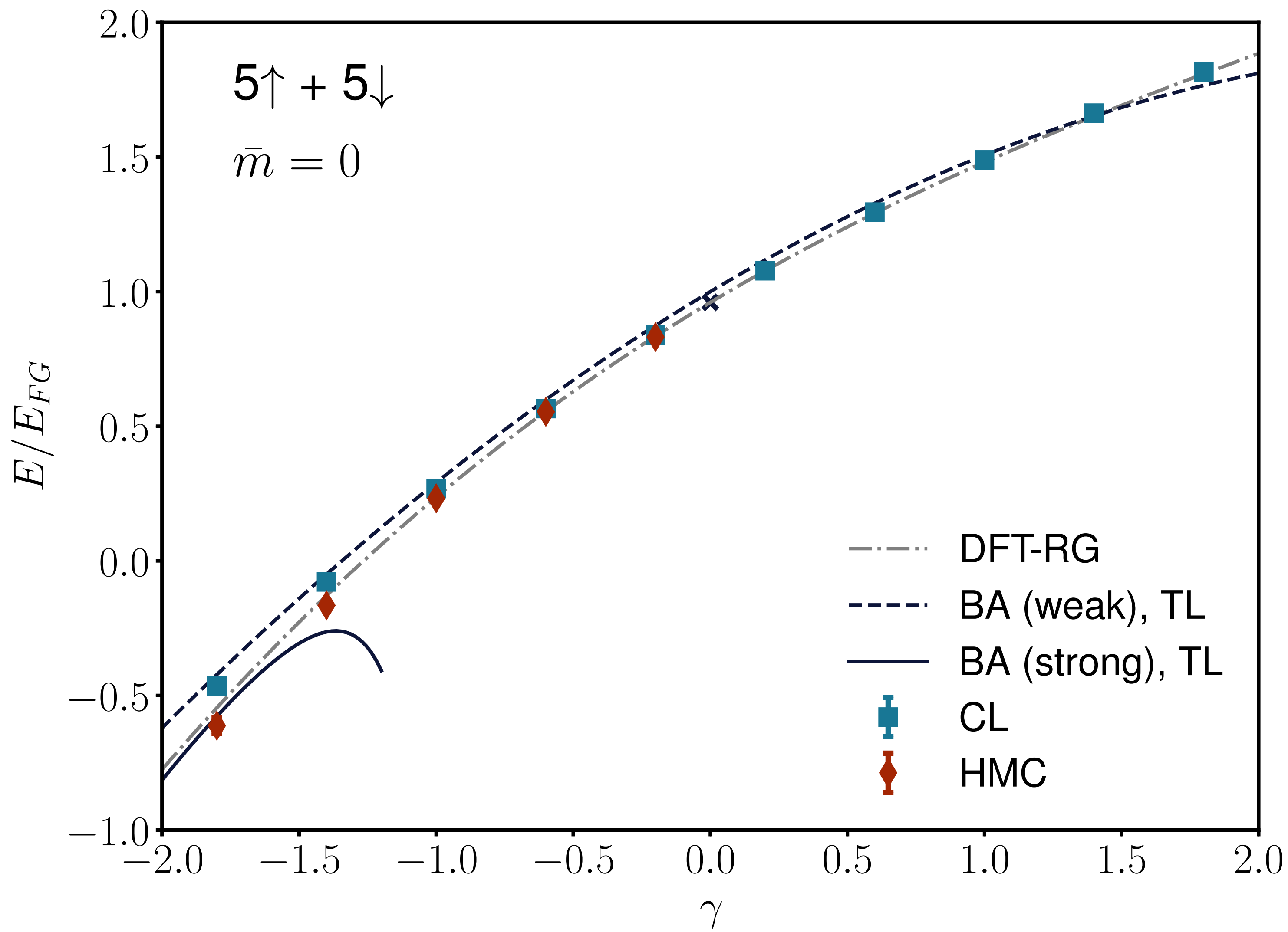
First step: compare to other methods

[LR, Porter, Drut, Braun '17]



$\gamma = g/n$

[BA: Iida, Wadati '07; Tracy, Widom '16]
[DFT-RG: Kemler, Pospiech, Braun '16]
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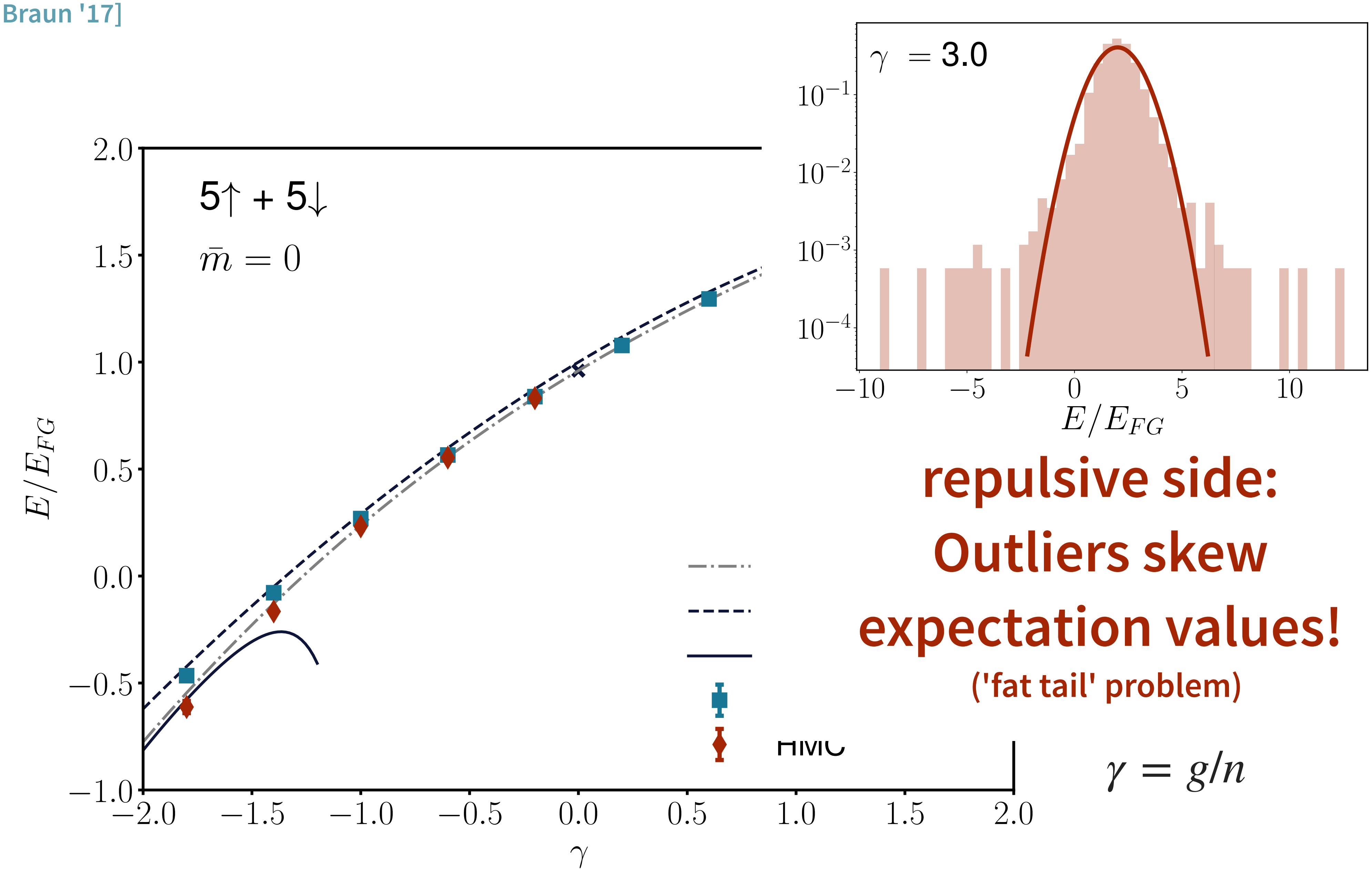

repulsive side:
Outliers skew expectation values!
('fat tail' problem)

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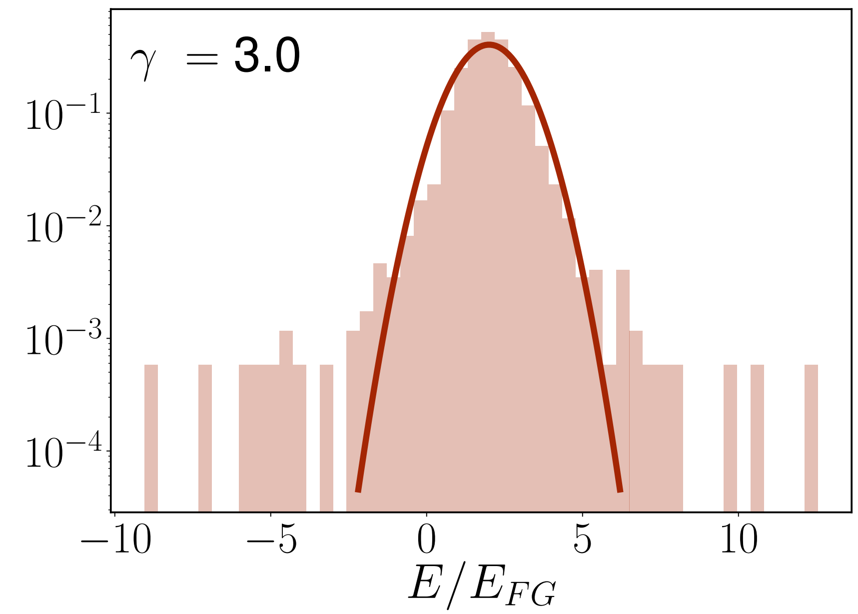
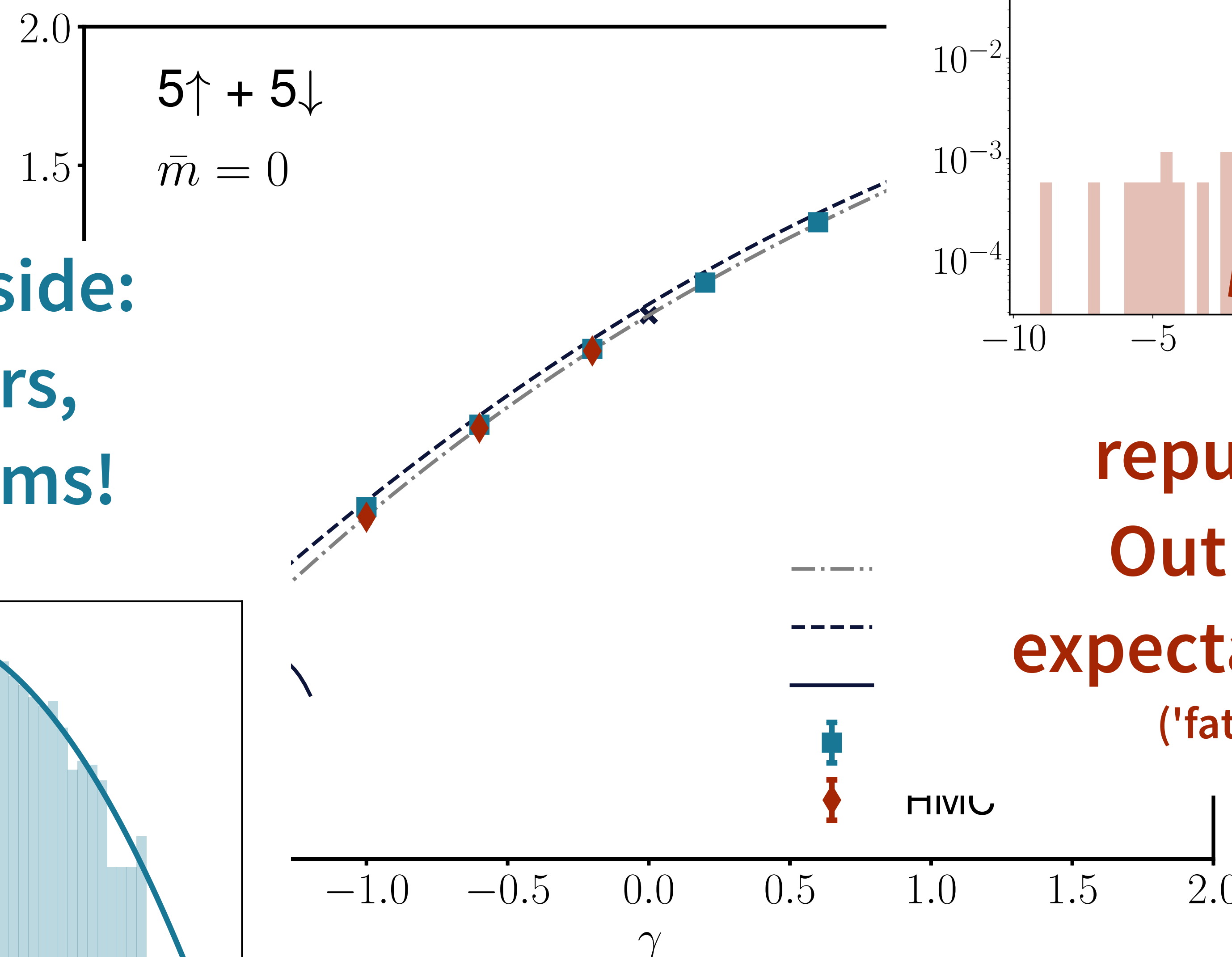


attractive side:
no outliers,
no problems!



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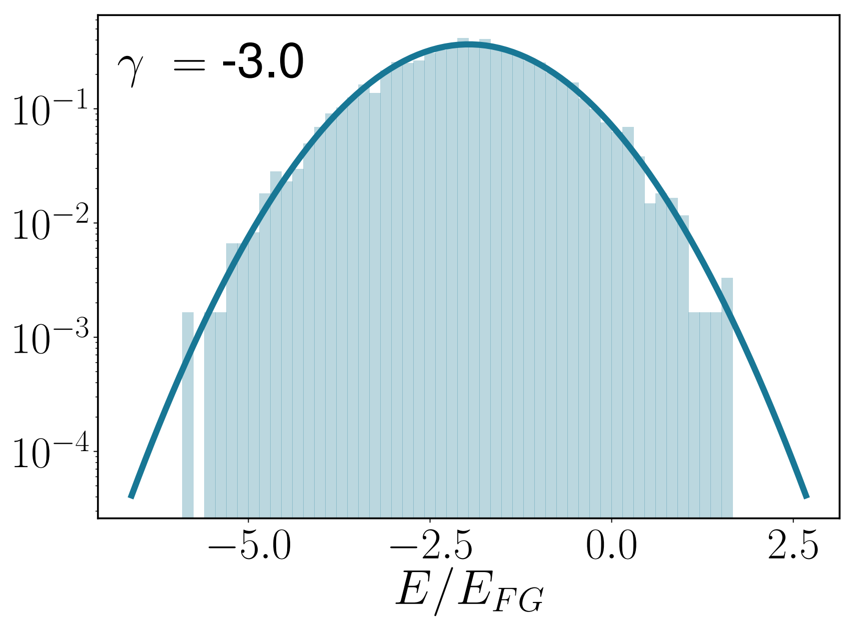

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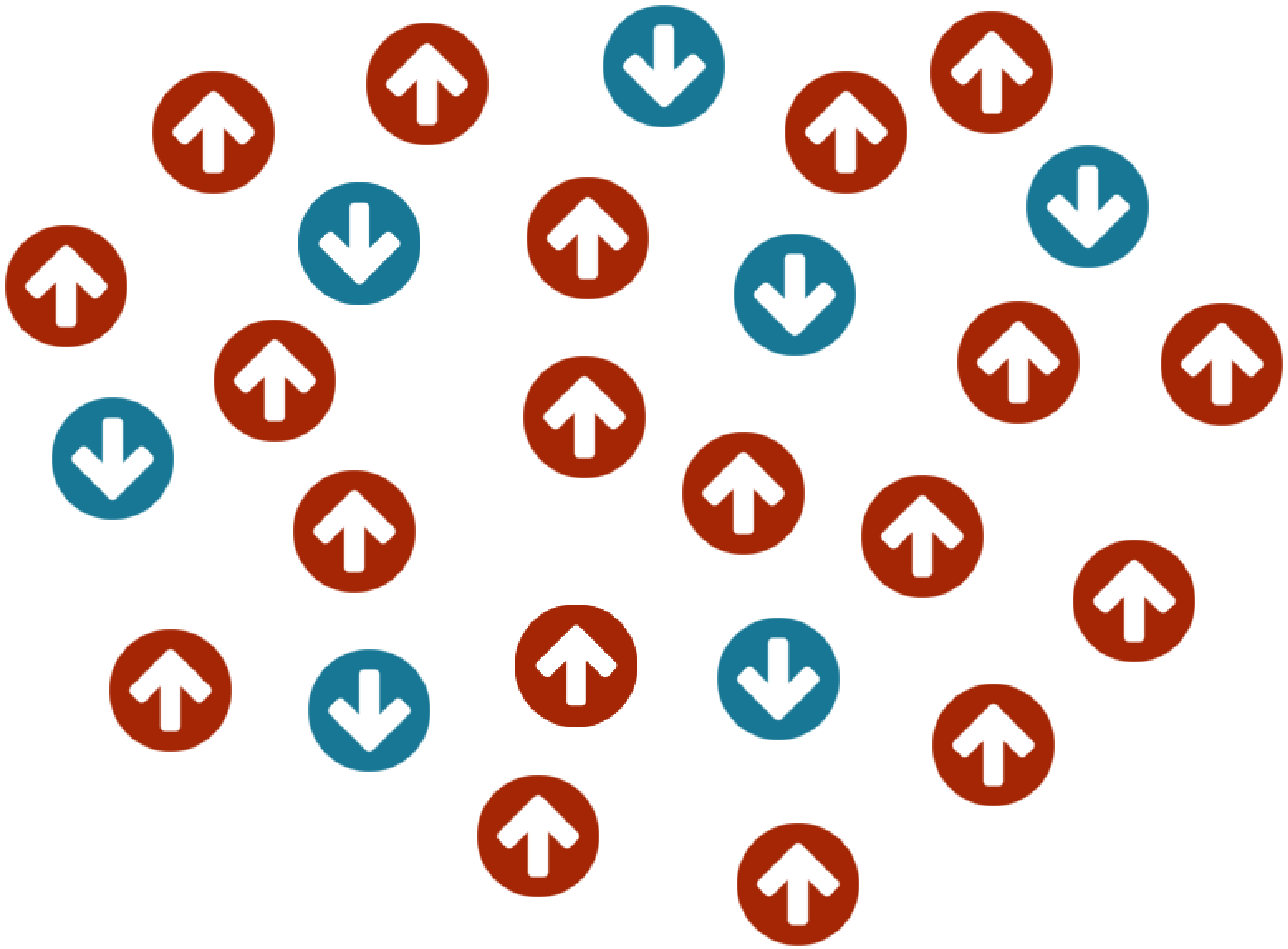
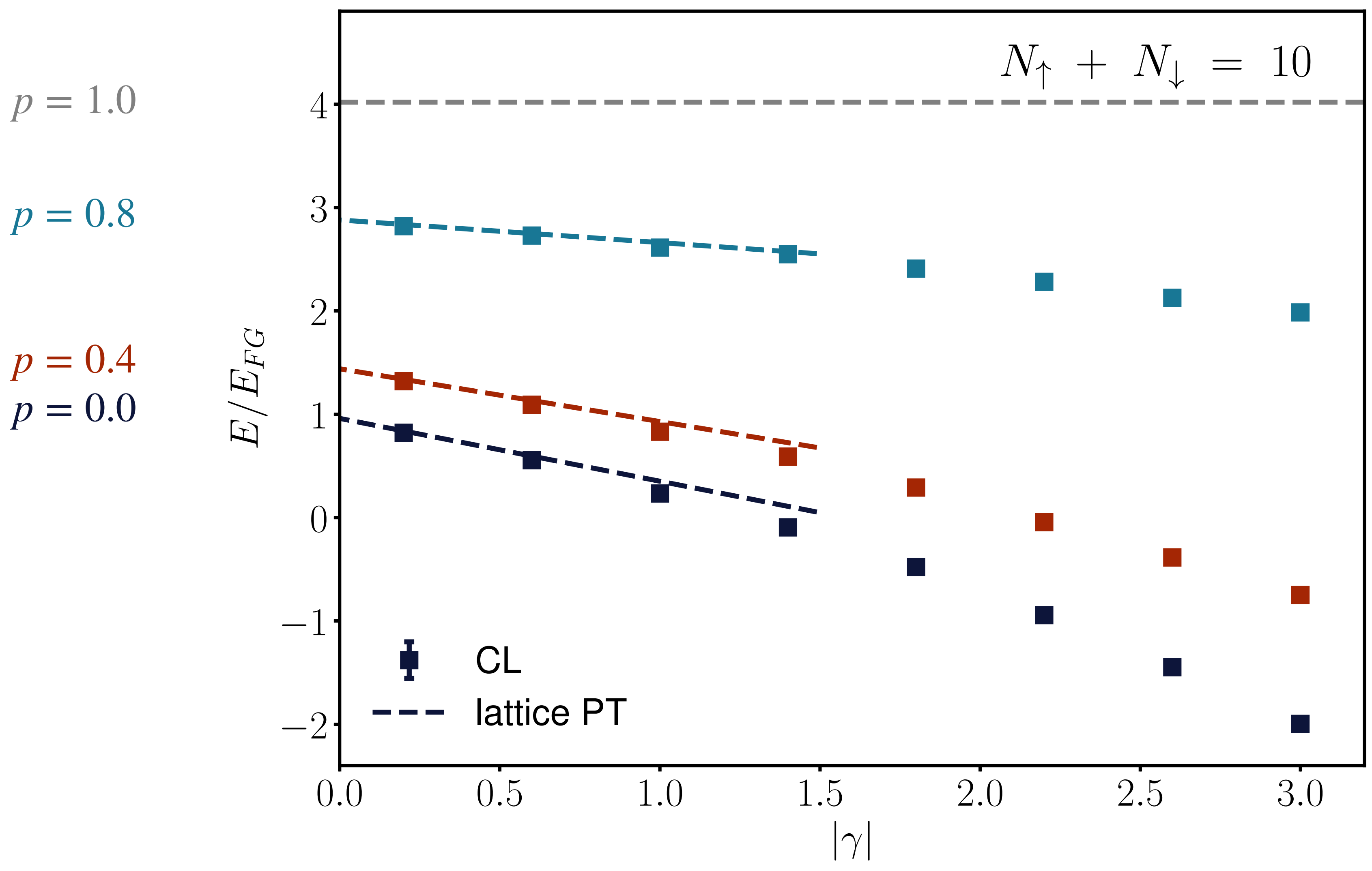
spin polarization



polarized 1D fermions: equation of state

[LR, Drut, Braun *in preparation*]



$\gamma = g/n$

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

polarized 1D fermions: pair correlation

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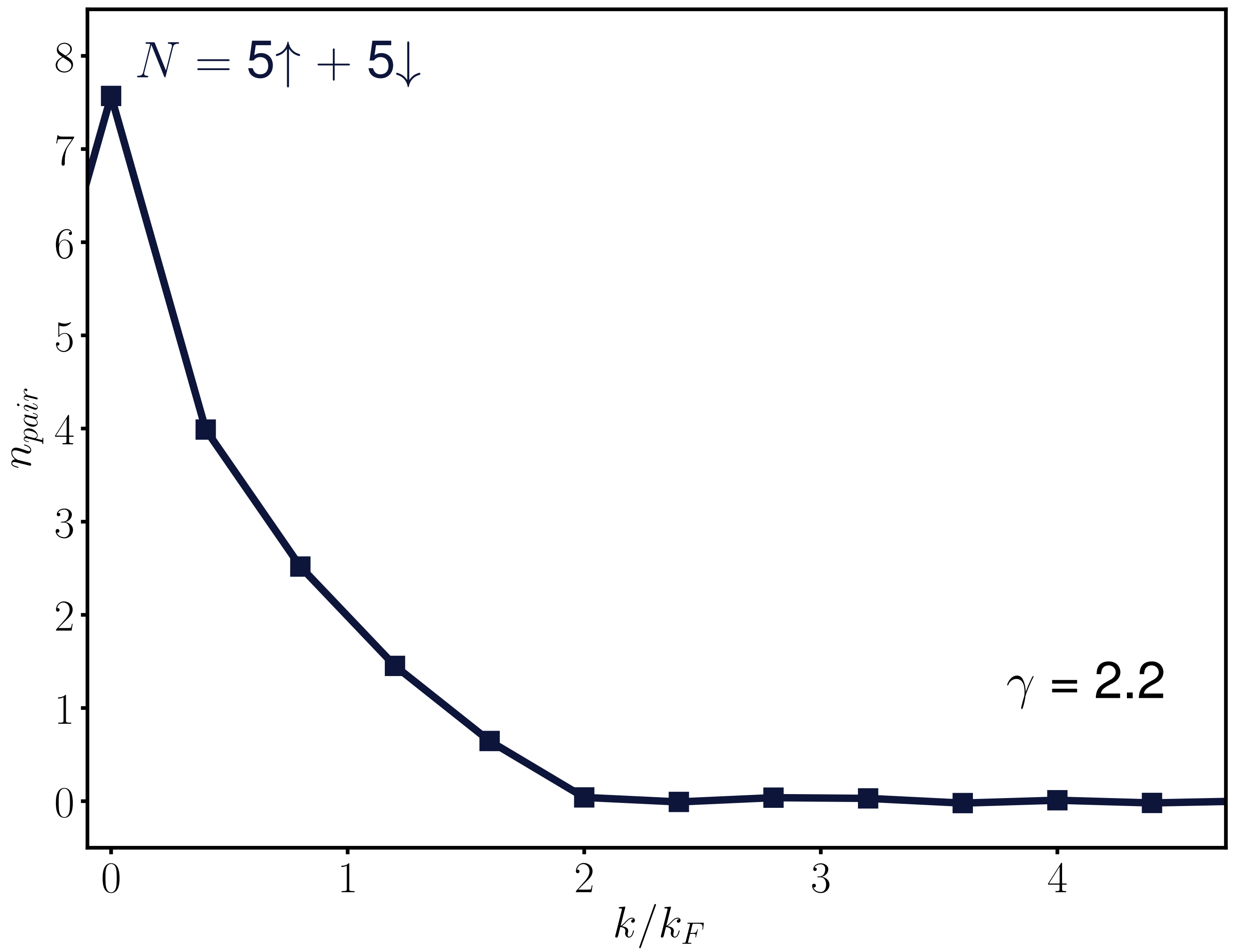

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$$n_{pair}(x, x') = \langle \hat{\psi}^\dagger_\uparrow(x)\, \hat{\psi}^\dagger_\downarrow(x)\, \hat{\psi}_\downarrow(x')\, \hat{\psi}_\uparrow(x') \rangle$$

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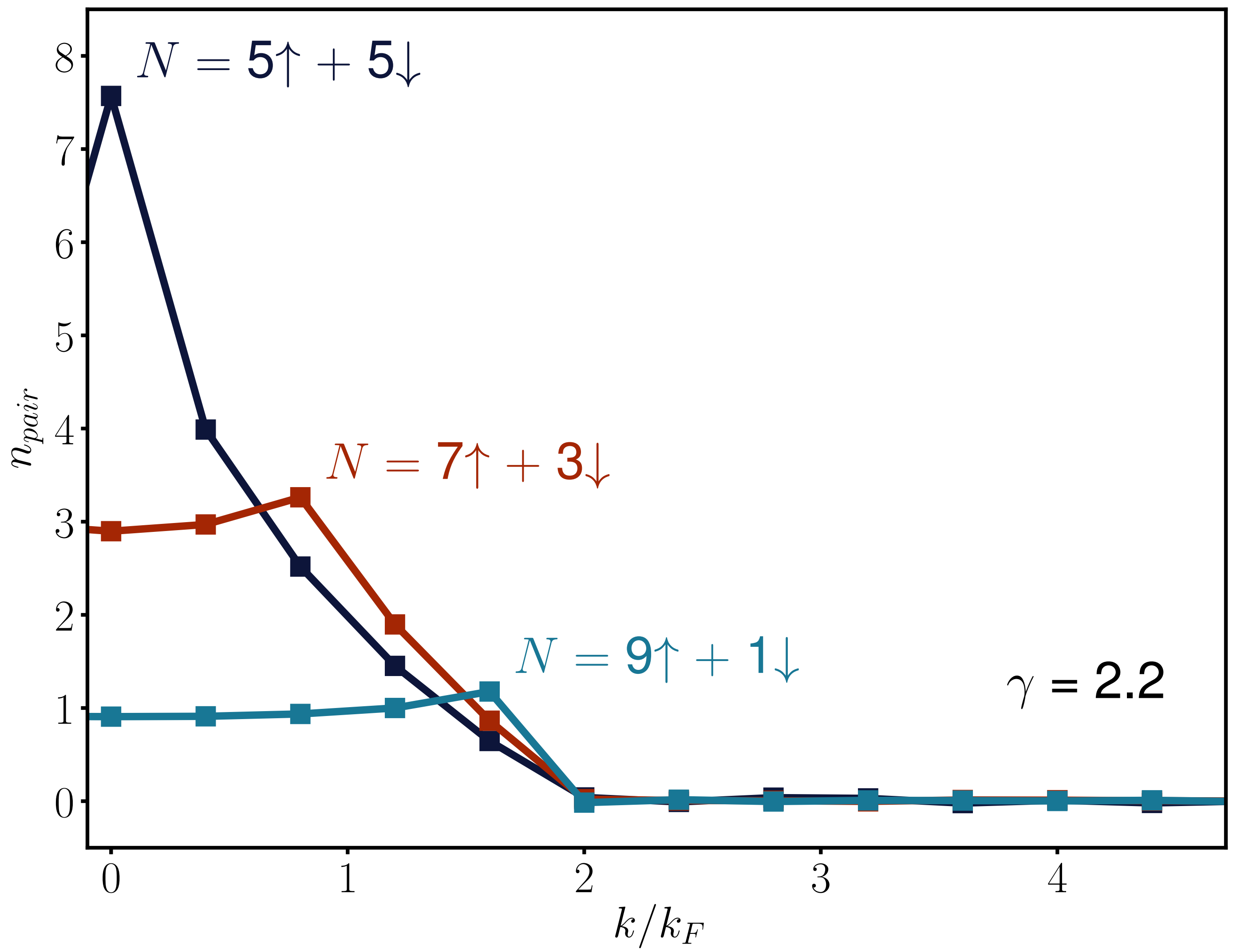

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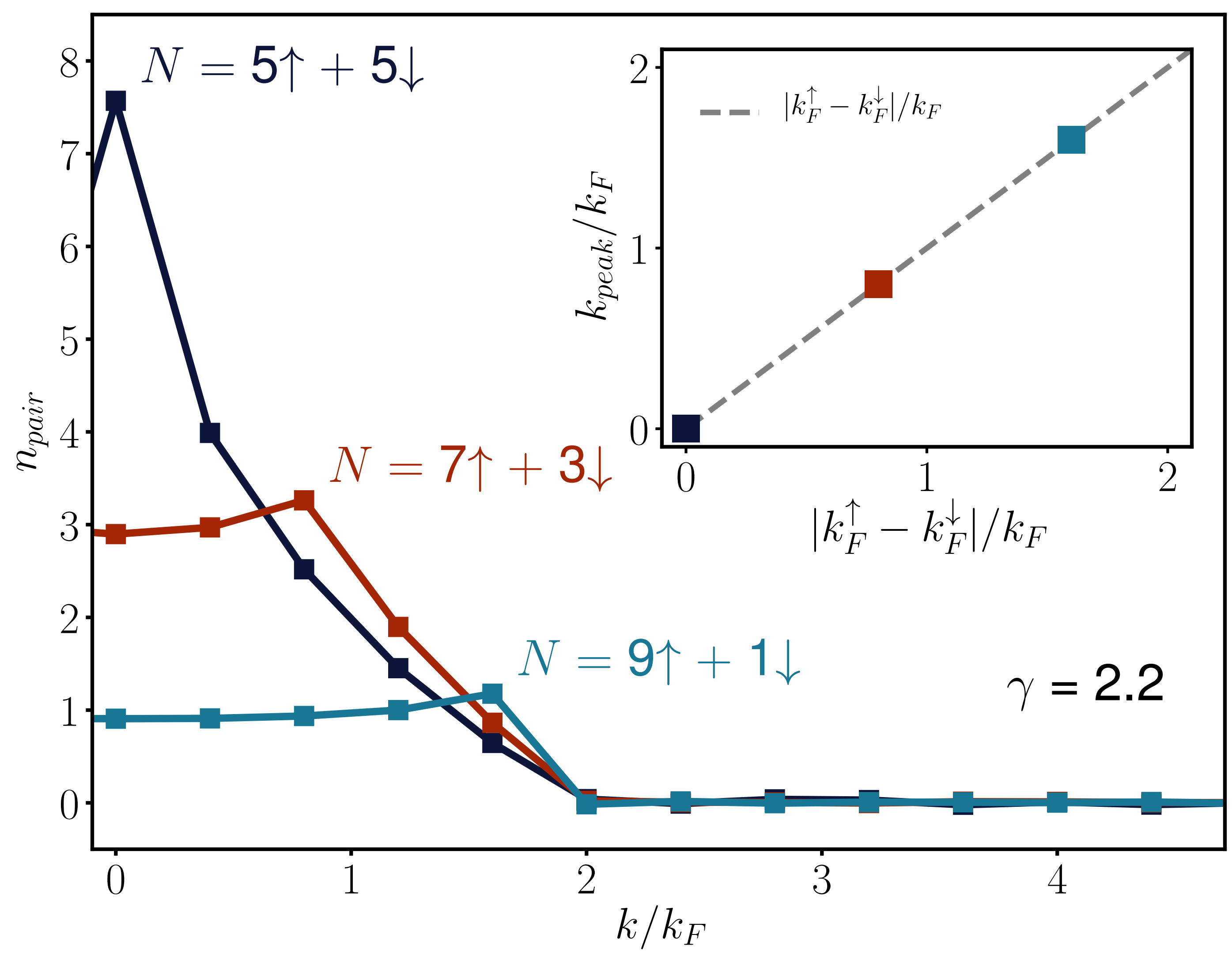

signature of FFLO type pairing

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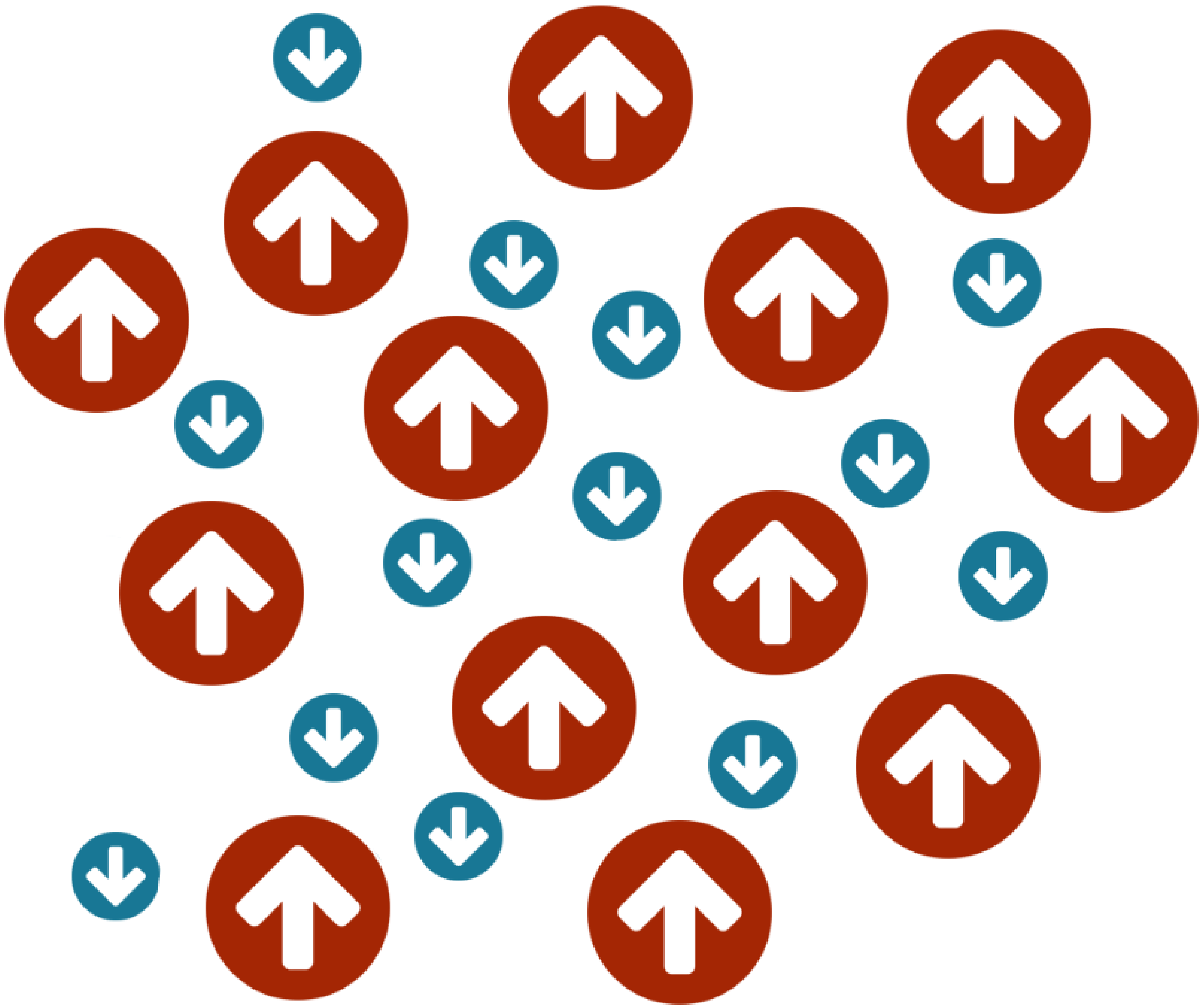
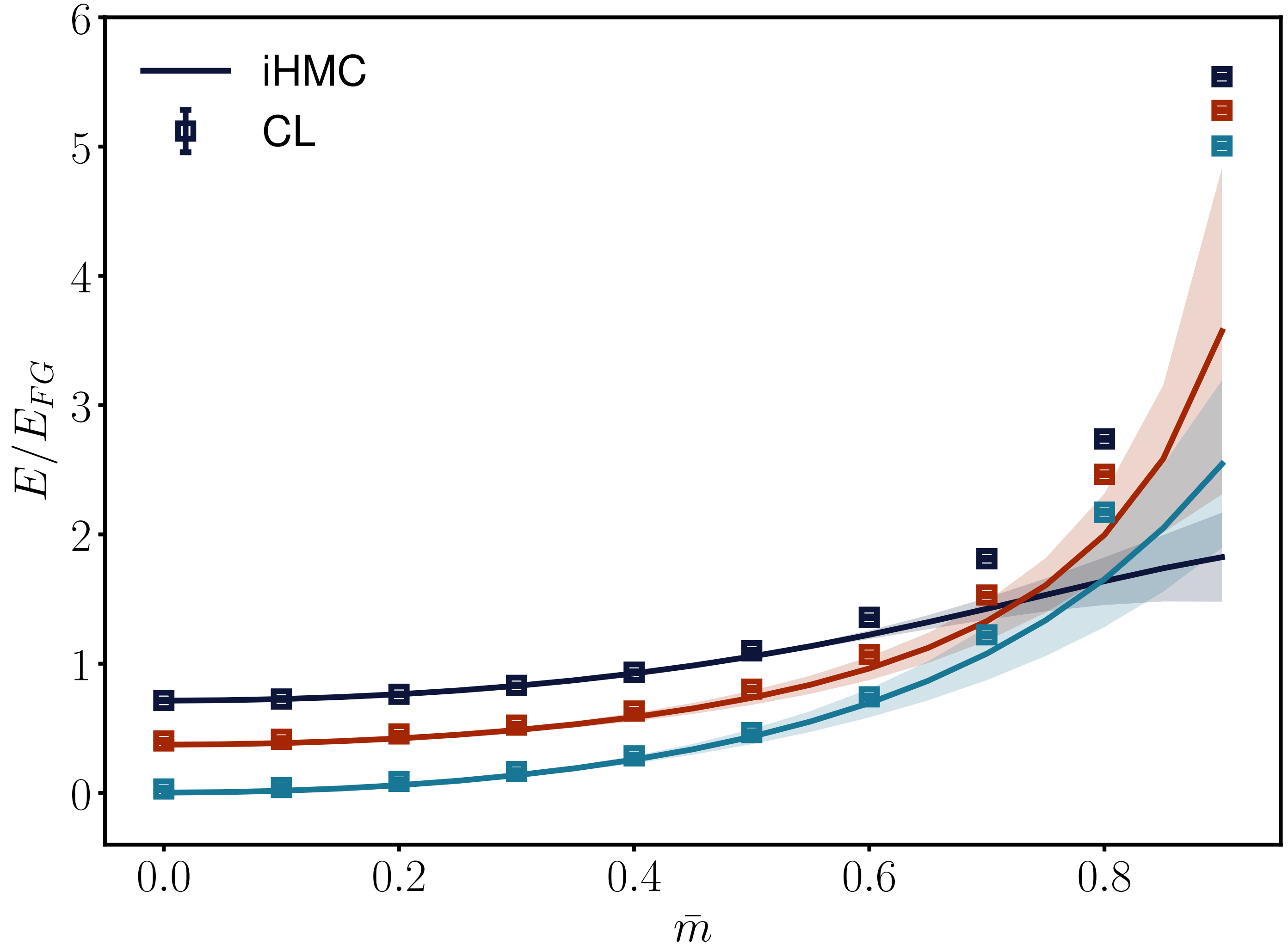
mass imbalance



mass-imbalanced 1D fermions: CL & iHMC

[LR, Porter, Drut, Braun '17]



$\gamma = 0.6$
$\gamma = 1.0$
$\gamma = 1.4$

$\gamma = g/n$

$\bar{m} = \frac{m_\uparrow - m_\downarrow}{m_\uparrow + m_\downarrow}$

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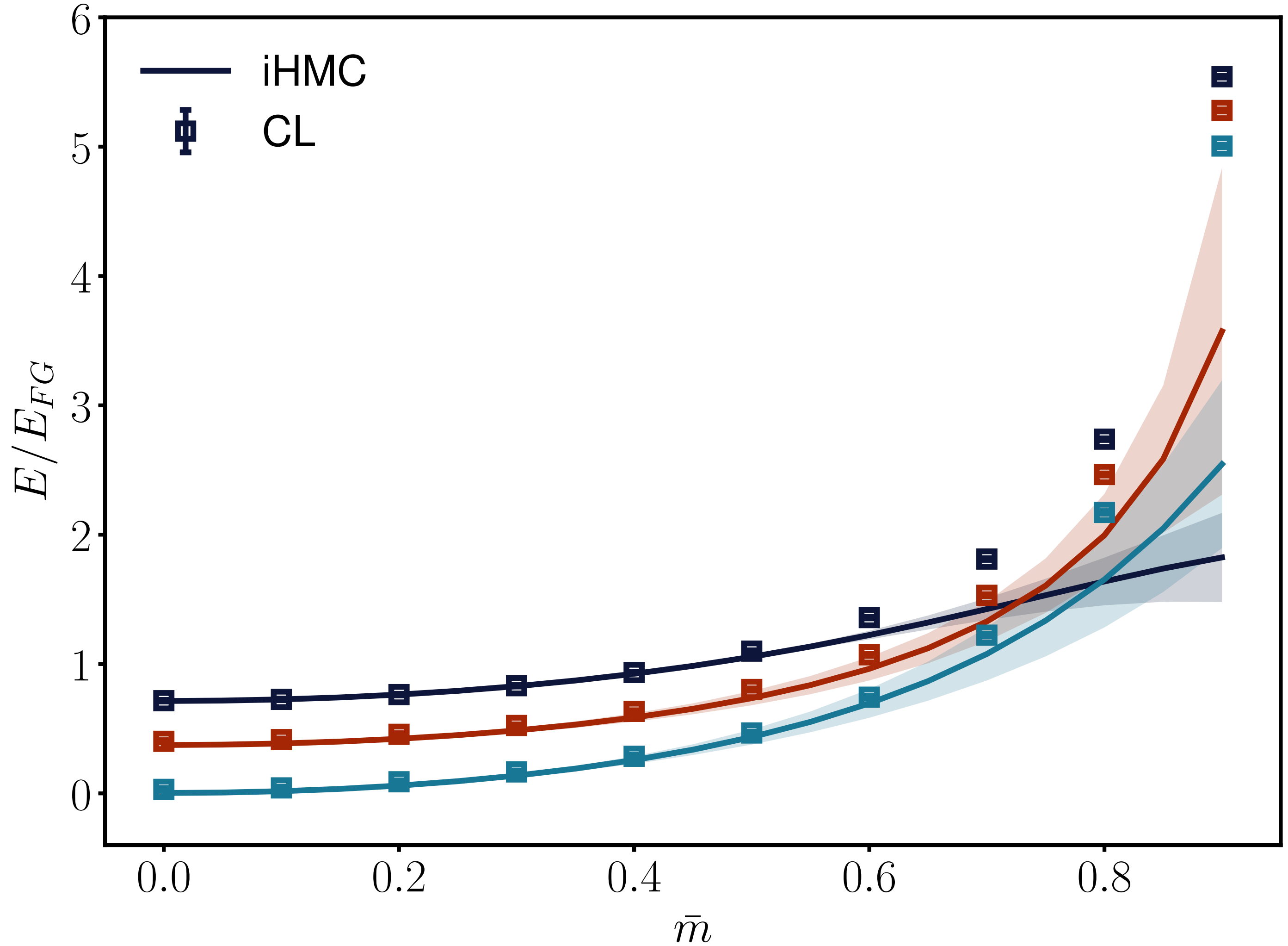
[LR, Porter, Drut, Braun '17]

excellent agreement for $\bar{m} \lesssim 0.6$



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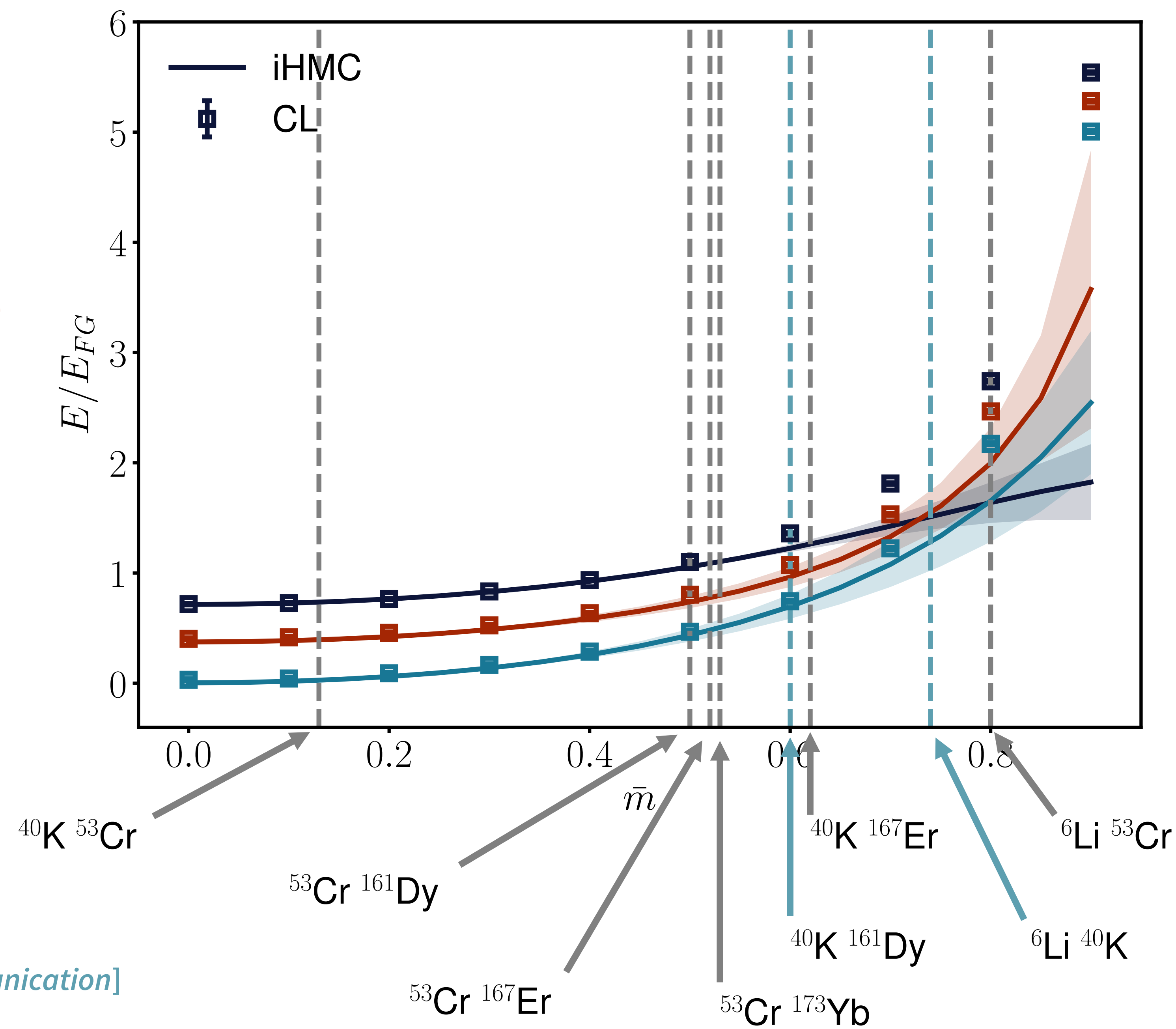

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experimental mixtures accessible!

$\gamma = g/n$

$\bar{m} = \frac{m_\uparrow - m_\downarrow}{m_\uparrow + m_\downarrow}$

[Grimm, *private communication*]

COMPLEX LANGEVIN IN 1D

very good agreement of CL & other methods (BA, DFT-RG, HMC, PT)

EOS of spin-imbalanced systems in agreement with perturbation theory

FFLO-type pairing at all polarizations in 1D (no breakdown)

mass-imbalance: EOS up to very high mass-imbalances
(no analytic solutions available!)

3D CALCULATIONS

same methods but computationally challenging!

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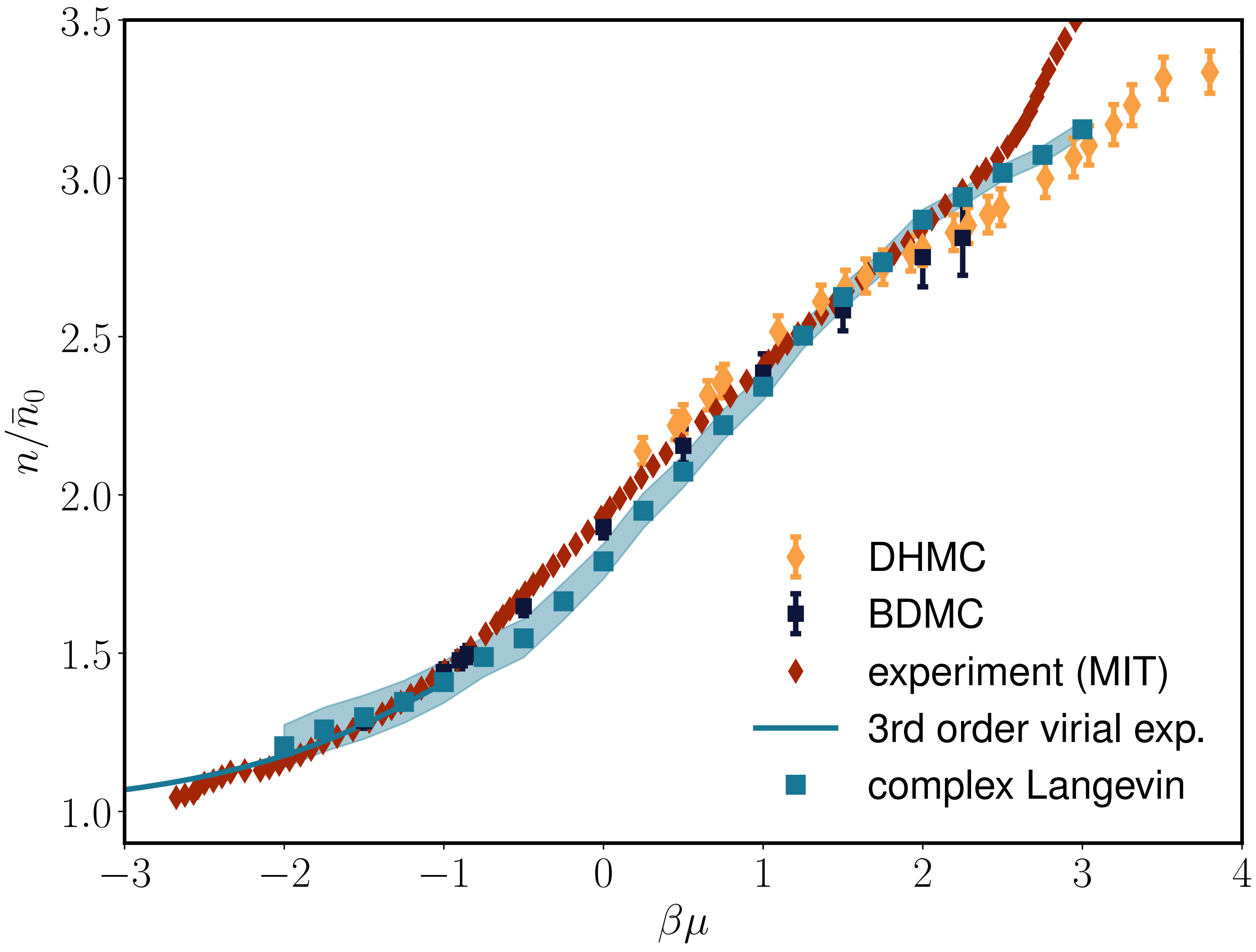
particularly interesting:

UNITARY FERMI GAS (UFG)

UFG at finite T: equation of state

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

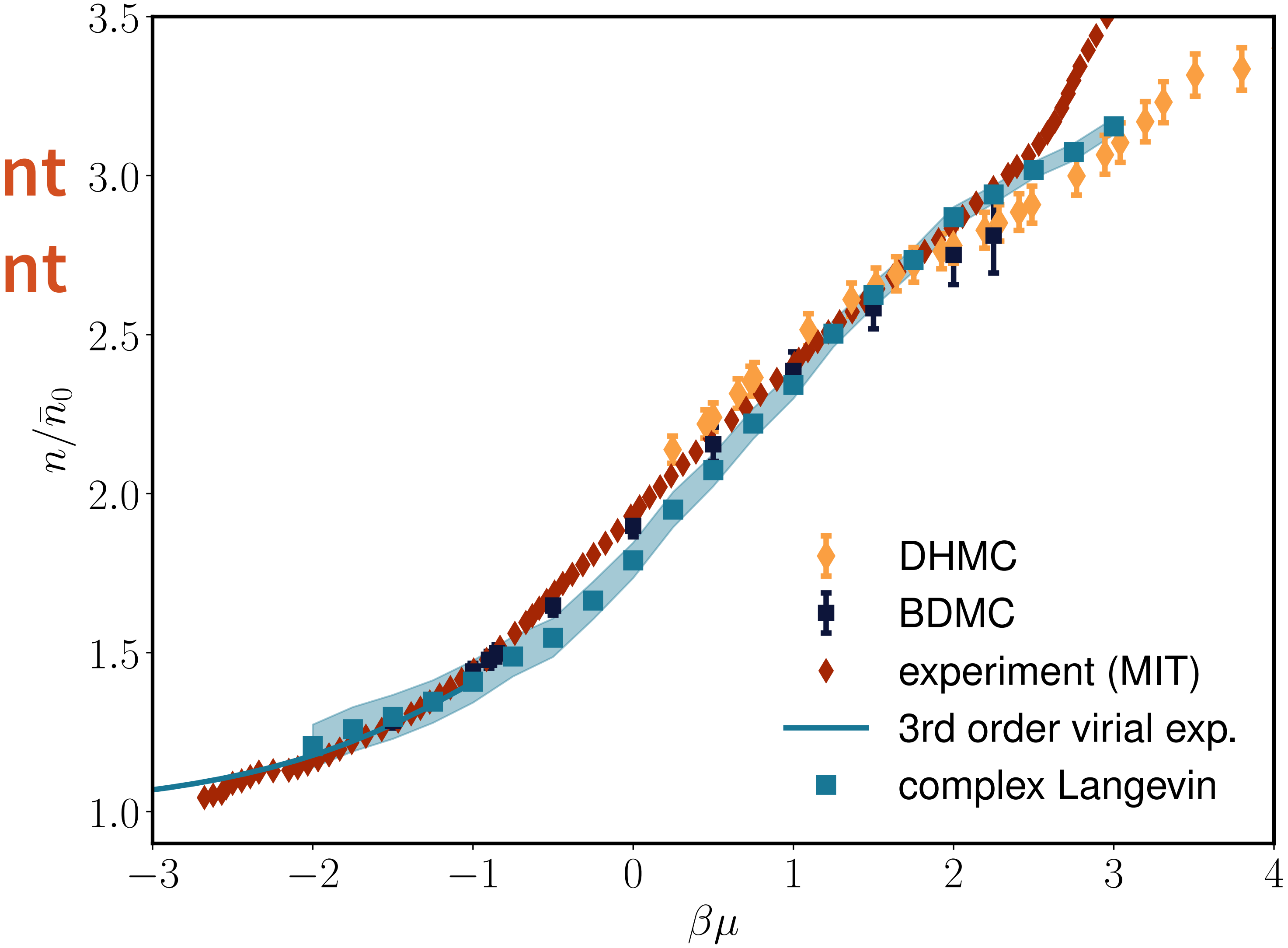


[experiment/BDMC: van Houcke+ '12]
[DHMC: Drut, Lähde, Wlazlowski, Magierski '12]

UFG at finite T: equation of state

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

good agreement with experiment and other methods!



CL results: finite lattice!

$(V = 9^3)$

[experiment/BDMC: van Houcke+ '12]
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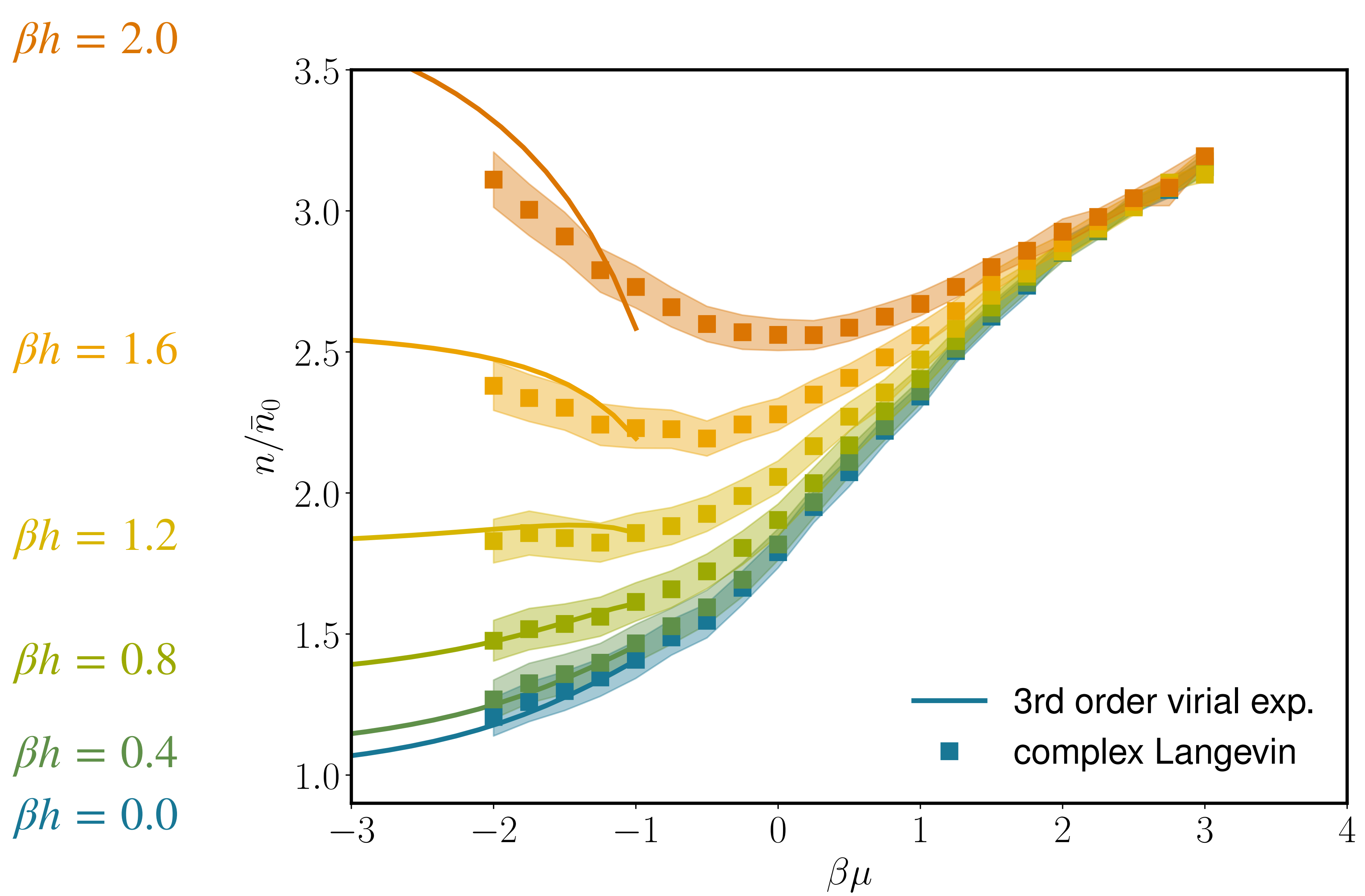

$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

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UFG at finite T: equation of state

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

$\beta h = 2.0$

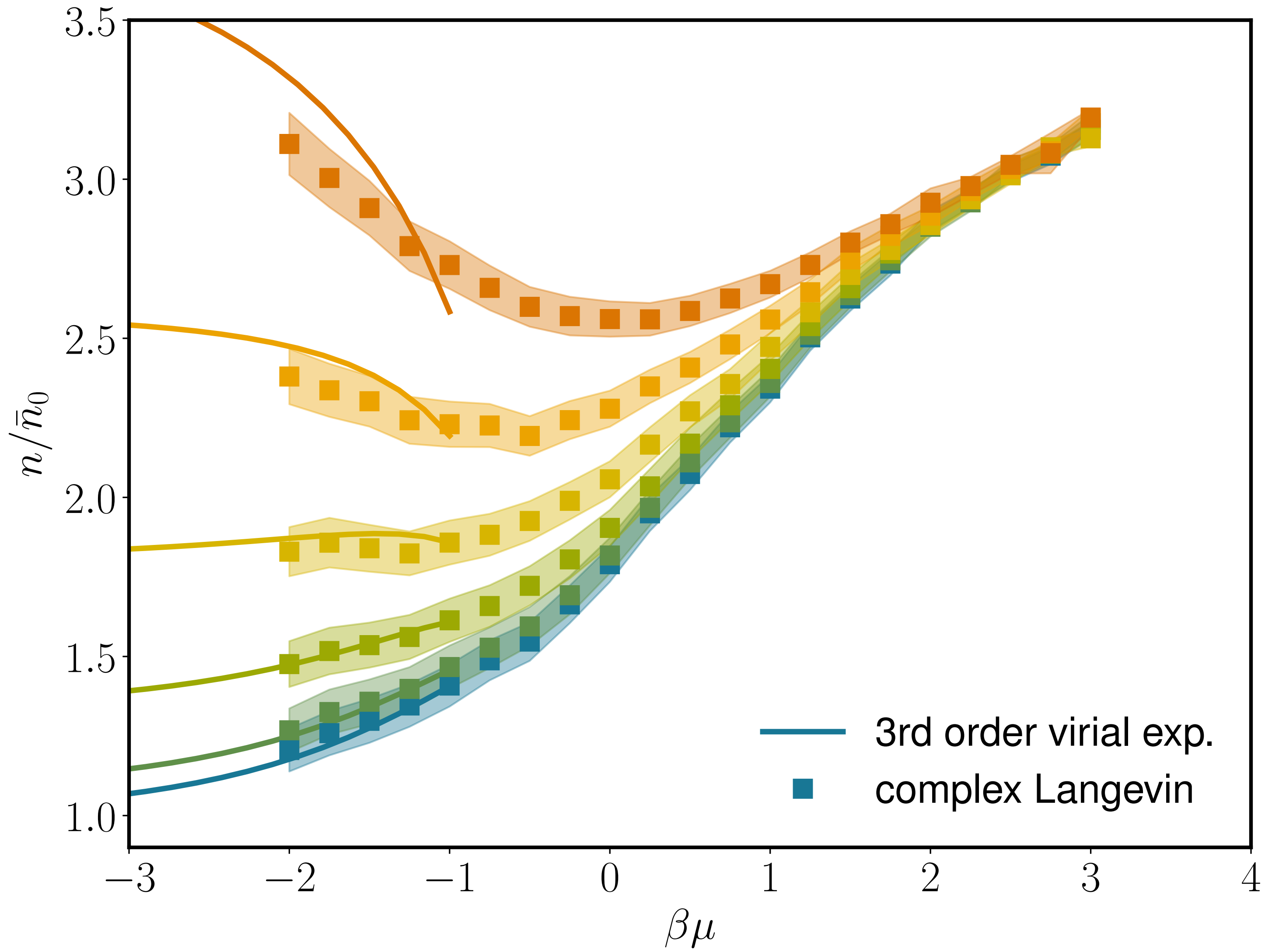
$\beta h = 1.6$

$\beta h = 1.2$

$\beta h = 0.8$

$\beta h = 0.4$

$\beta h = 0.0$



results match 3rd order virial expansion at large temperature

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

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RECAP

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

CL compares well with other methods wherever possible

EOS & correlation functions accessible
for systems with spin- and mass-imbalance

first *ab initio* results for the
UFG with finite polarization at $T > 0$