ULTRACOLD FERMIONS AWAY FROM BALANCED SYSTEMS

Lukas Rammelmüller, TU Darmstadt

Heidelberg, February 6th, 2018

[LR, Loheac, Drut, Braun *in preparation*]
[LR, Porter, Drut, Braun *Phys. Rev. D* 96, 094506, 2017]
[LR, Porter, Drut *Phys. Rev. A* 93, 033639, 2016]

THE PLAN

motivation: what do we want to do and why is it interesting?

method: how to get numbers?

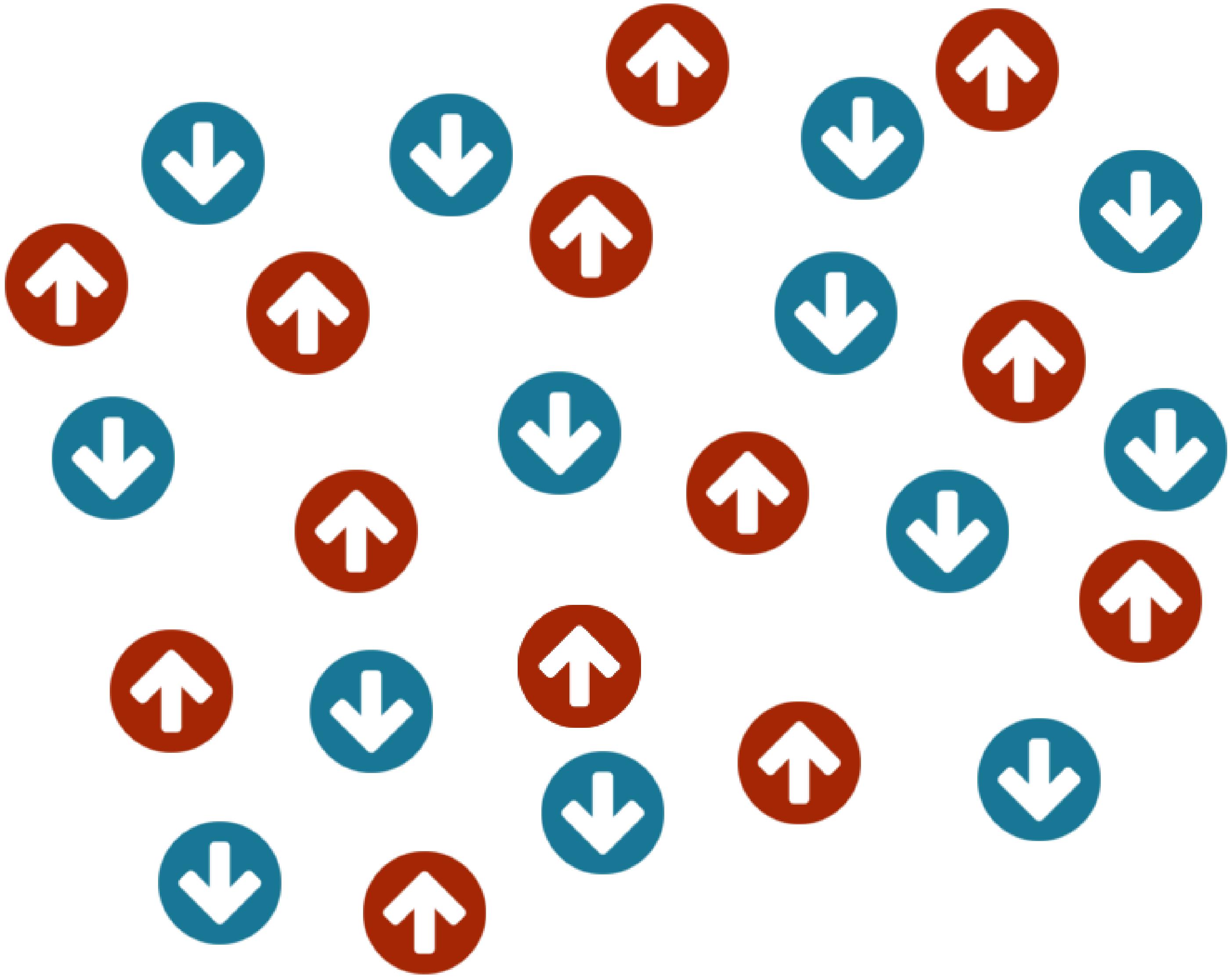
results: 1D, 2D & 3D Fermi gases

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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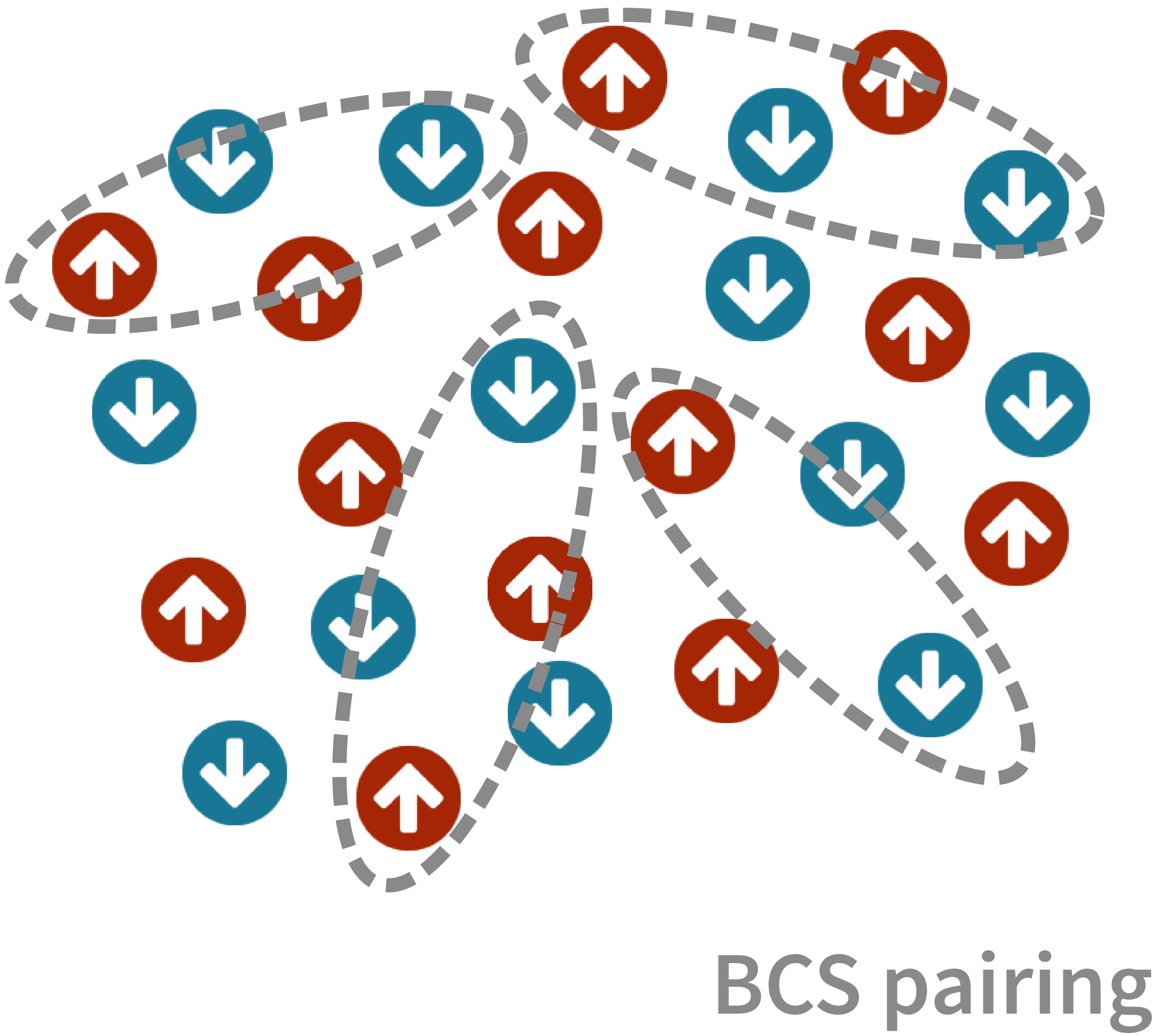

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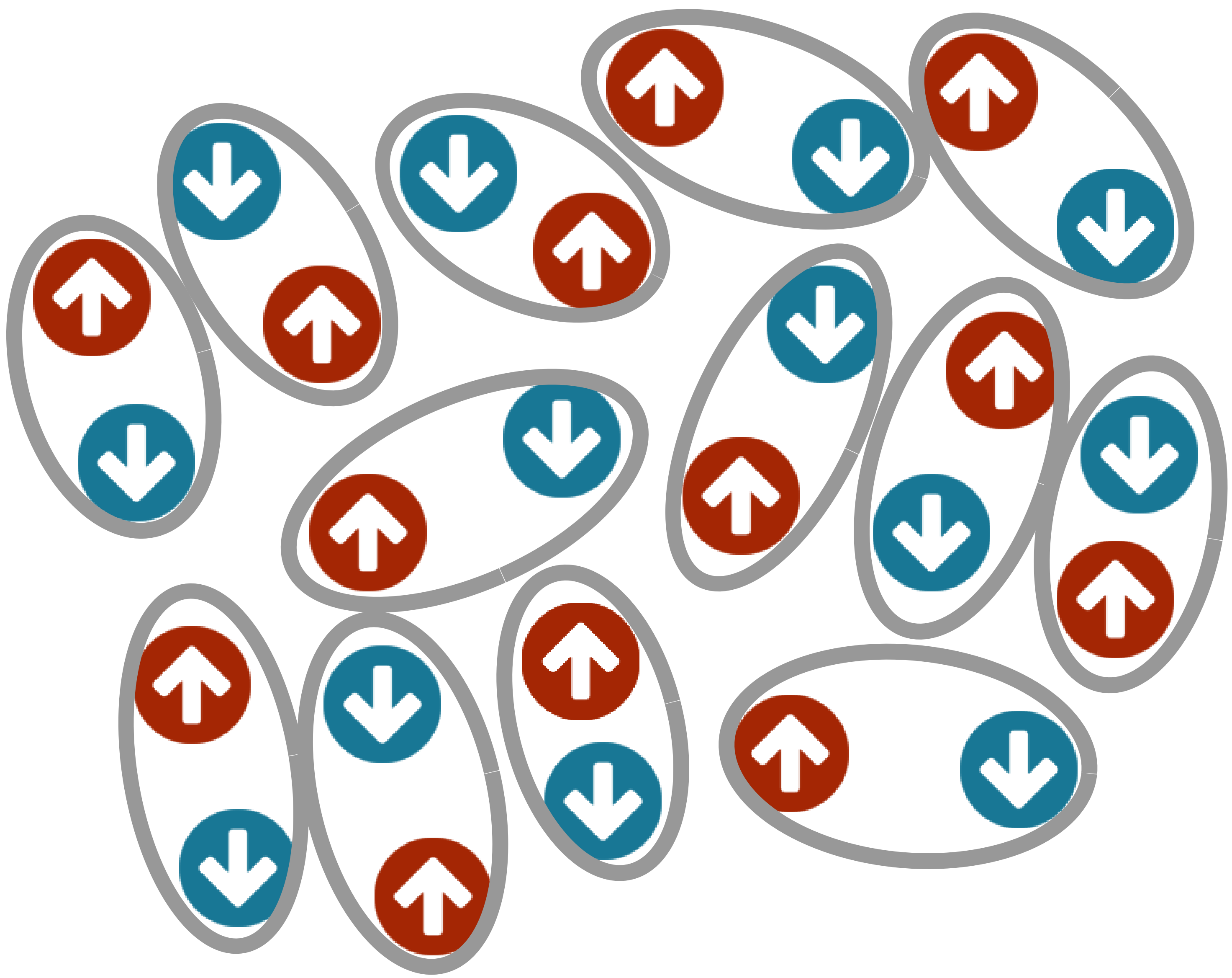
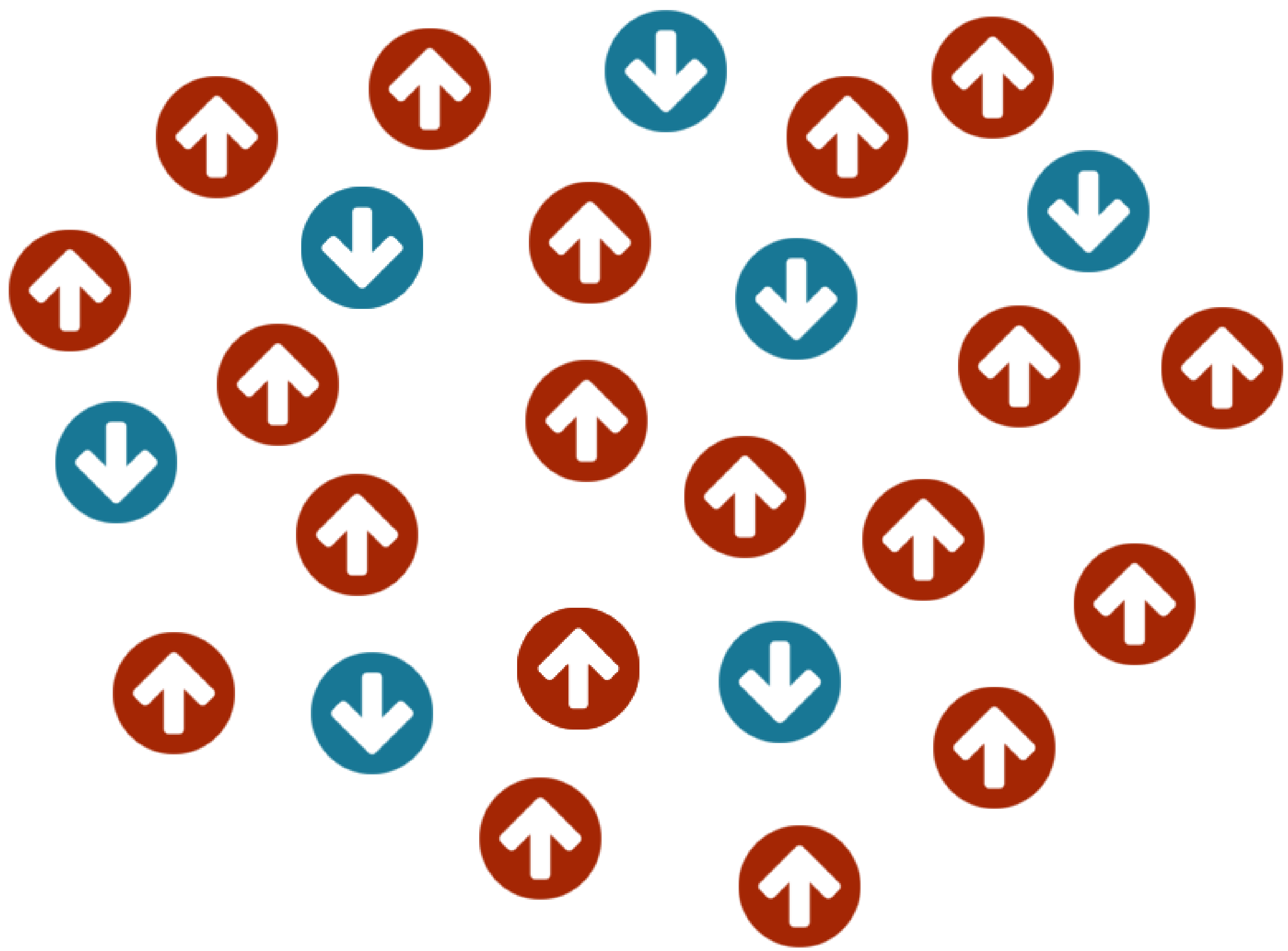
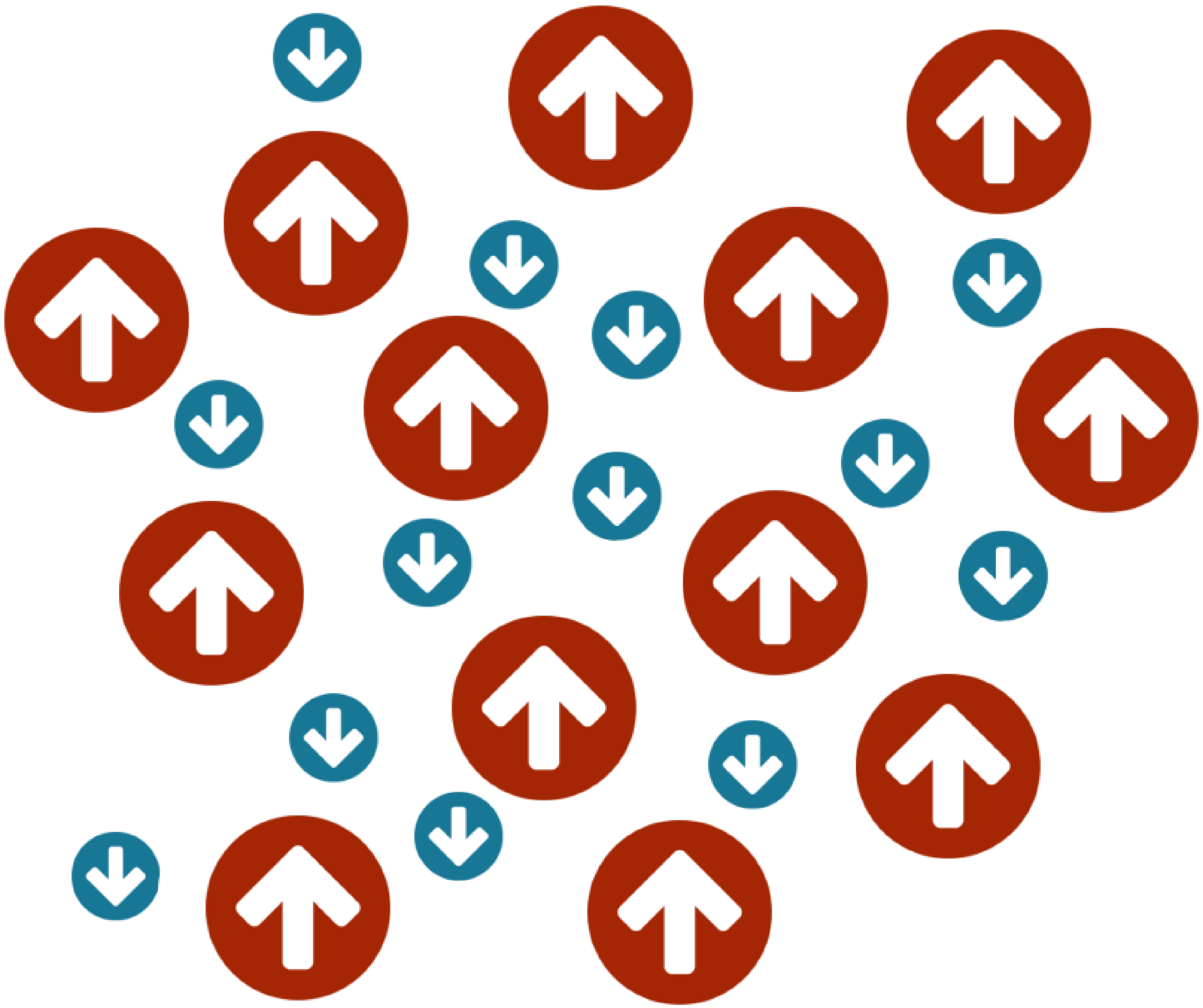


BEC pairing

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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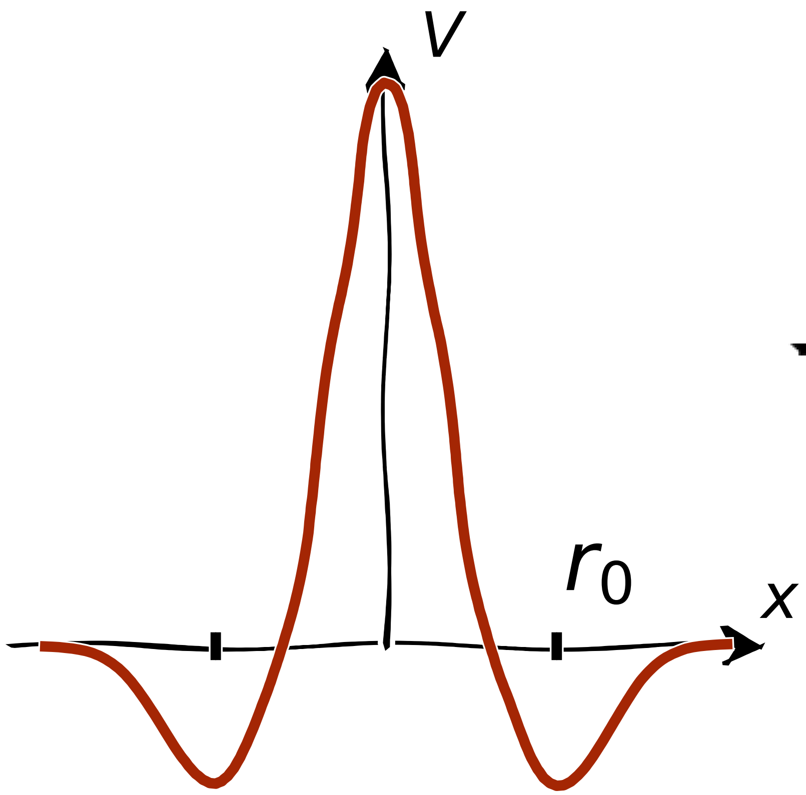
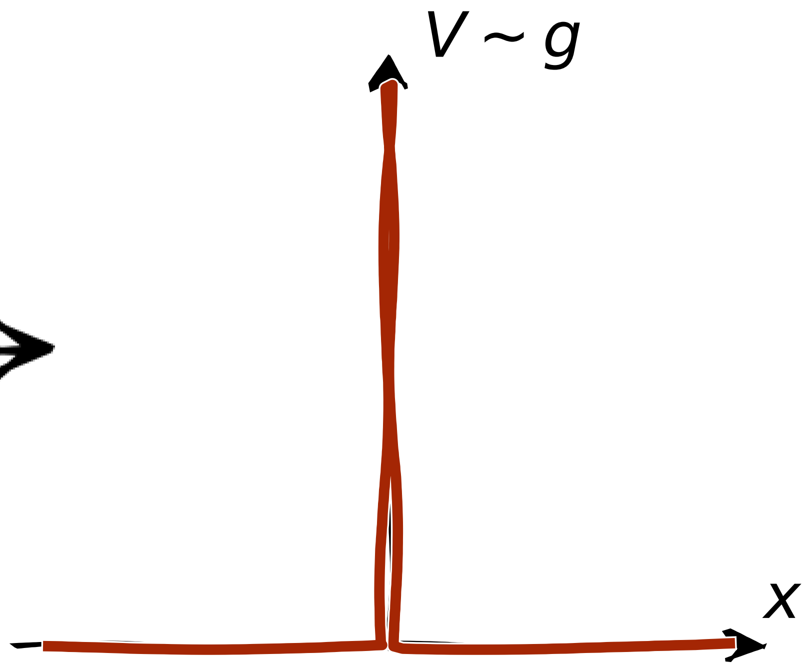
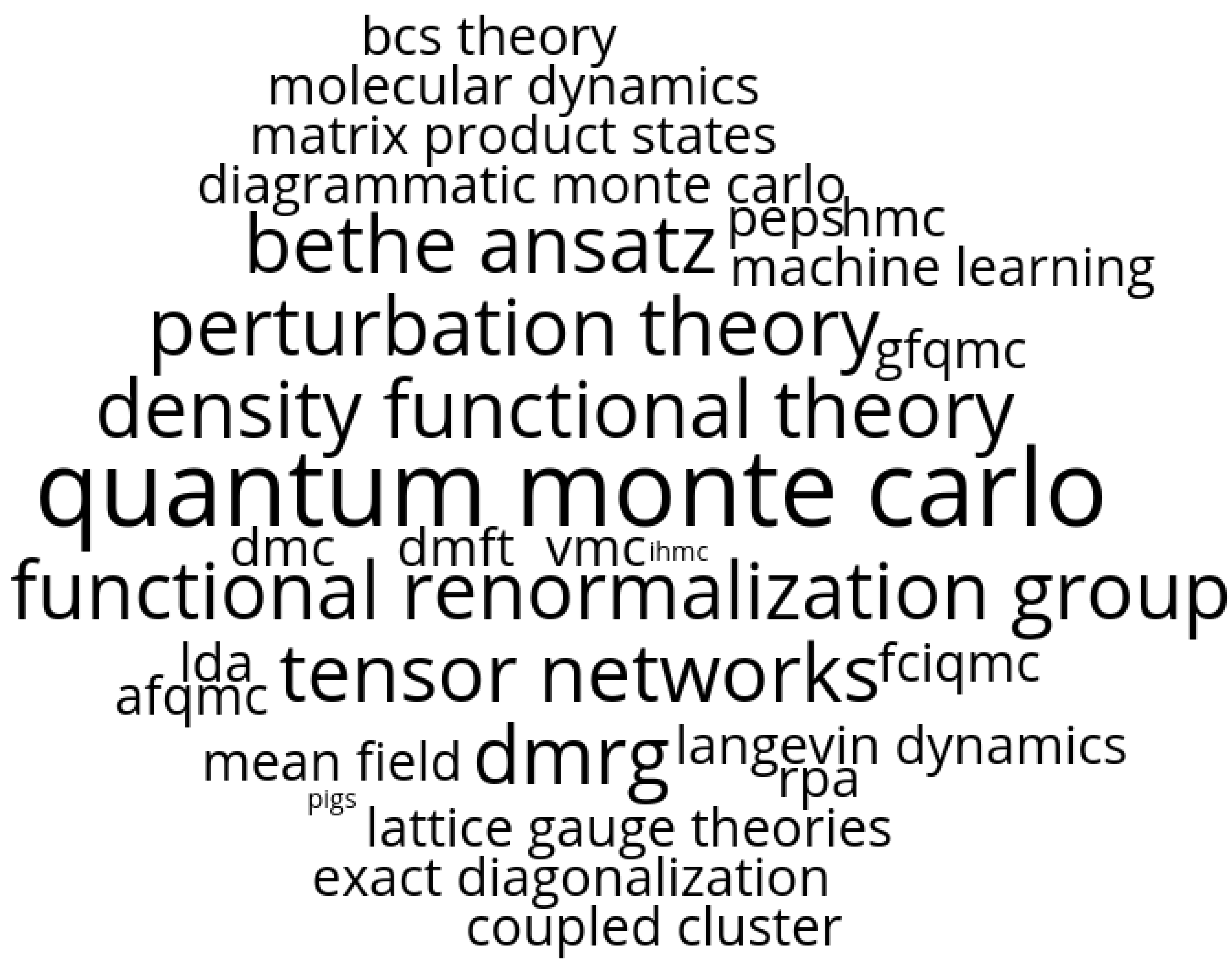


$$k_F^{-1} \gg r_0$$





*not exhaustive

what do we need to compute?

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

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

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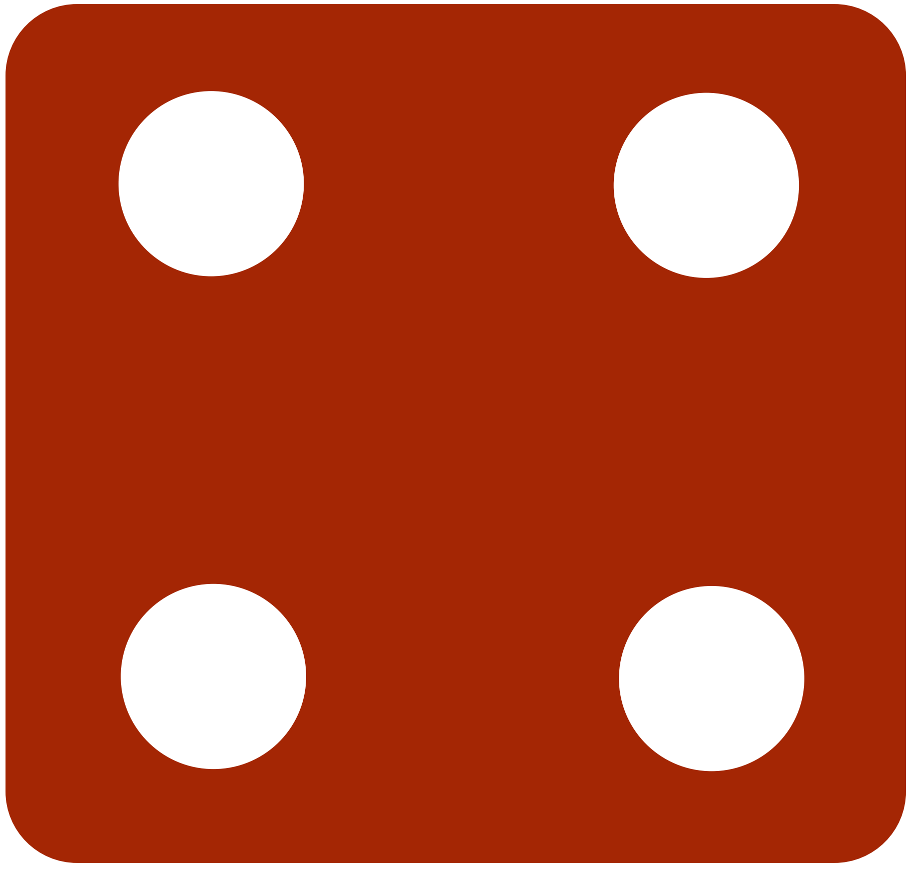
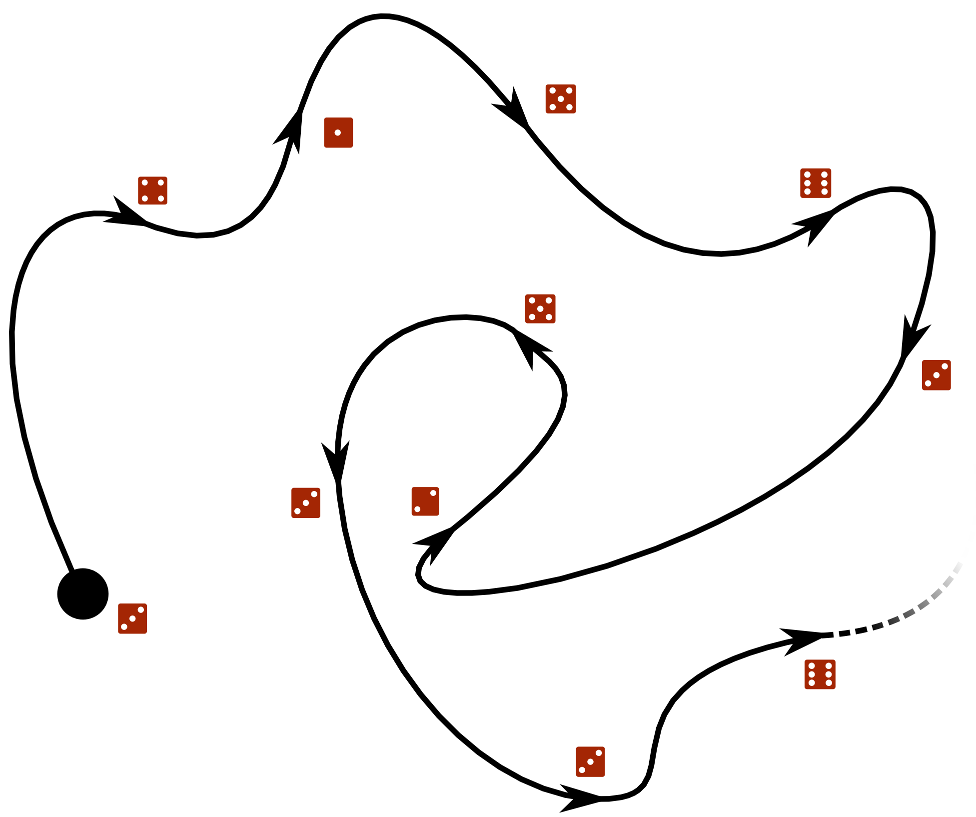
"all" that is left to do: evaluate high-dimensional integral

roll some dice



(create random auxiliary field configurations)

Quantum Monte Carlo (QMC)



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

i. produce a random sample of the auxiliary field ϕ

ii. evaluate the integrand with that value

iii. save result & repeat

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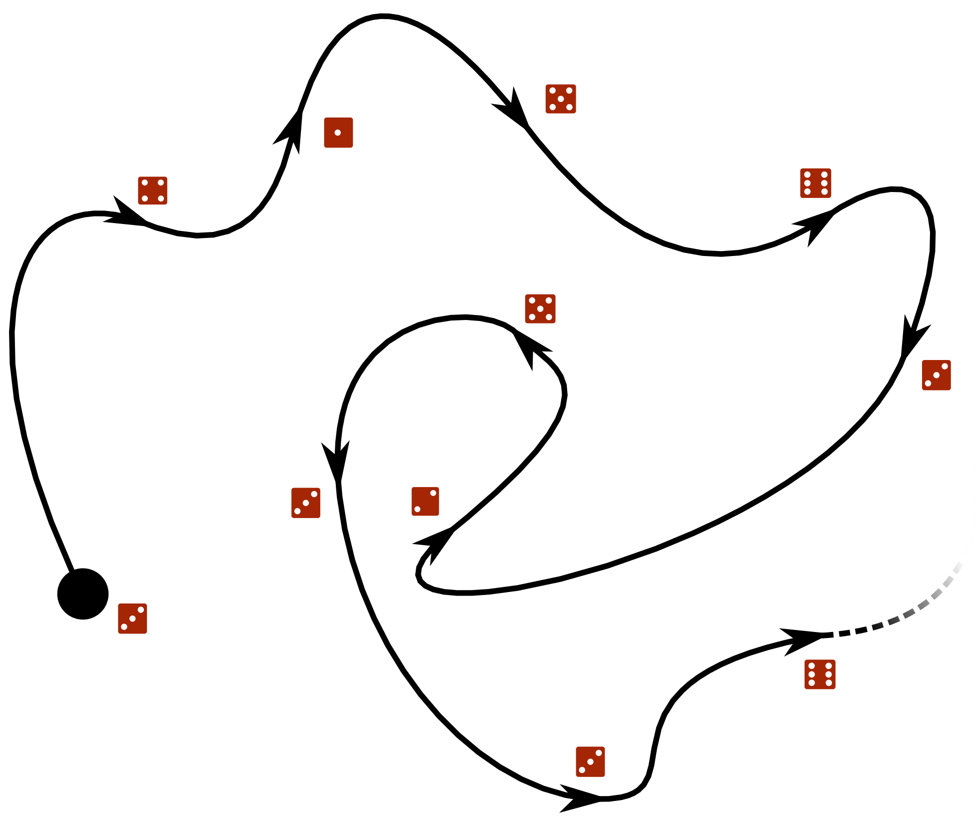

Markov chain produced with hybrid Monte Carlo (HMC)
[Duane, Kennedy, Pendleton, Roweth '87]

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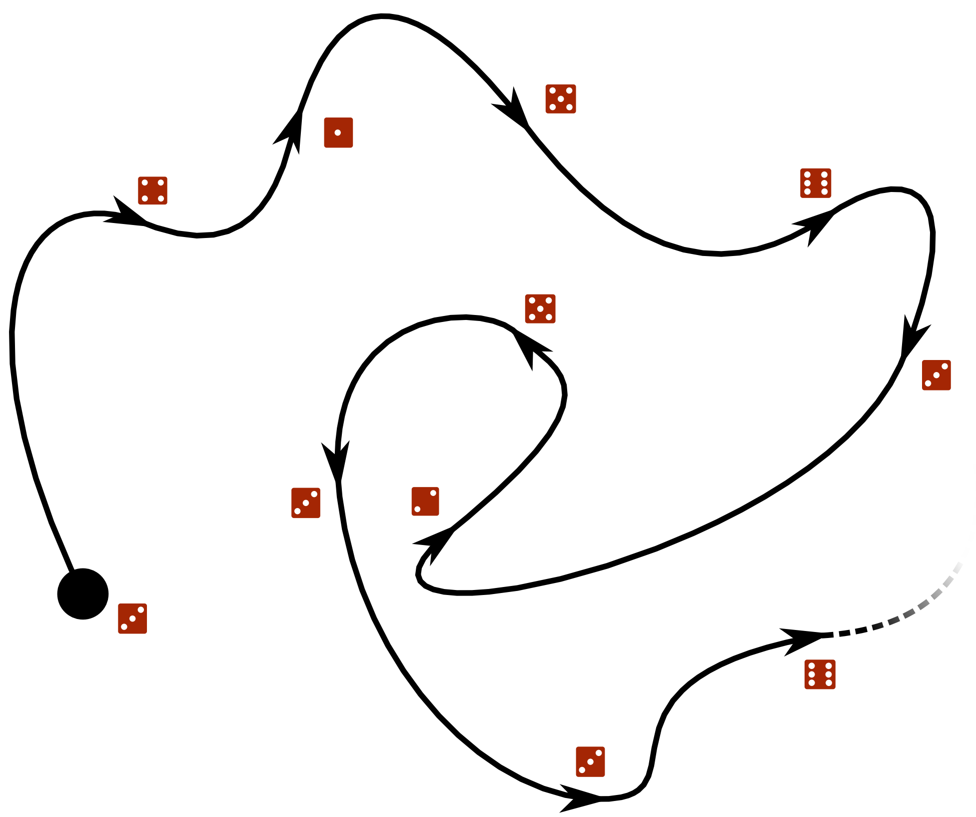

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i. produce a random sample of the auxiliary field ϕ

ii. evaluate the integrand with that value

iii. save result & repeat

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

statistical uncertainties

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

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EXAMPLE: COIN FLIPS

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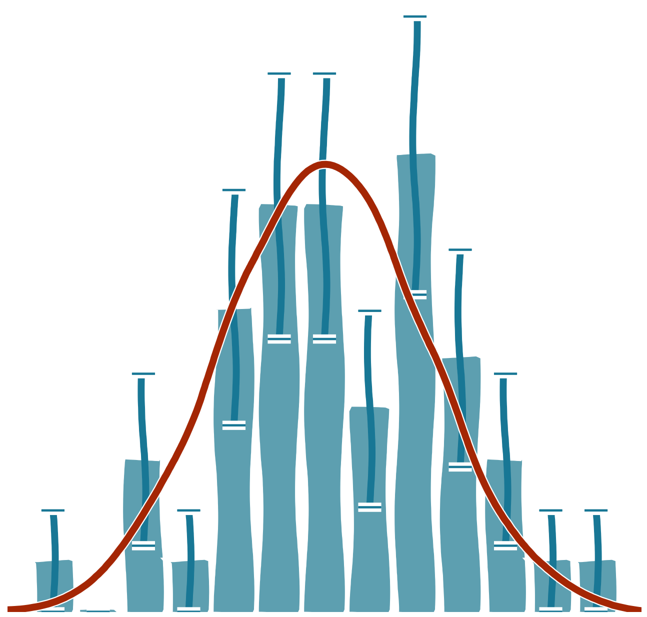

x 50

statistical uncertainties

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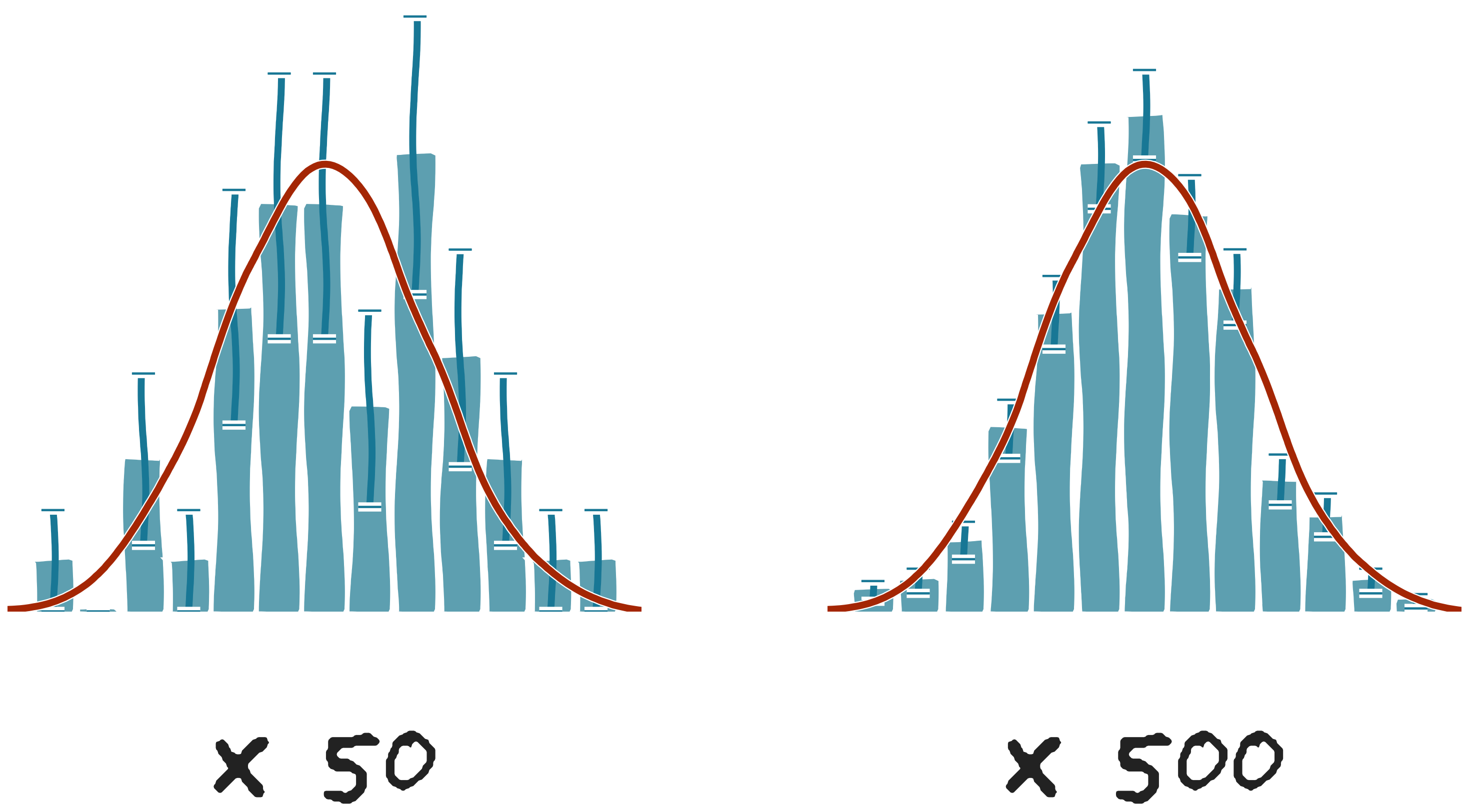
EXAMPLE: COIN FLIPS



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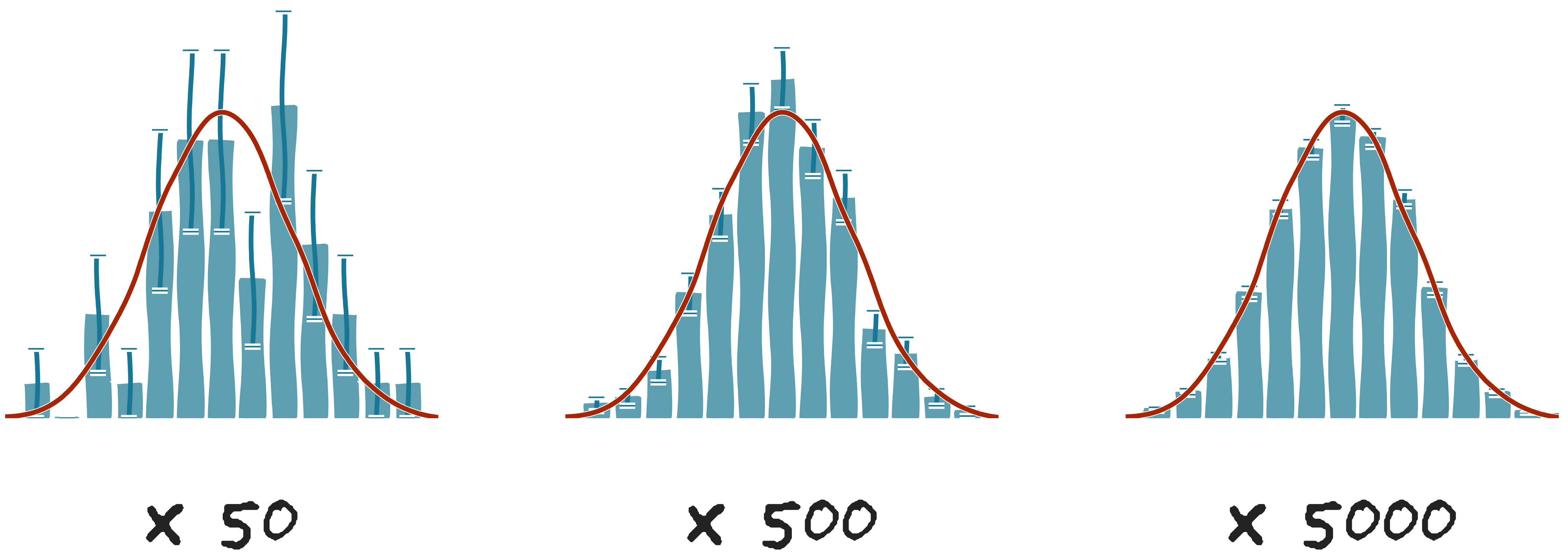

THE SIGN PROBLEM

(computational effort increases exponentially with system size)

[Troyer, Wiese '05]

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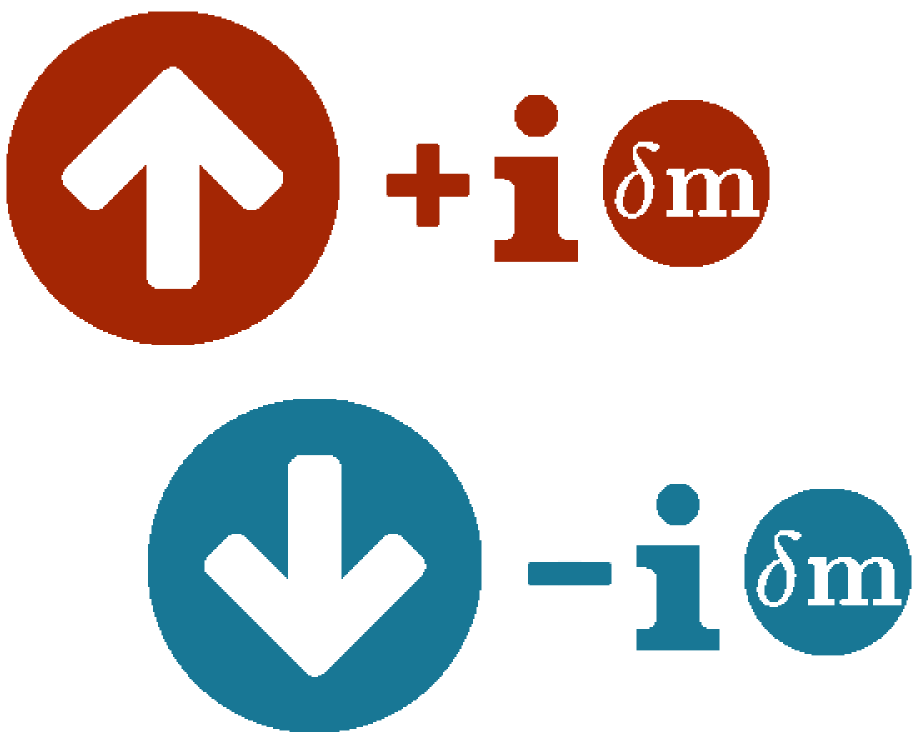
$$\mathcal{Z} = \int \mathcal{D}\phi \, \det M_\phi^\uparrow \, \det M_\phi^\downarrow$$

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

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

option I: imaginary mass imbalance (iHMC)



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

[Braun et al. '13]
[Roscher, Braun, Chen, Drut '13]
[Braun, Drut, Roscher '15]

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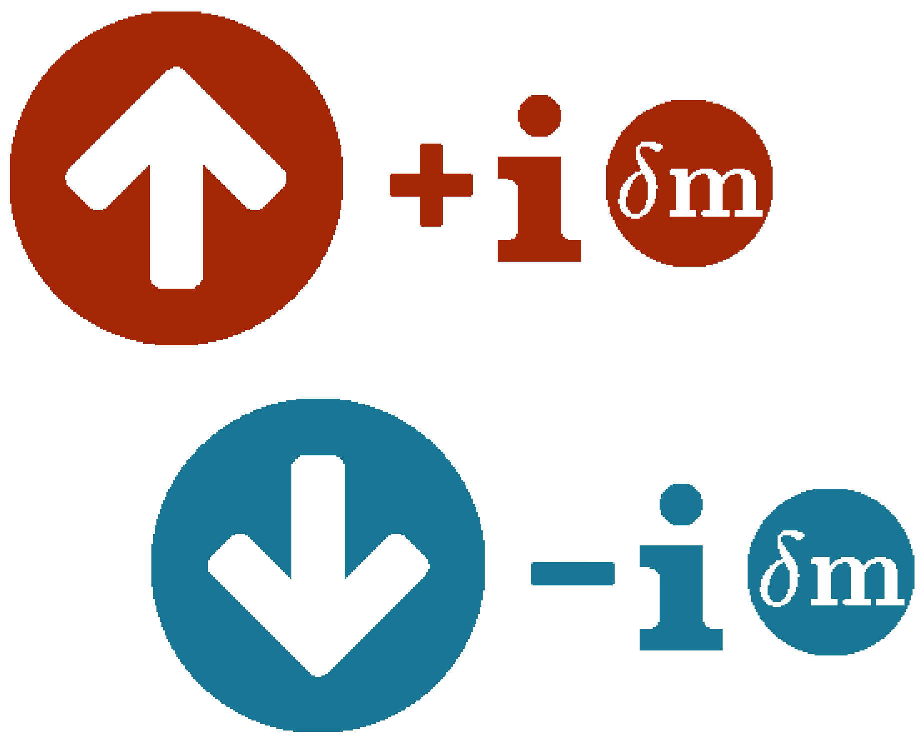

masses have an imaginary part and are **complex conjugate** to each other

probability measure non-negative:

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

analytic continuation: $\quad i\bar{m} \;\rightarrow\; \bar{m}$

to obtain results for real imbalances

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

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

[Braun et al. '13]
[Roscher, Braun, Chen, Drut '13]
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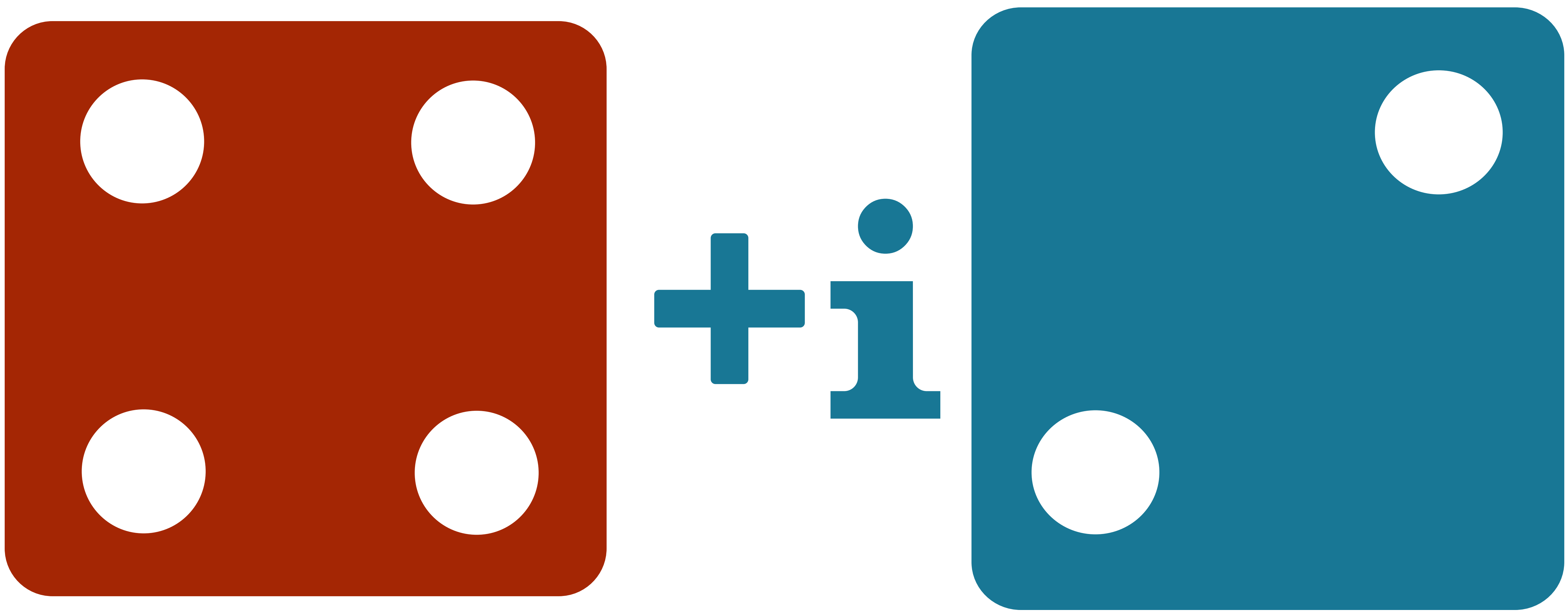
option II: roll dice with imaginary sides



(complexified auxiliary fields)

Complex Langevin (CL)

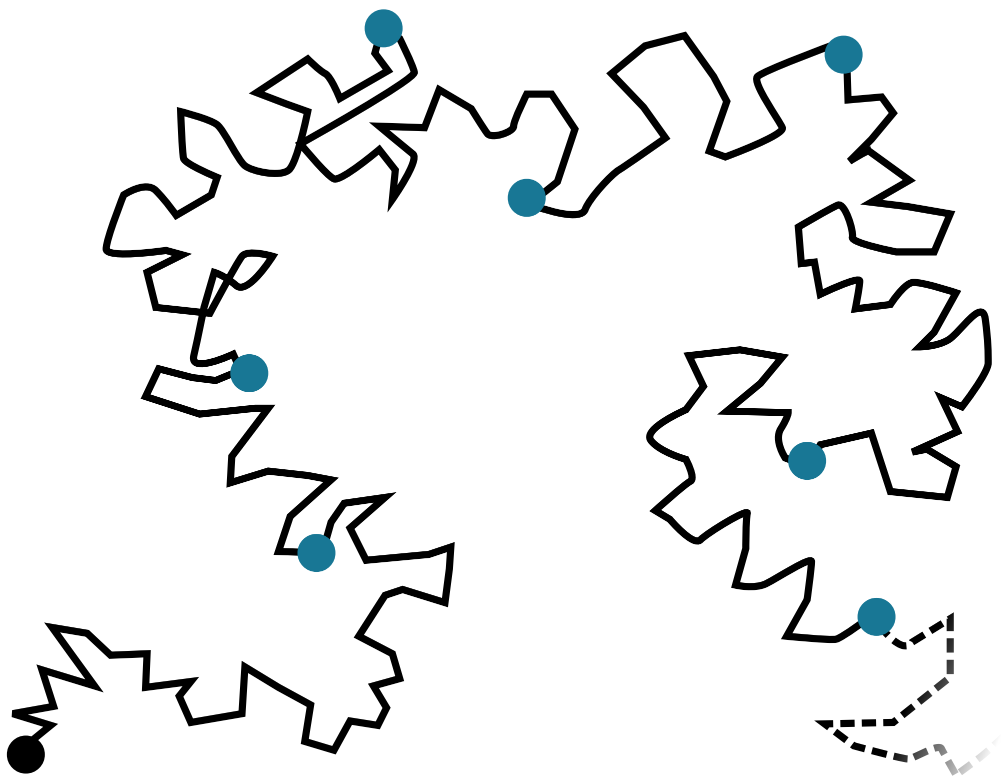
stochastic quantization: equilibrium distribution of a $(d+1)$-dimensional random process is identified with the probability measure of our d-dimensional path integral

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

Complex Langevin (CL)



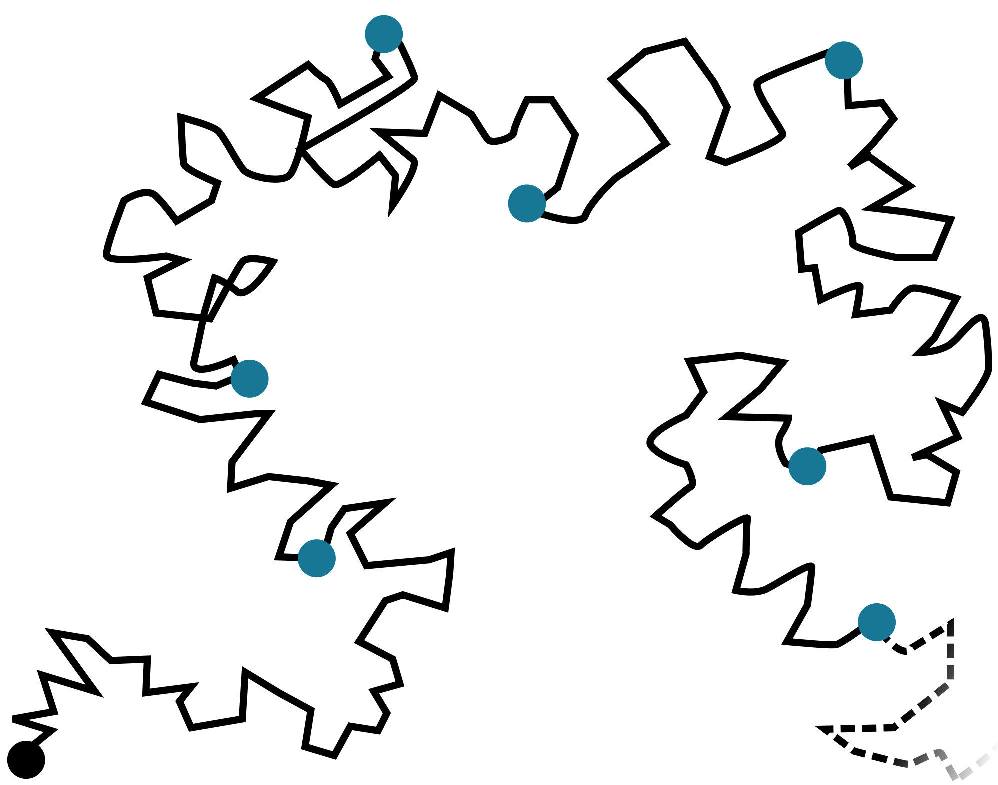
discretized Langevin equations:

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

$$\delta\phi_R = -\mathrm{Re}[\frac{\partial S[\phi]}{\partial\phi}]\delta t + 2\xi\phi_R\delta t + \eta(t)\sqrt{\delta t}$$

$$\delta\phi_I = -\mathrm{Im}[\frac{\partial S[\phi]}{\partial\phi}]\delta t + 2\xi\phi_I\delta t$$

Complex Langevin (CL)



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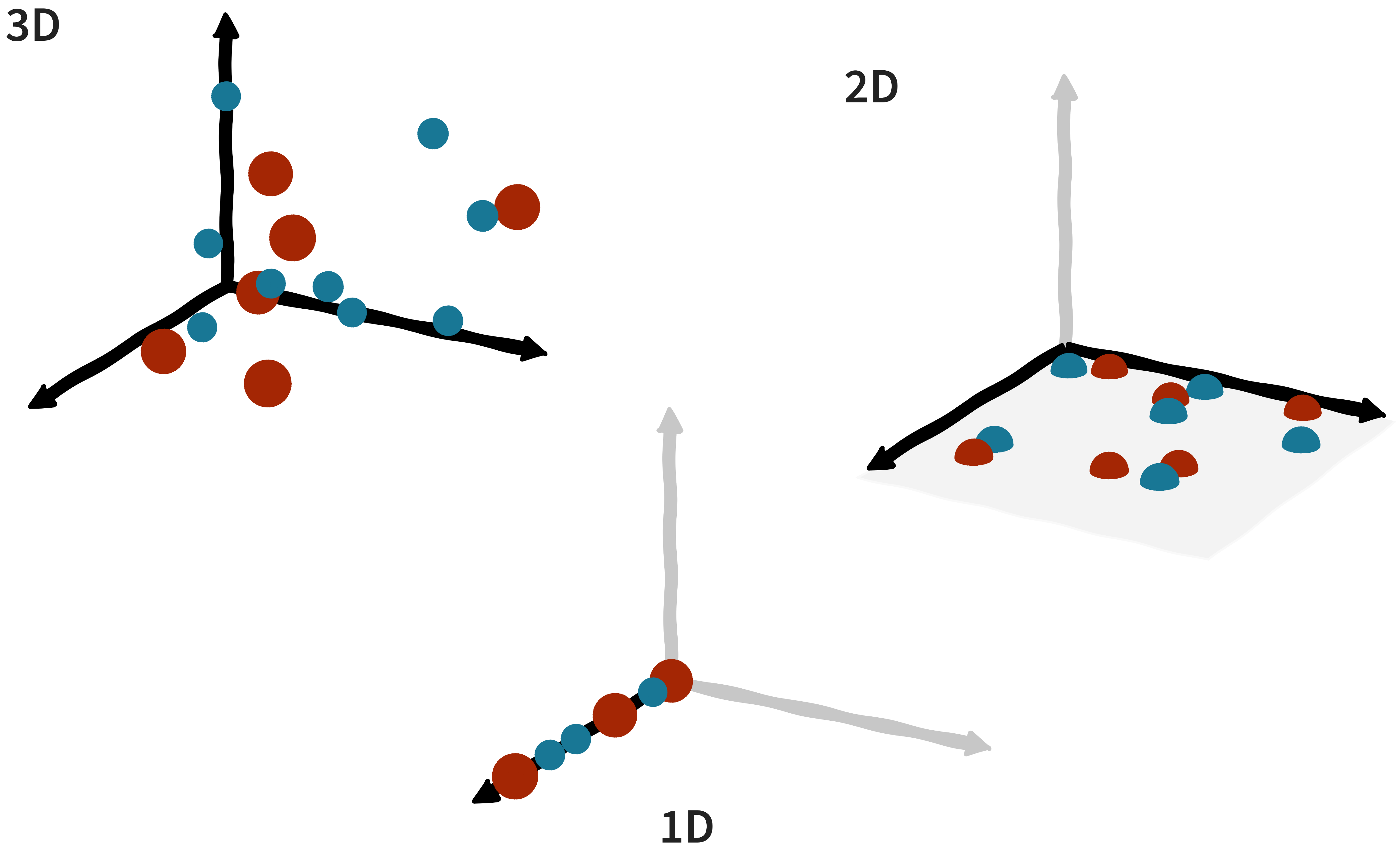
condition: $S[\phi]$ must be bounded from below!

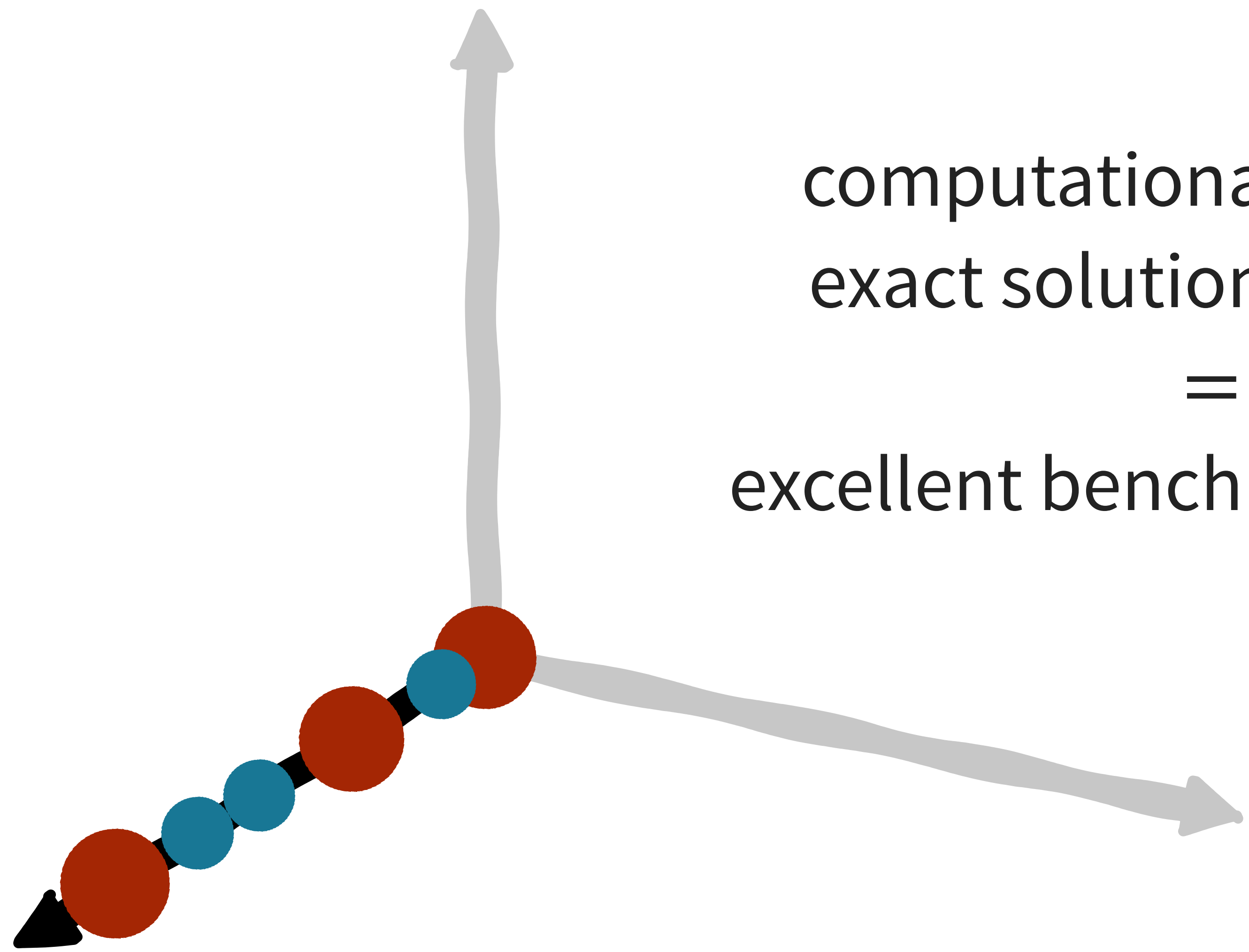
$$S[\phi] \equiv \ln\left(\det M_\phi^\uparrow \ \det M_\phi^\downarrow\right)$$

[Aarts, Seiler, Sexty, Stamatescu '16; '17]

methods work in any dimension



one-dimensional systems



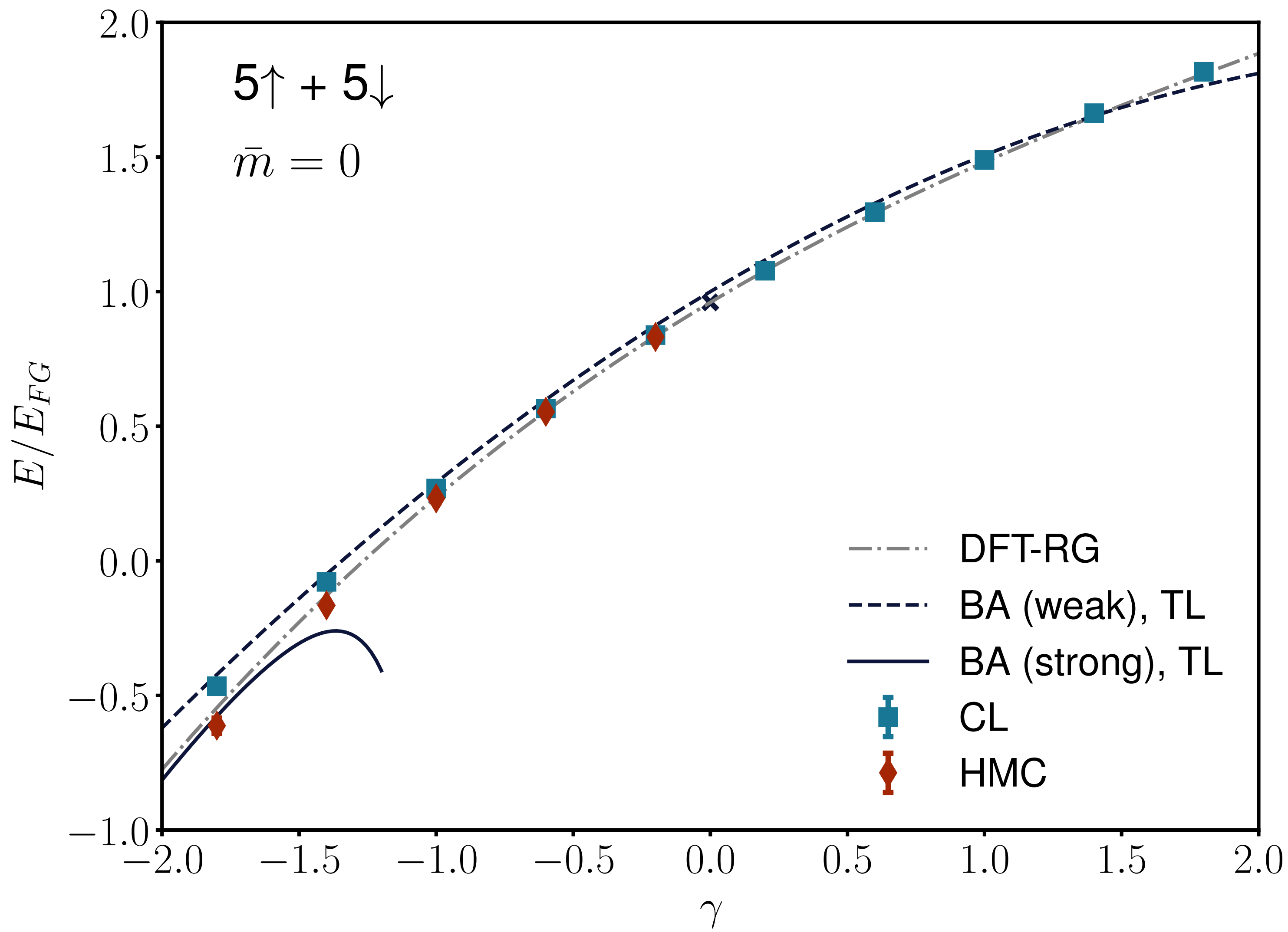
computationally cheap &
exact solutions available
=
excellent benchmark systems

accessible in experiment

[Wenz et al. '13; Zürn et al. '13; Murmann et al. '15]

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 '17; Kemler '17]
[HMC: LR, Porter, Loheac, Drut '15]

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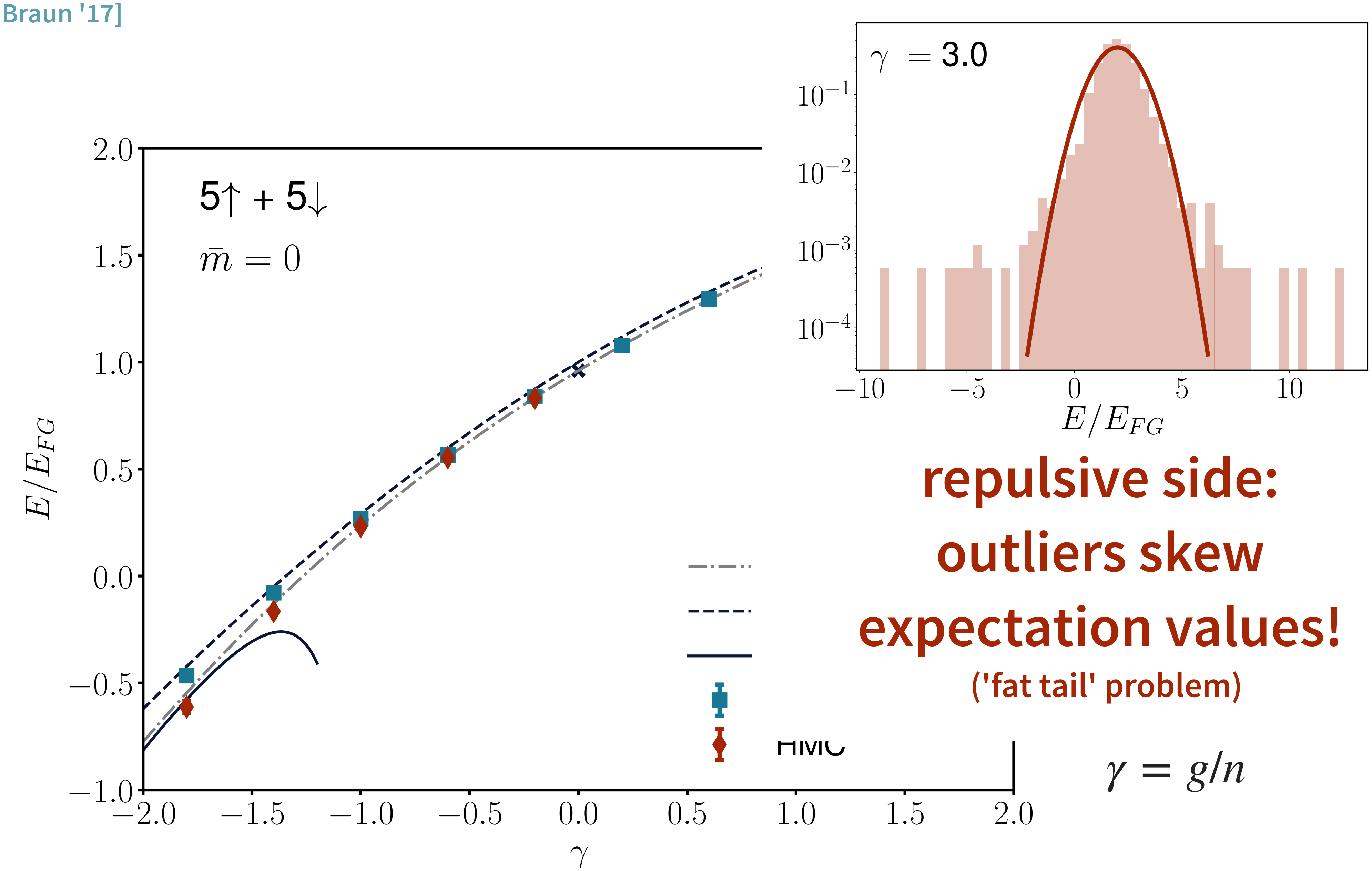

repulsive side: outliers skew expectation values!

('fat tail' problem)

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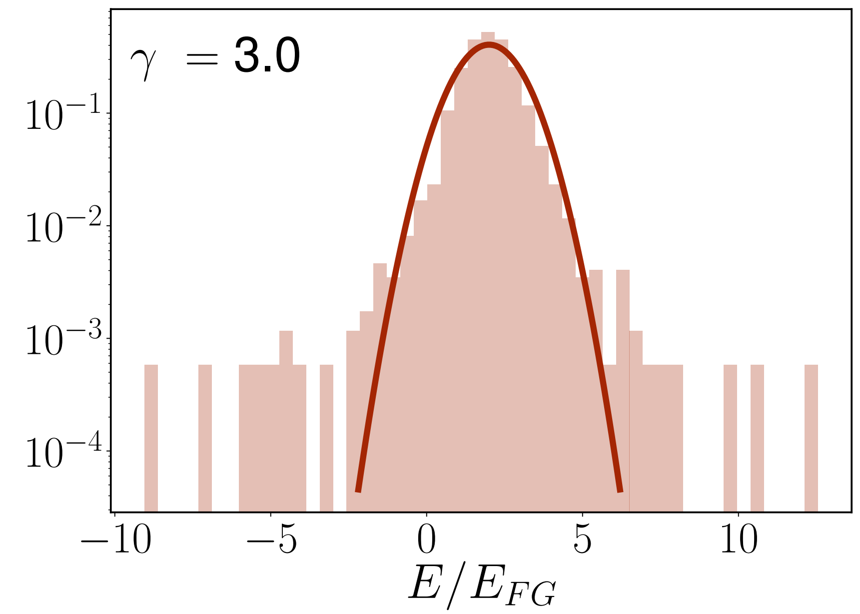
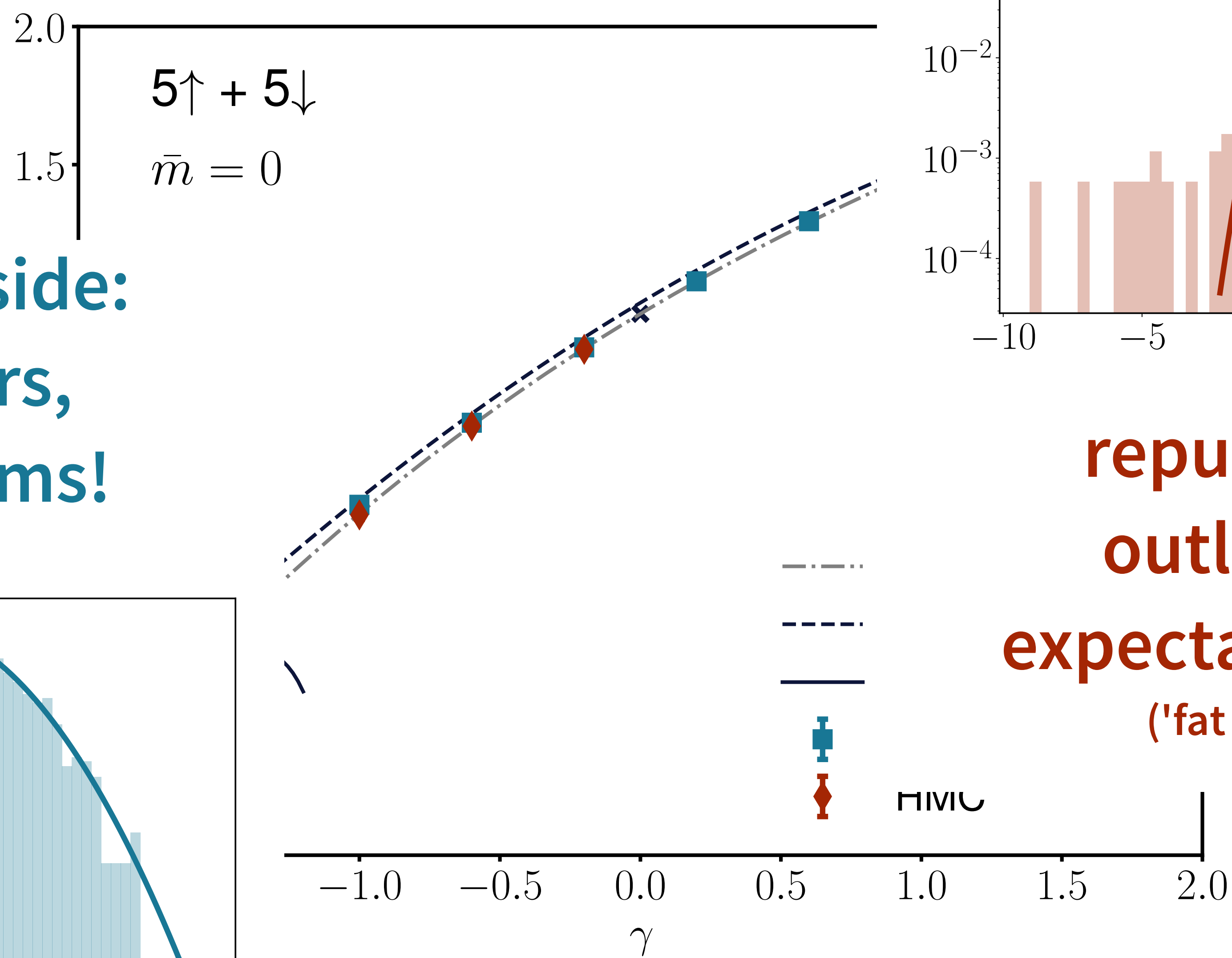
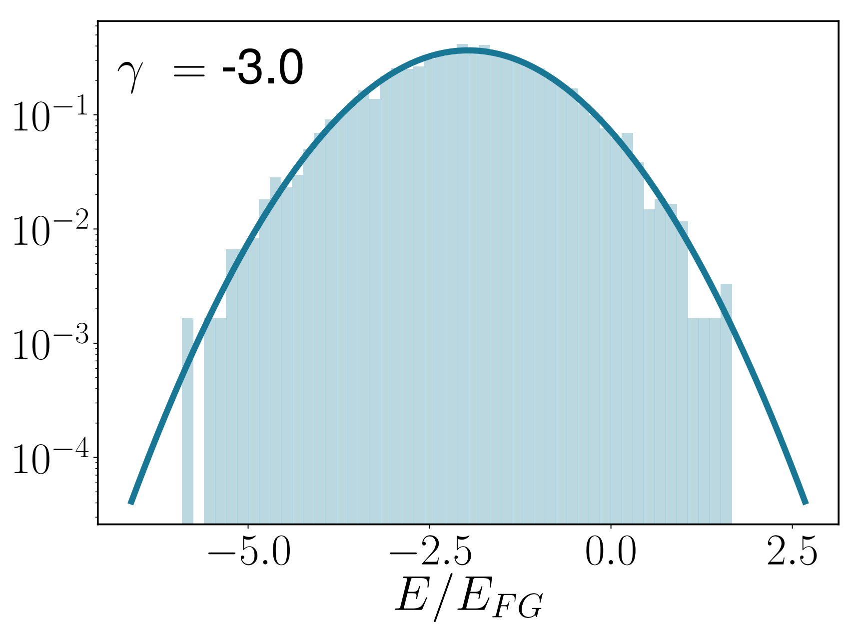




attractive side:
no outliers,
no problems!

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



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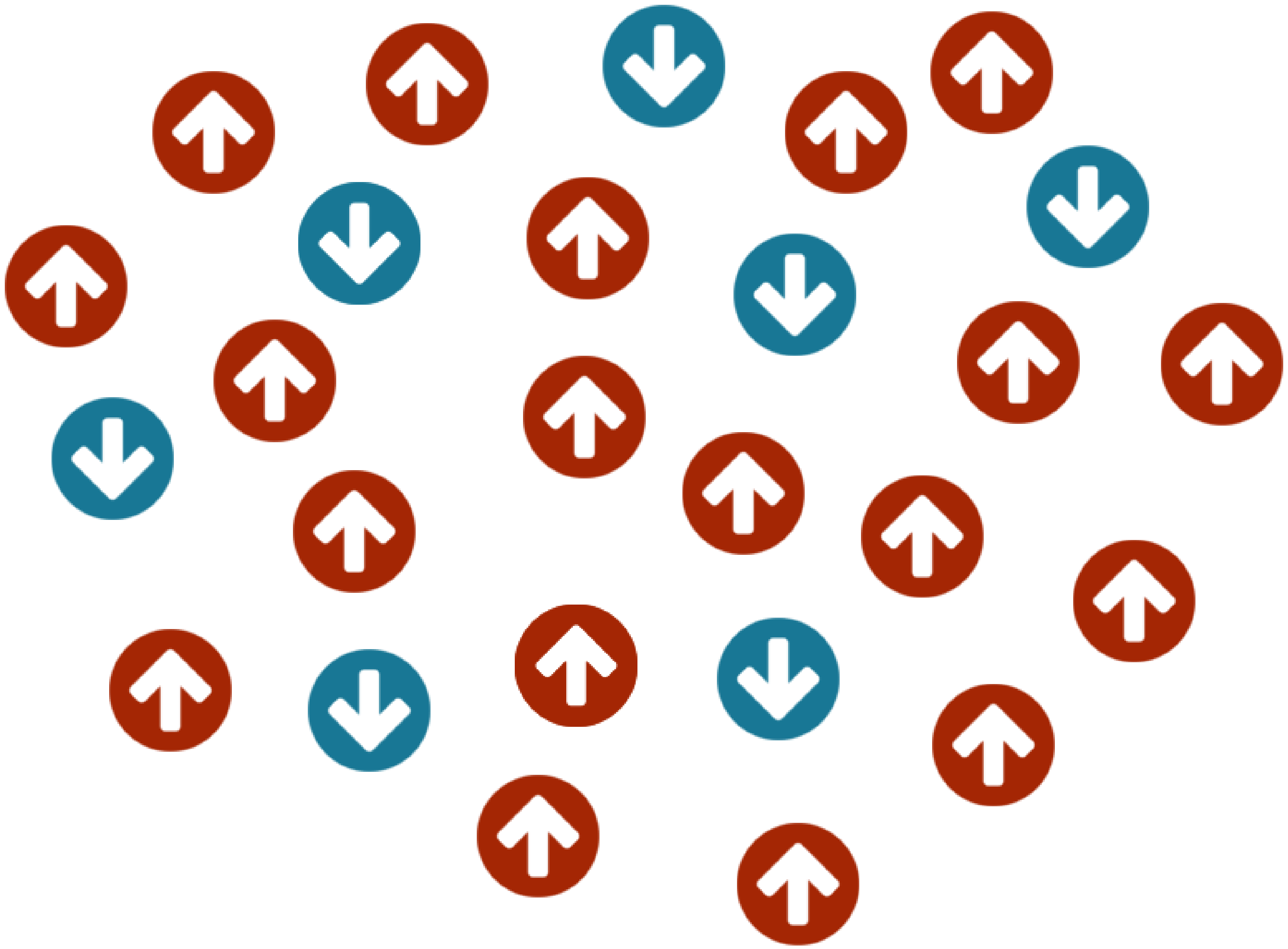
spin polarization



polarized 1D fermions: equation of state

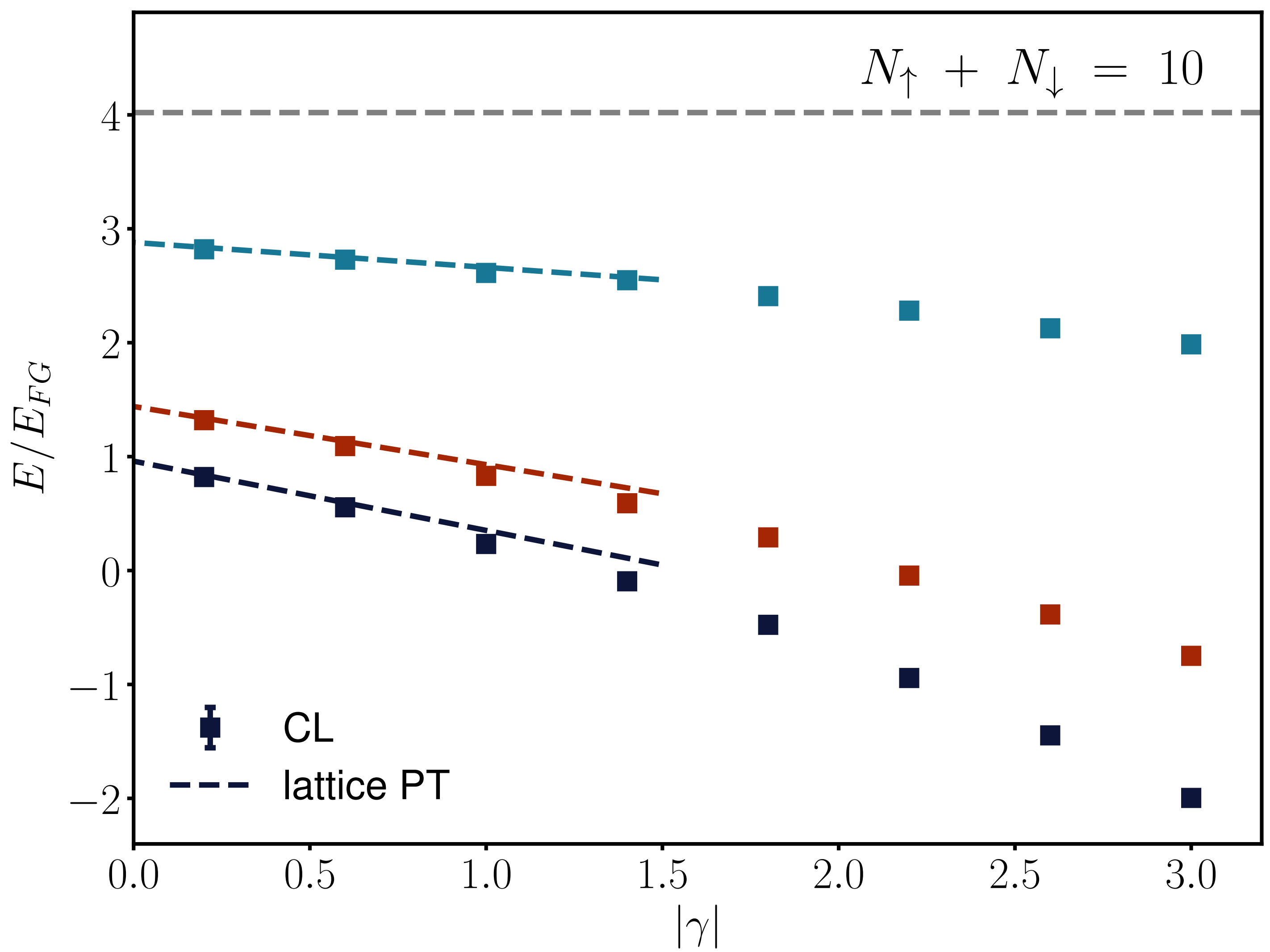
[LR, Drut, Braun *in preparation*]

$p = 1.0$

$p = 0.8$

$p = 0.4$

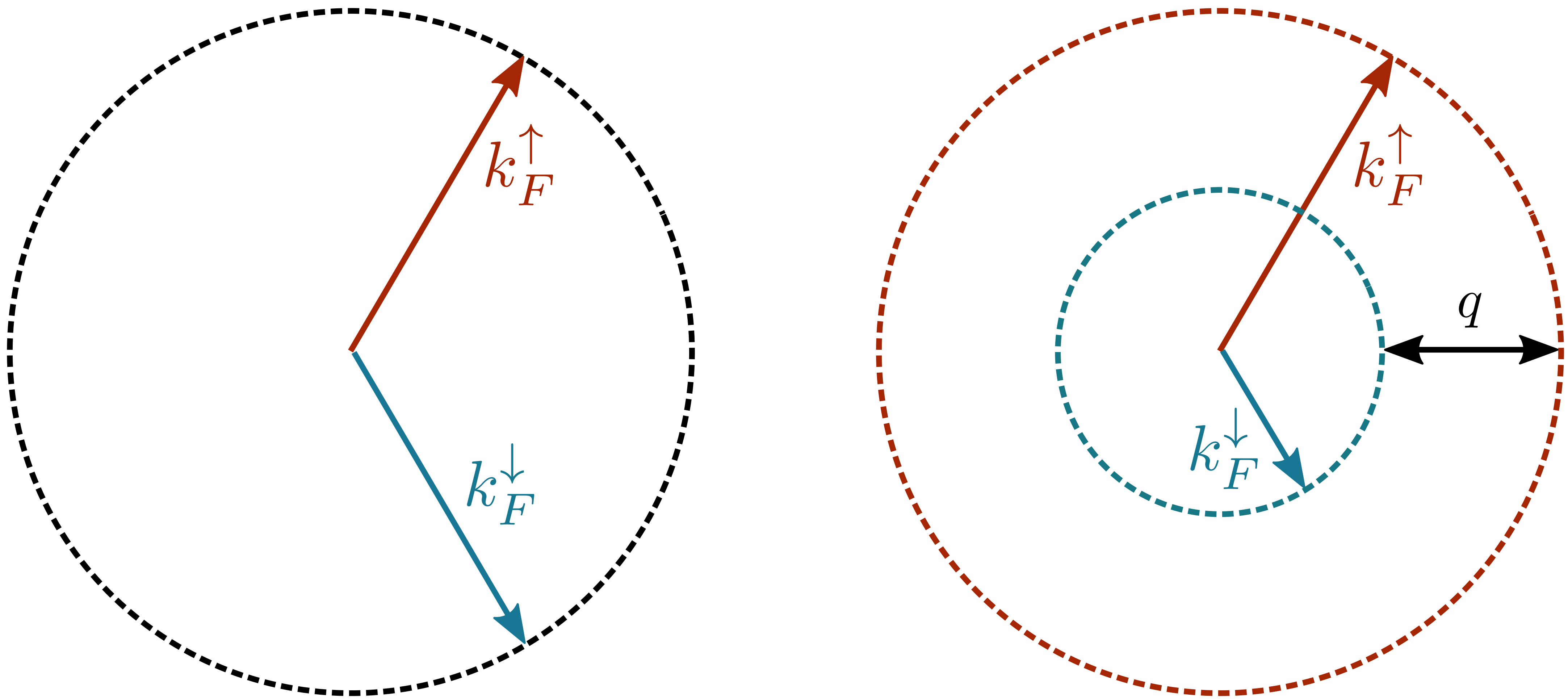
$p = 0.0$



$\gamma = g/n$

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

interlude: pairing (schematically)



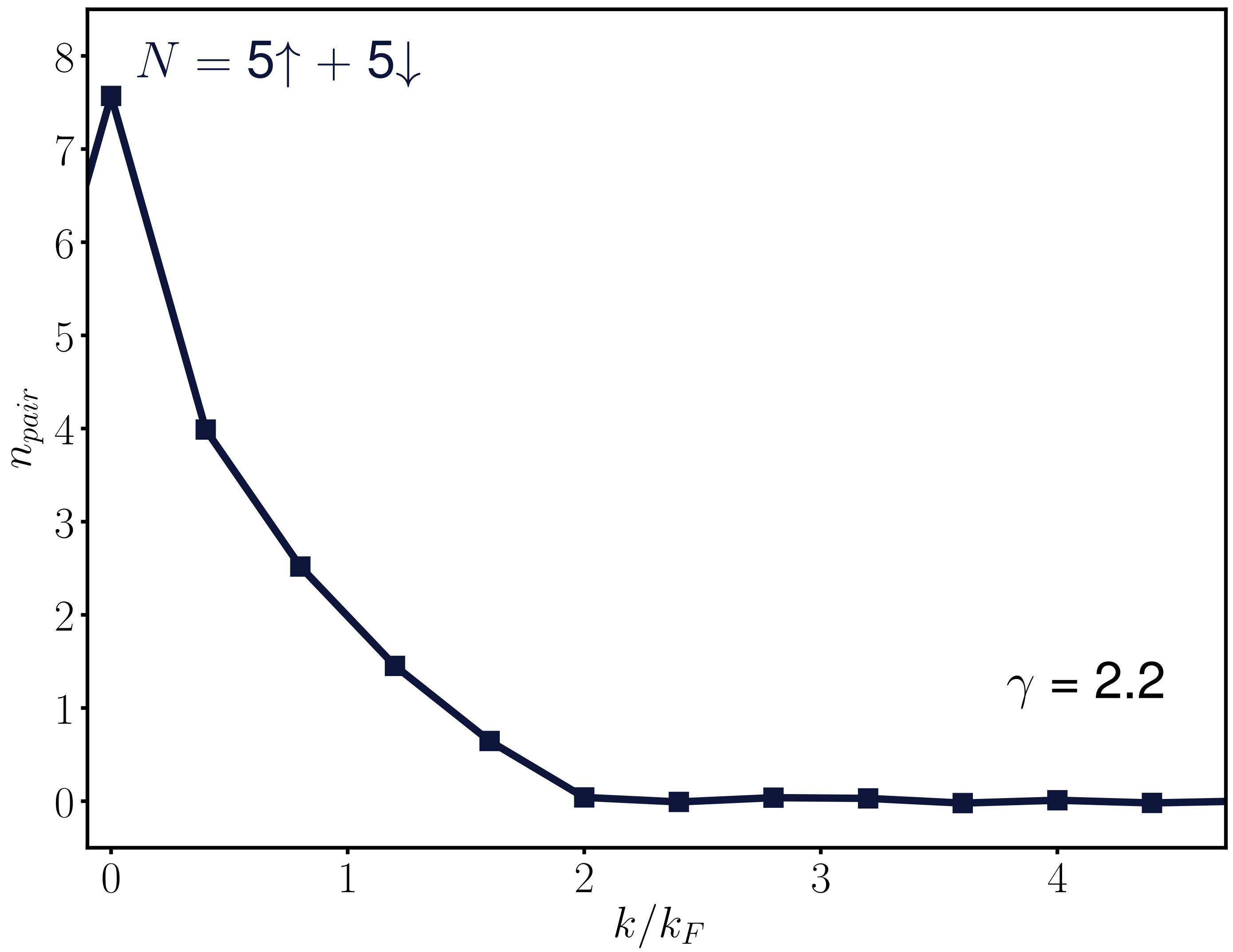
$$\vec{q} \equiv \vec{k}_F^\uparrow - \vec{k}_F^\downarrow = 0$$

$$\vec{q} \neq 0$$

[Fulde, Ferrell '64; Larkin, Ovchinnikov '65]

polarized 1D fermions: pair correlation

[LR, Drut, Braun *in preparation*]



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

polarized 1D fermions: pair correlation

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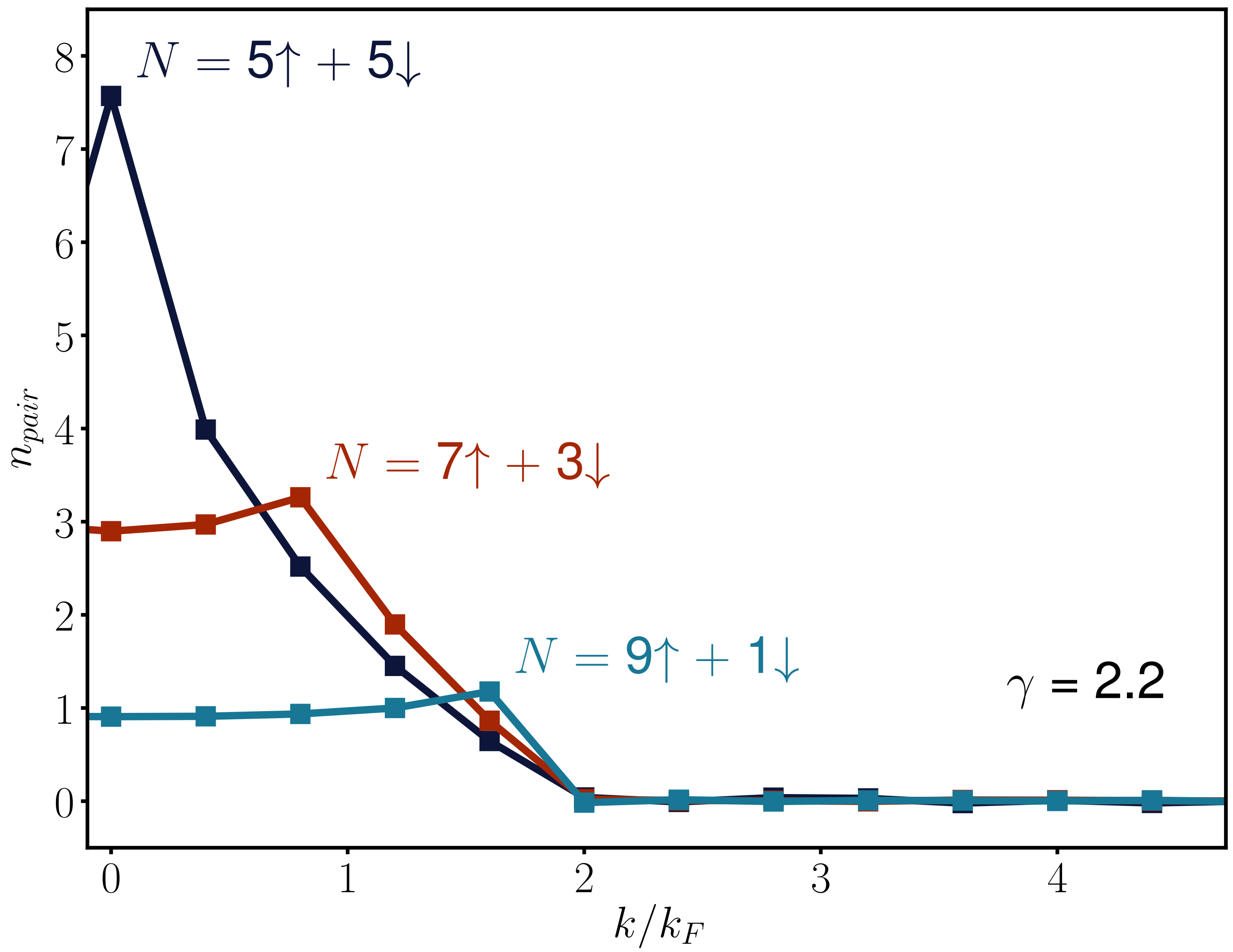

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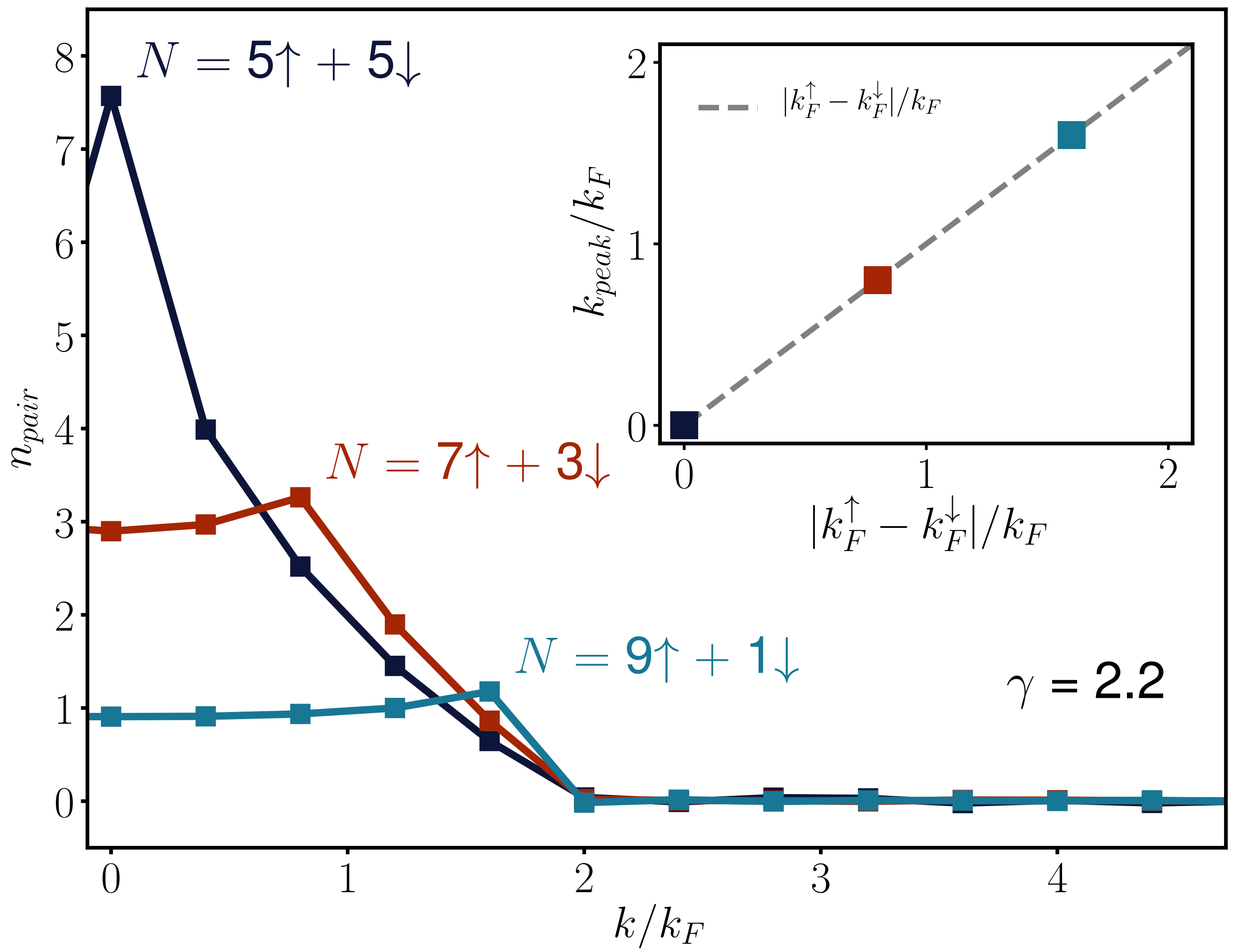

signature of FFLO type pairing

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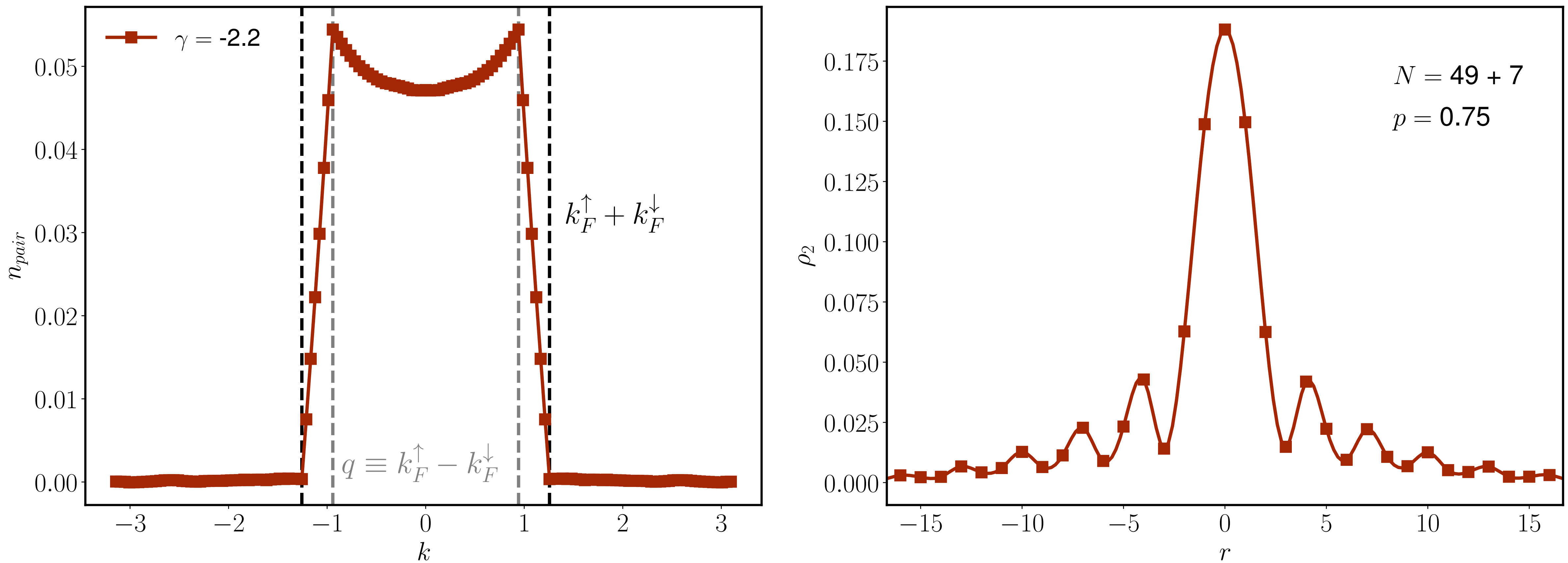
$$n_{pair}(x, x') = \langle \hat{\psi}_\uparrow^\dagger(x)\, \hat{\psi}_\downarrow^\dagger(x)\, \hat{\psi}_\downarrow(x')\, \hat{\psi}_\uparrow(x') \rangle$$

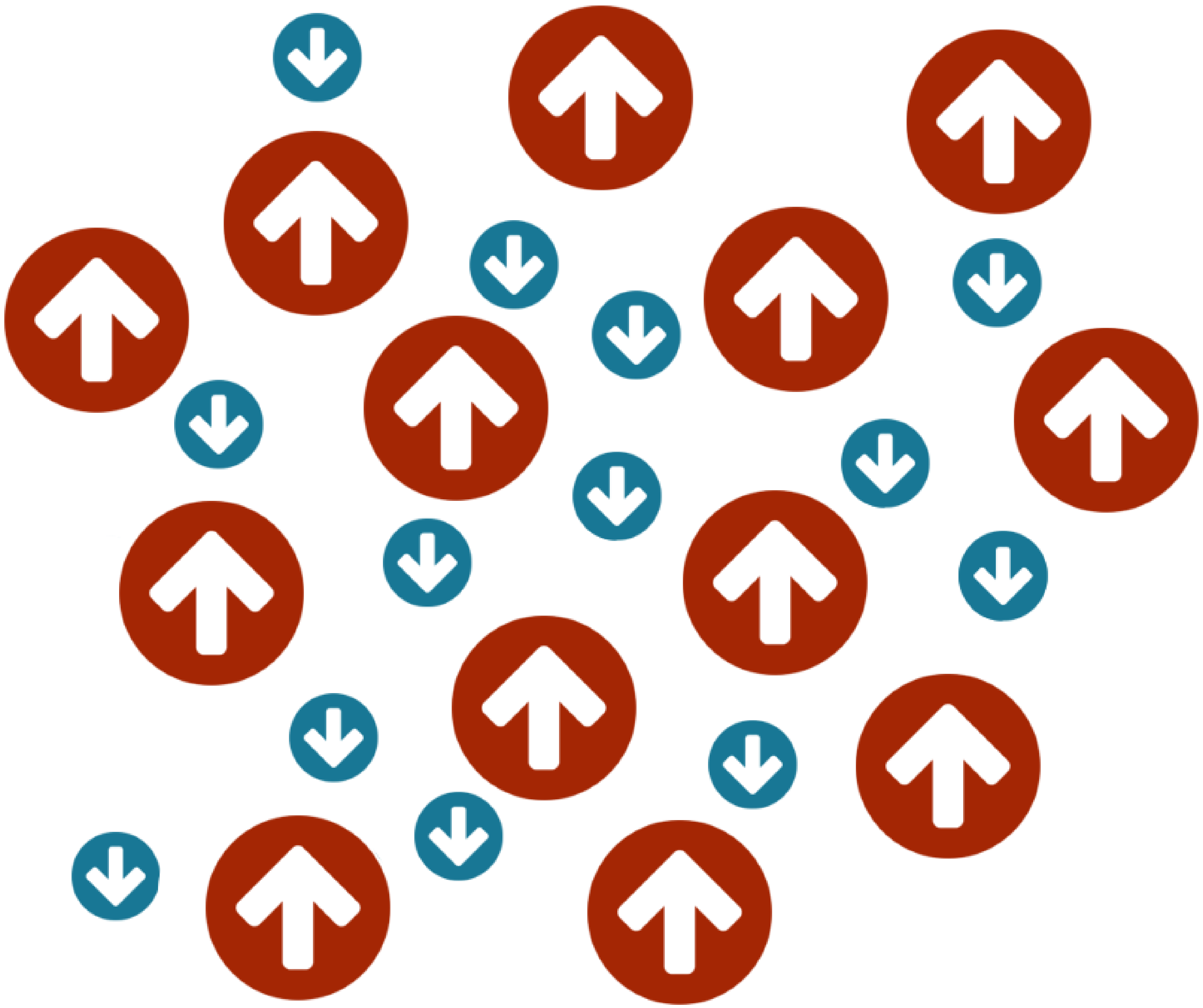
polarized 1D fermions: order parameter

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



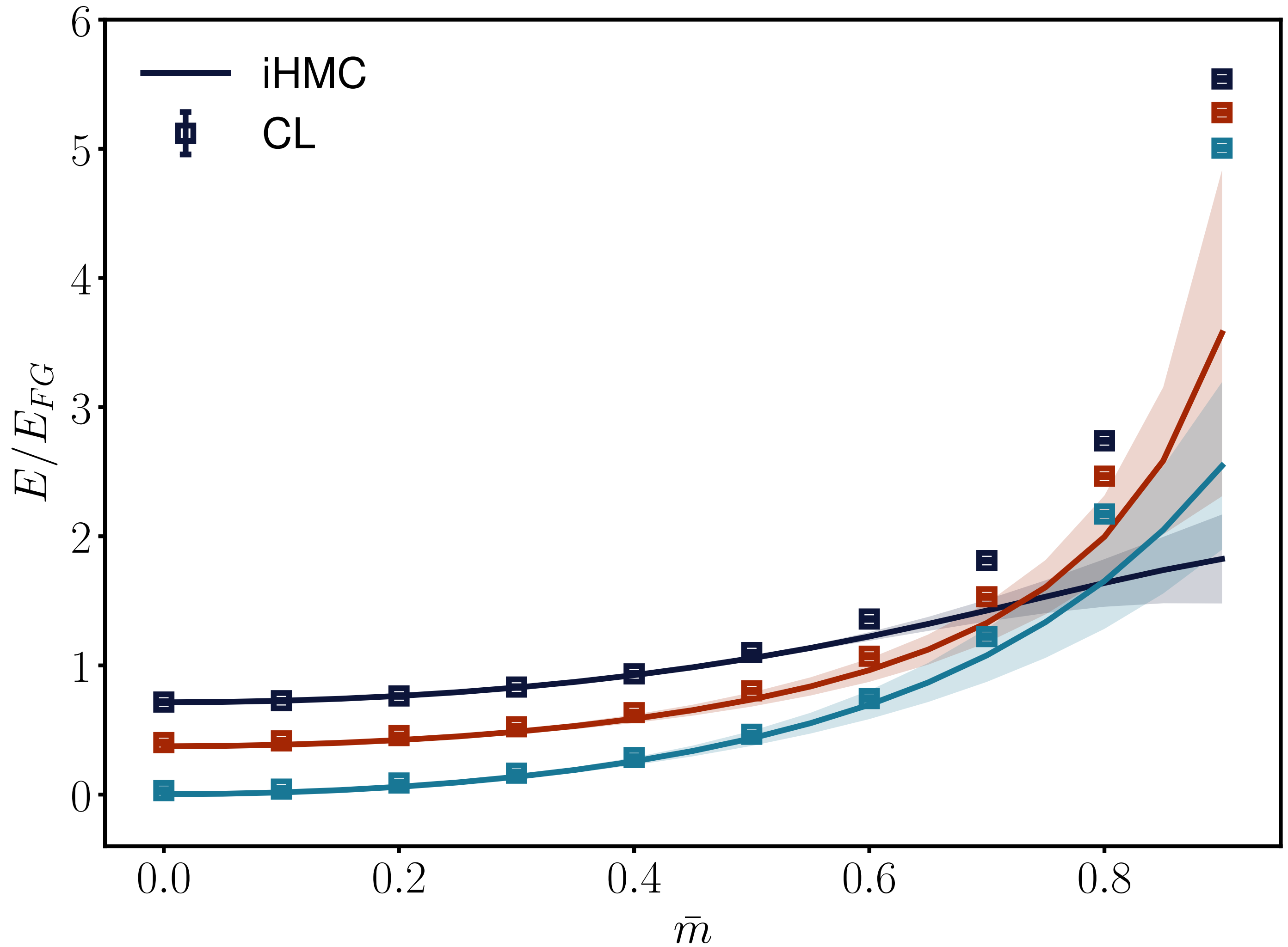
$$|\rho_2(x)| \sim |\cos(qx)| \,/\, x^\Delta$$

mass imbalance



mass-imbalanced 1D fermions: CL & iHMC

[LR, Porter, Drut, Braun '17]



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$\gamma = 1.0$

$\gamma = 1.4$

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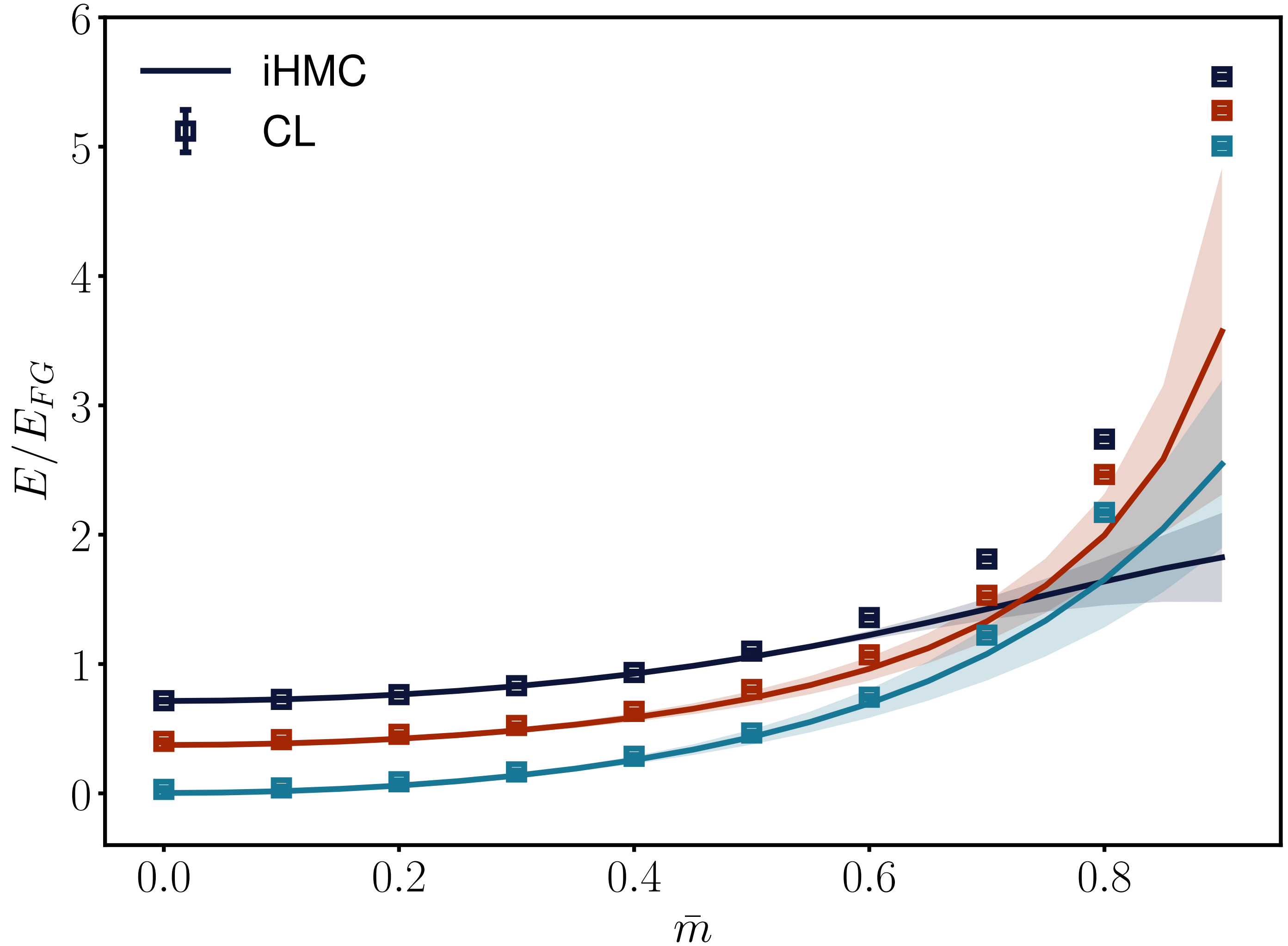
mass-imbalanced 1D fermions: CL & iHMC

[LR, Porter, Drut, Braun '17]

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



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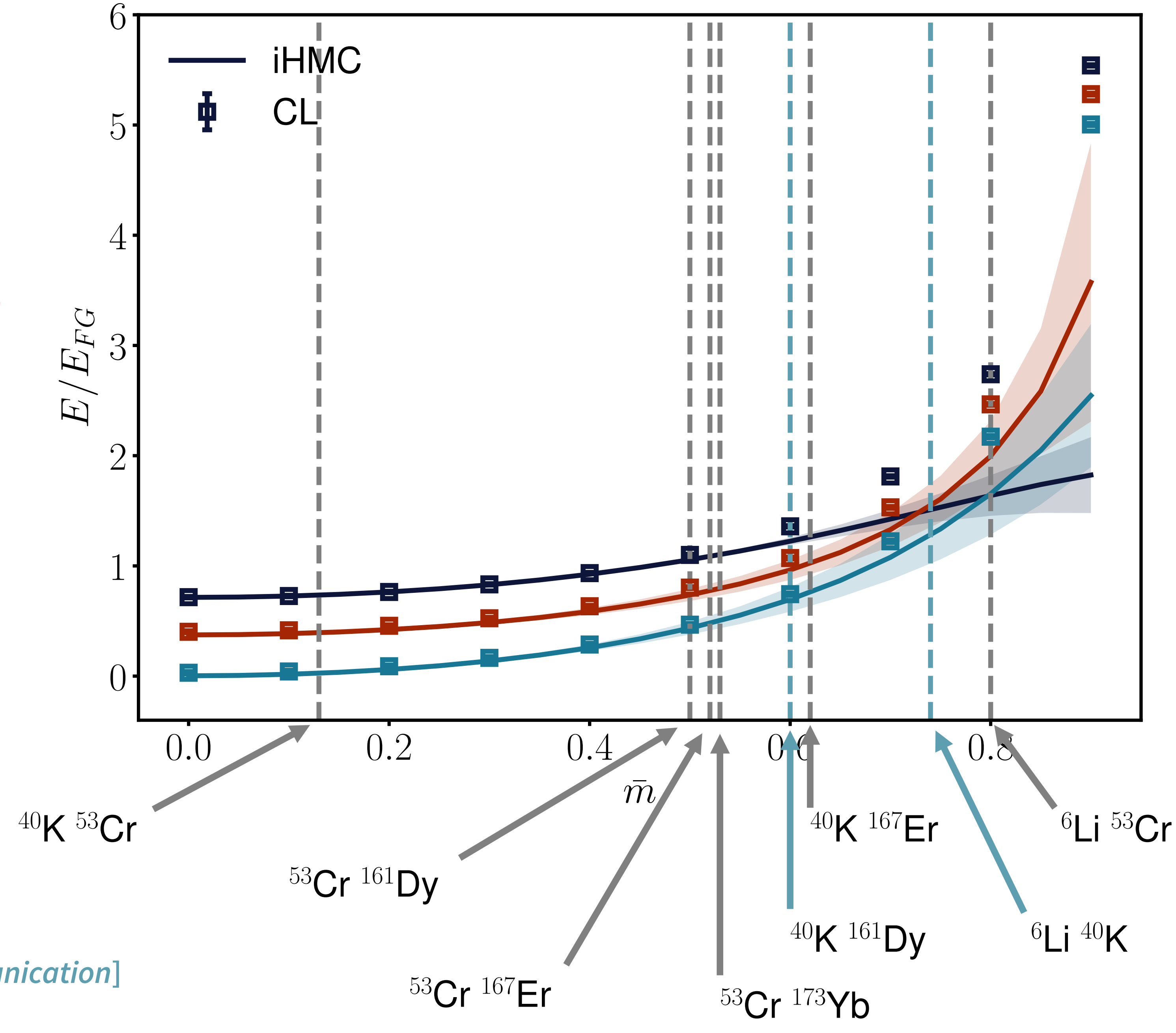


experimental mixtures accessible!

$\gamma = g/n$

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

[Grimm, *private communication*]

COMPLEX LANGEVIN IN 1D

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

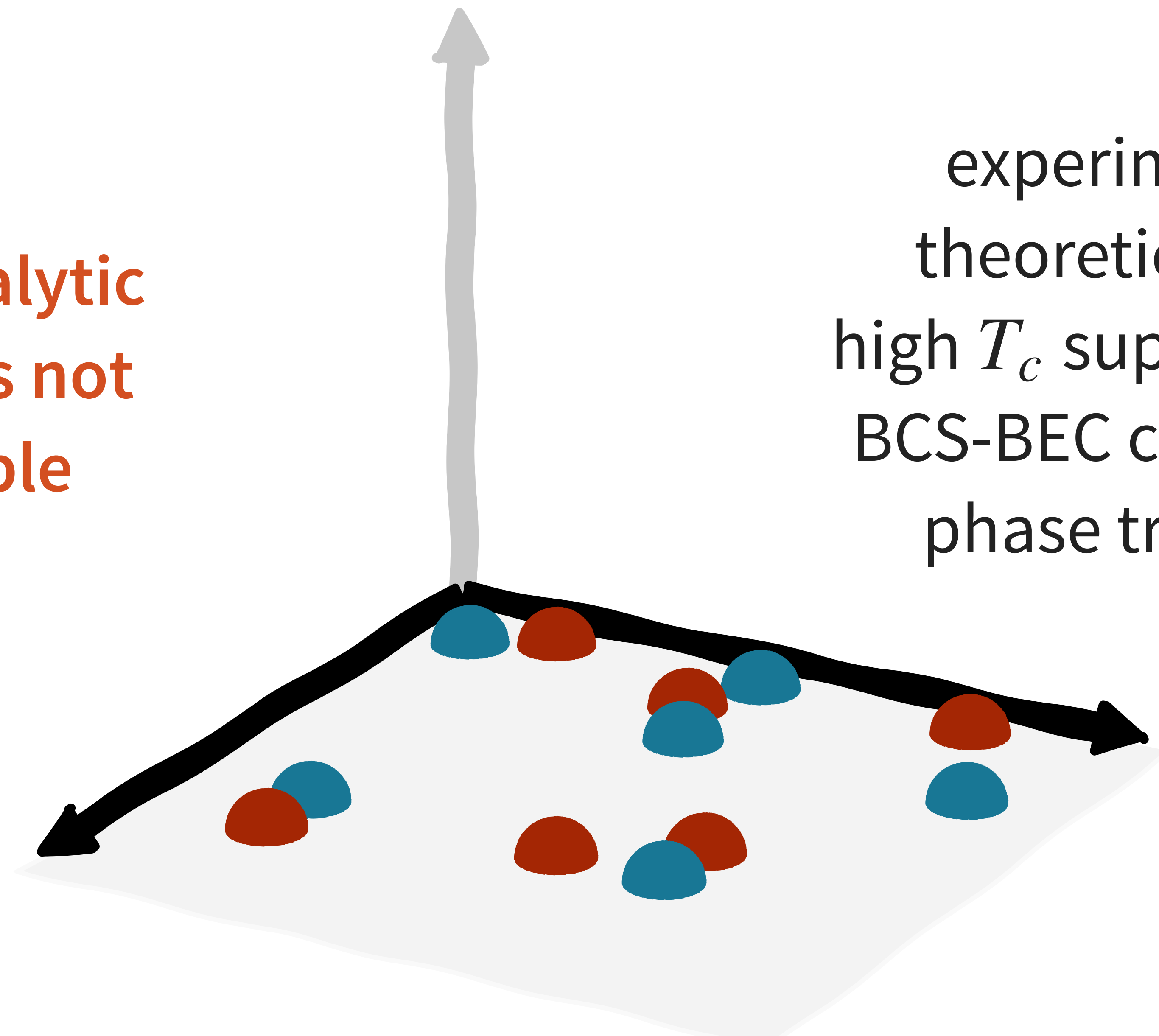
EOS of spin-imbalanced systems in agreement with perturbation theory

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

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

two-dimensional systems

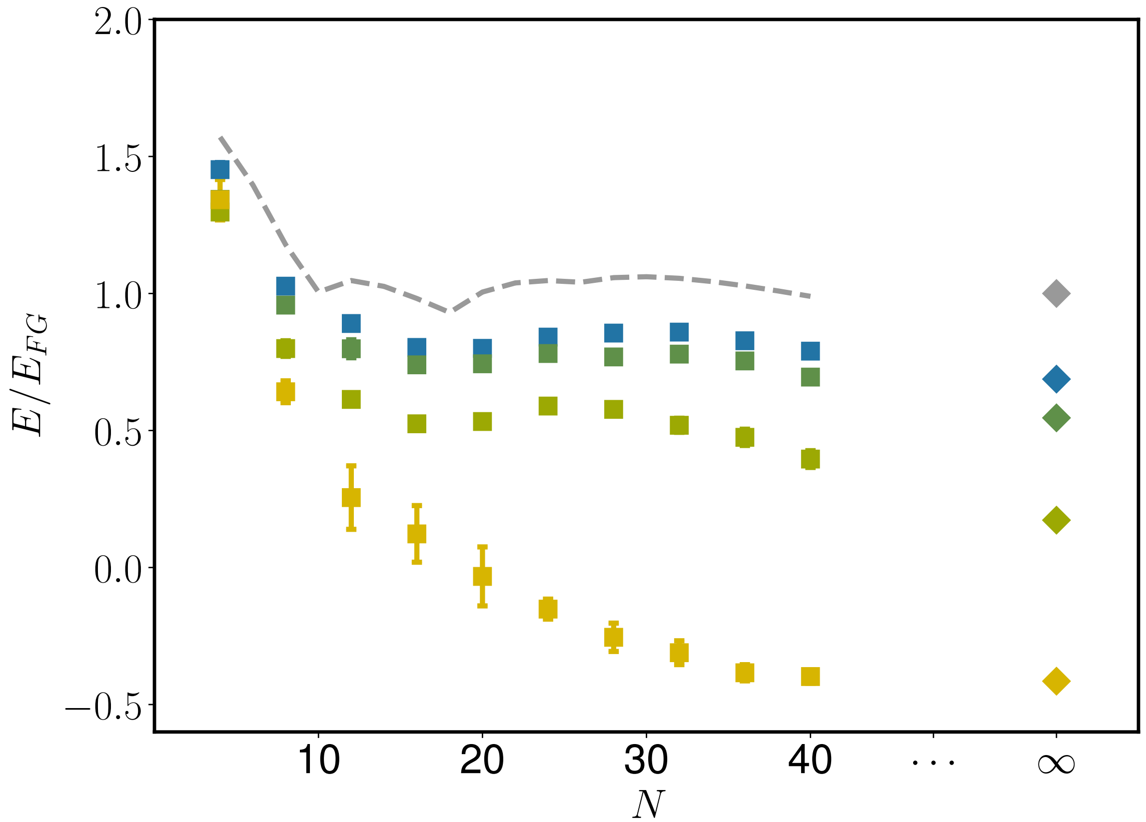
exact analytic solutions not available



experimental and theoretical interest: high T_c superconductors, BCS-BEC crossover, BKT phase transition, ...

2D ground state: from few to many body

[LR, Porter, Drut '16]



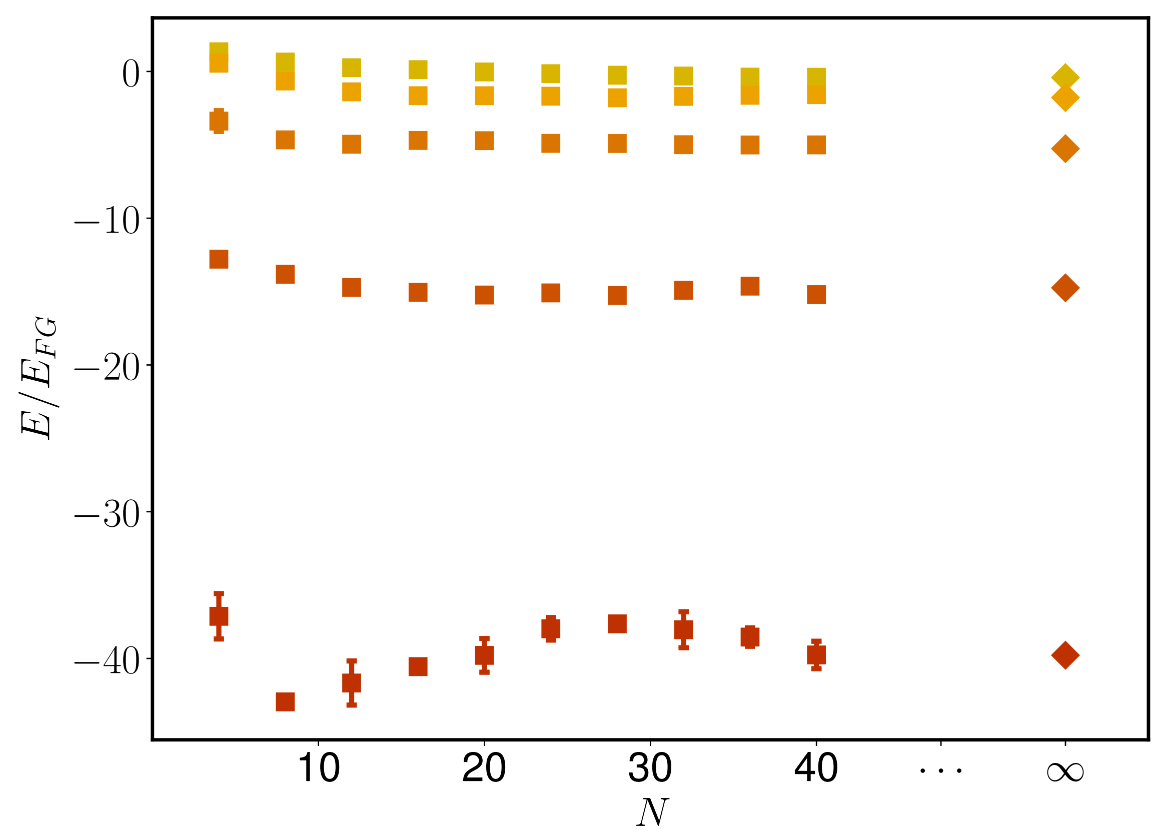
$$\eta = \ln(k_F a)$$

$\eta = \infty$ $\eta = 3.0$ $\eta = 2.0$

$\eta = 1.0$ $\eta = 0.5$ $\eta = 0.0$

$\eta = -0.5$ $\eta = -1.0$ $\eta = -1.5$

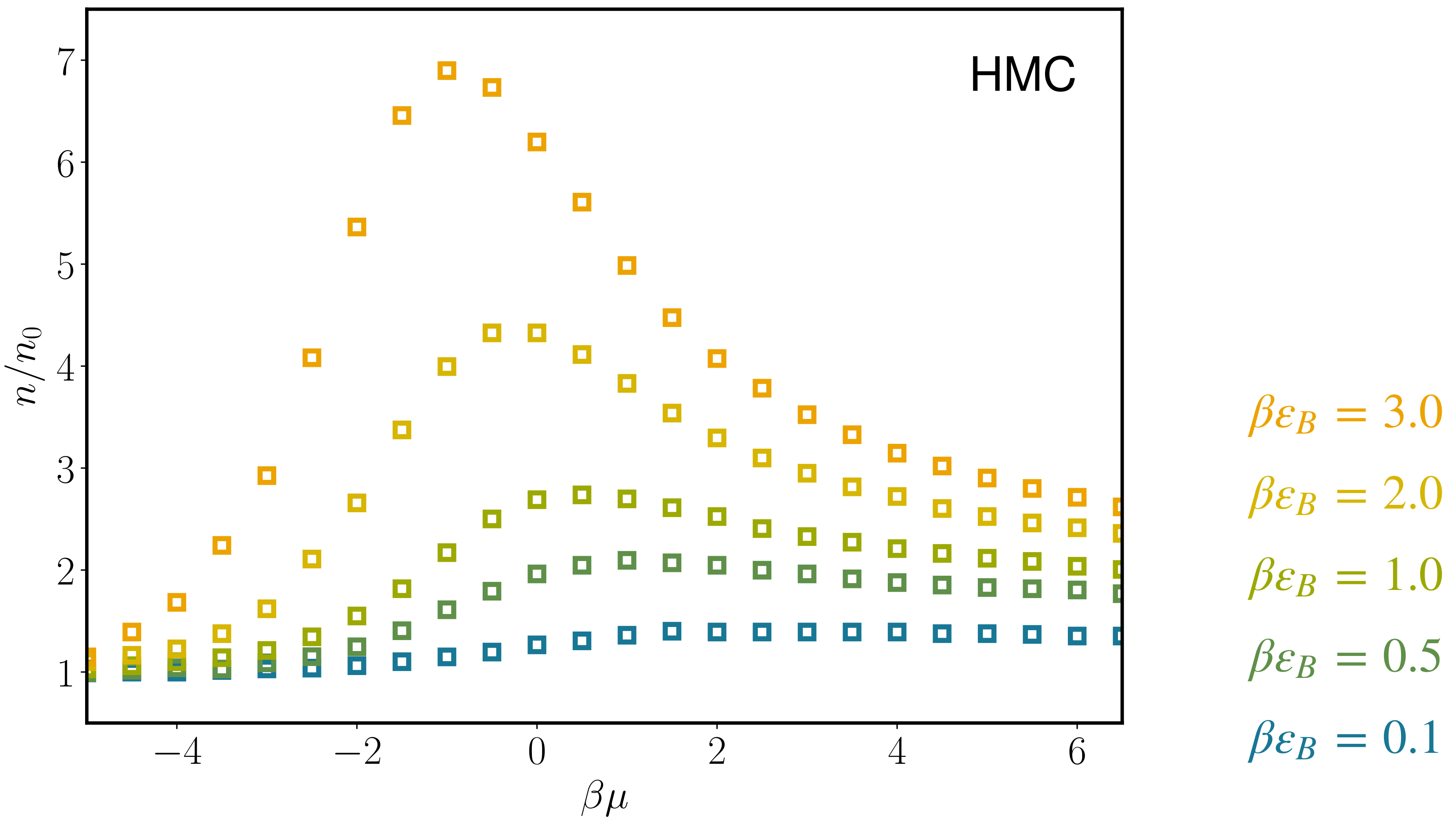
strongly coupled BEC regime
dominated by binding energy ε_B



[TL values: Bertaina, Giorgini '12]

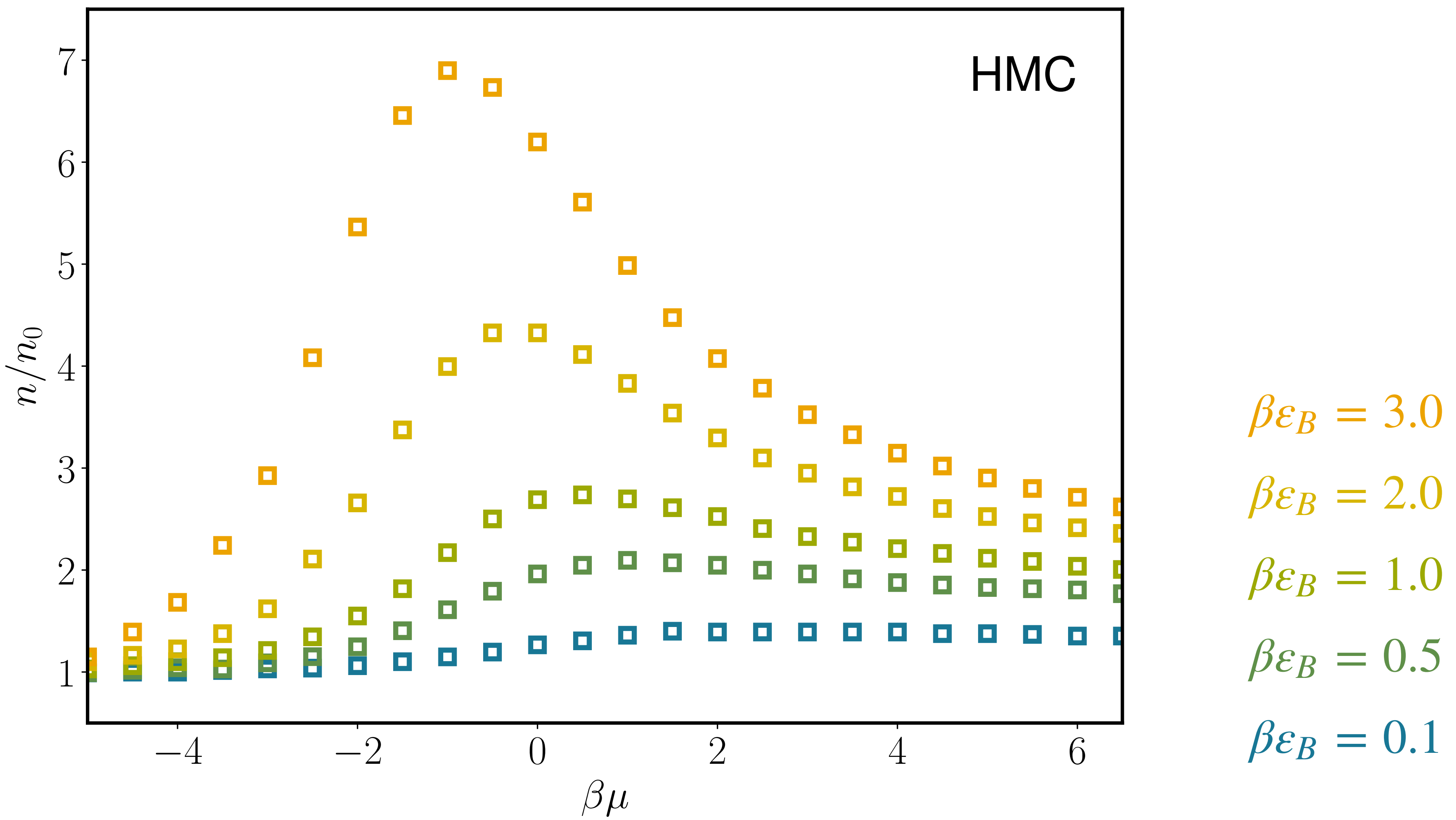
2D at finite T: equation of state

[Anderson, Drut '15]



2D at finite T: equation of state

[Anderson, Drut '15]

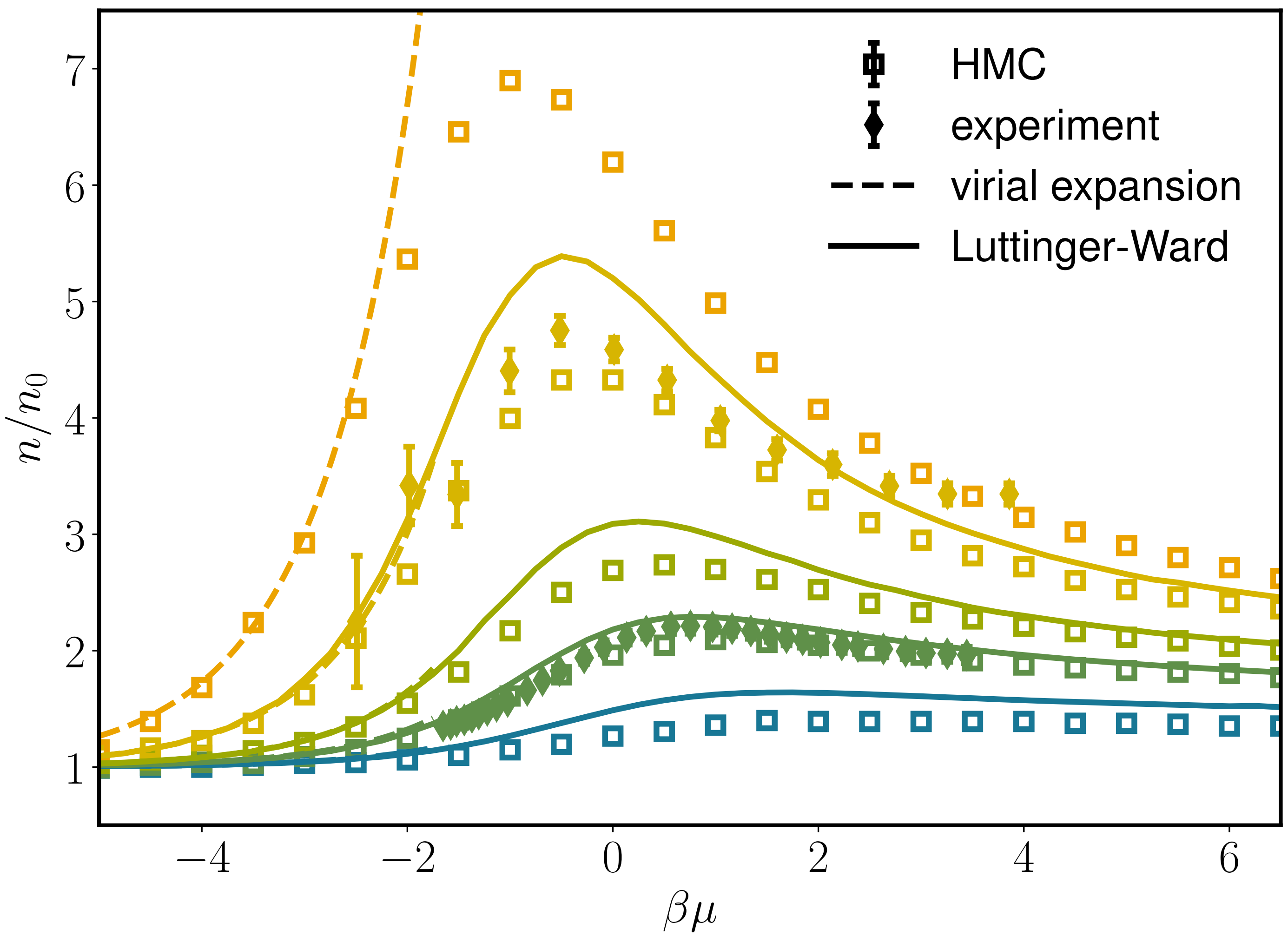


classical regime:
$k_B T$ dominates

quantum regime:
E_F dominates

2D at finite T: equation of state

[Anderson, Drut '15]



$\beta\varepsilon_B = 3.0$
$\beta\varepsilon_B = 2.0$
$\beta\varepsilon_B = 1.0$
$\beta\varepsilon_B = 0.5$
$\beta\varepsilon_B = 0.1$

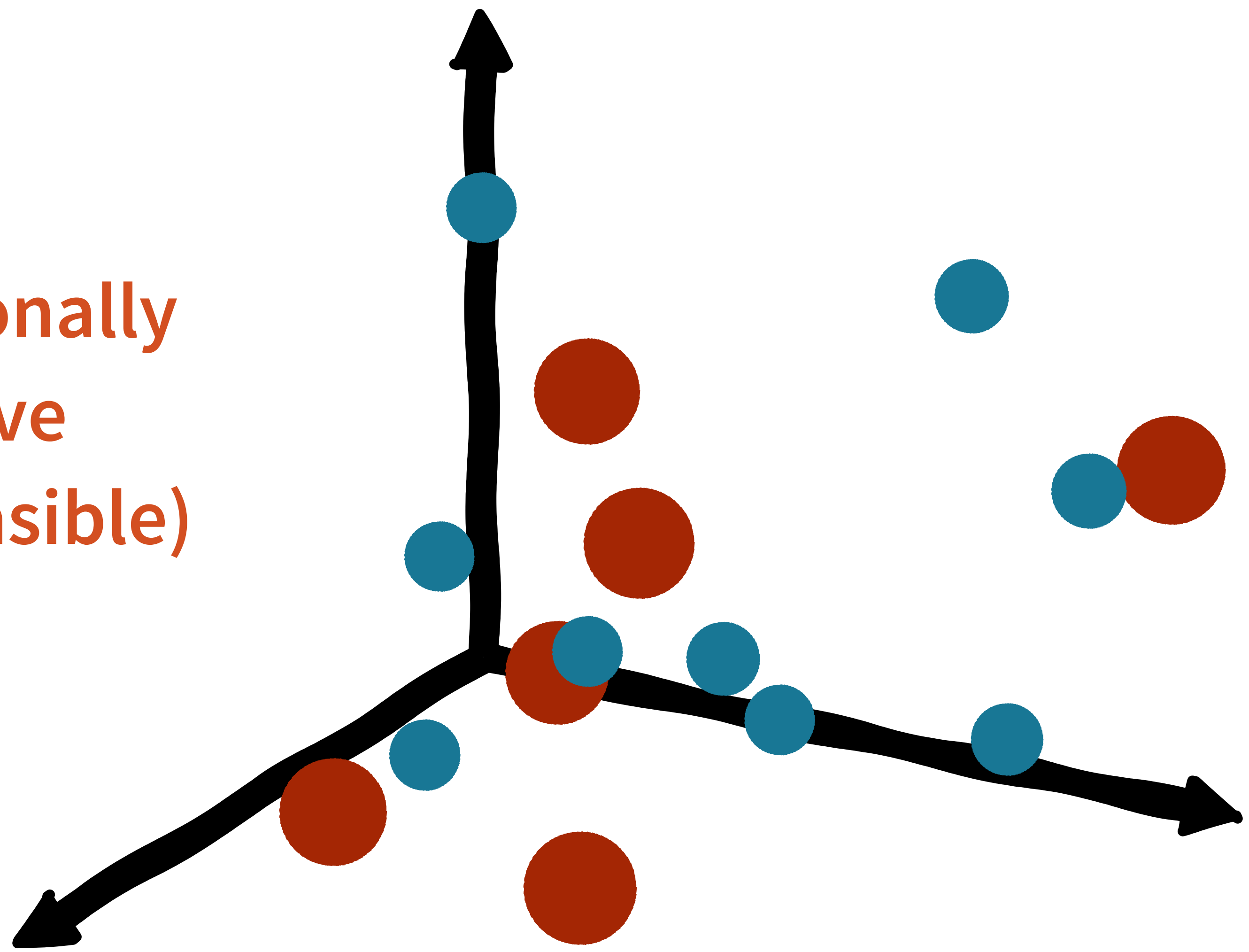
virial expansion:

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

[experiment: Fenech et al. '16; Boettcher et al. '16]
[LW: Bauer, Parish, Enss '14]

three-dimensional systems

computationally
expensive
(but still feasible)

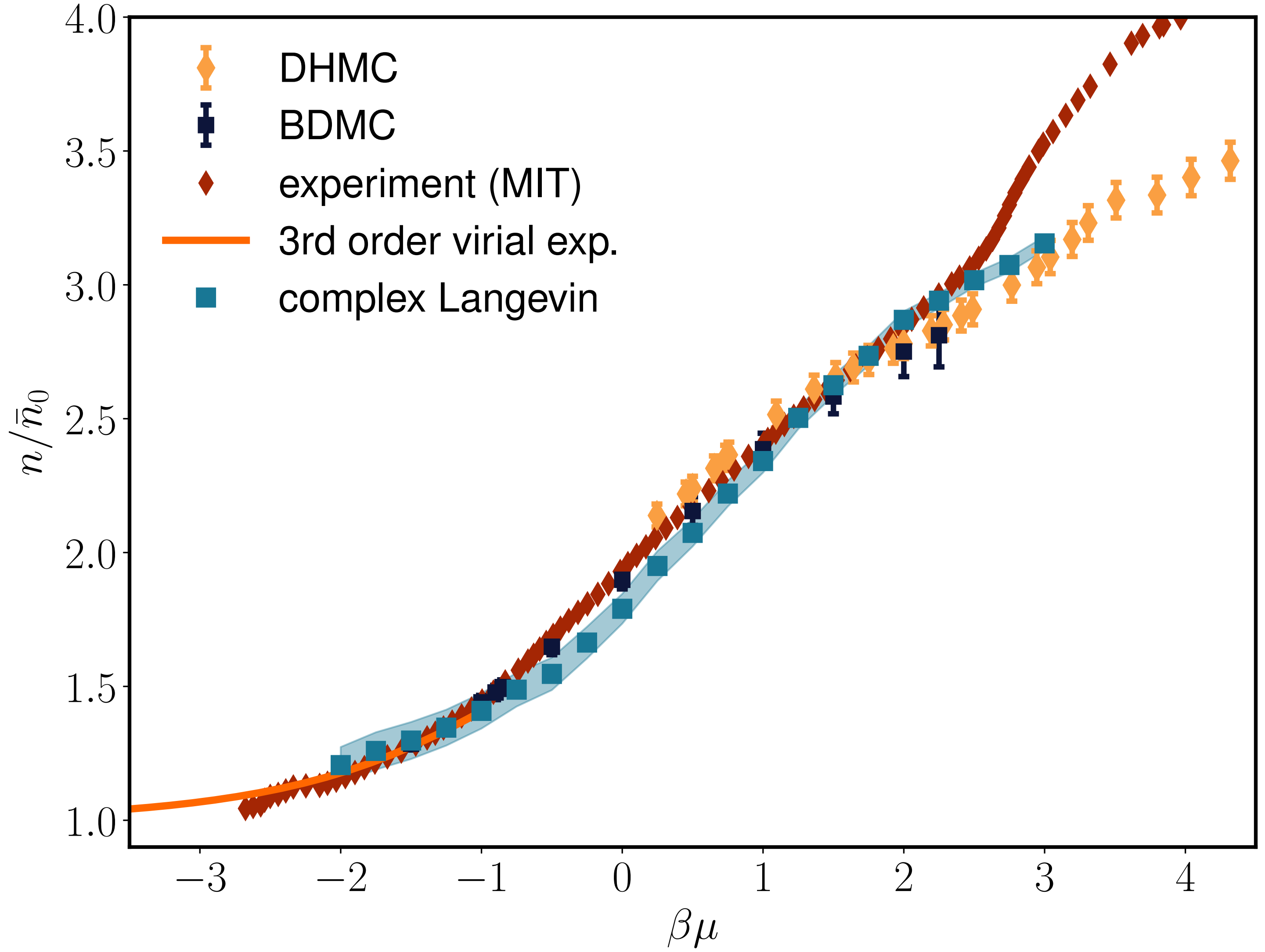


particularly interesting:

UNITARY FERMI GAS (UFG)

UFG at finite T: equation of state

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

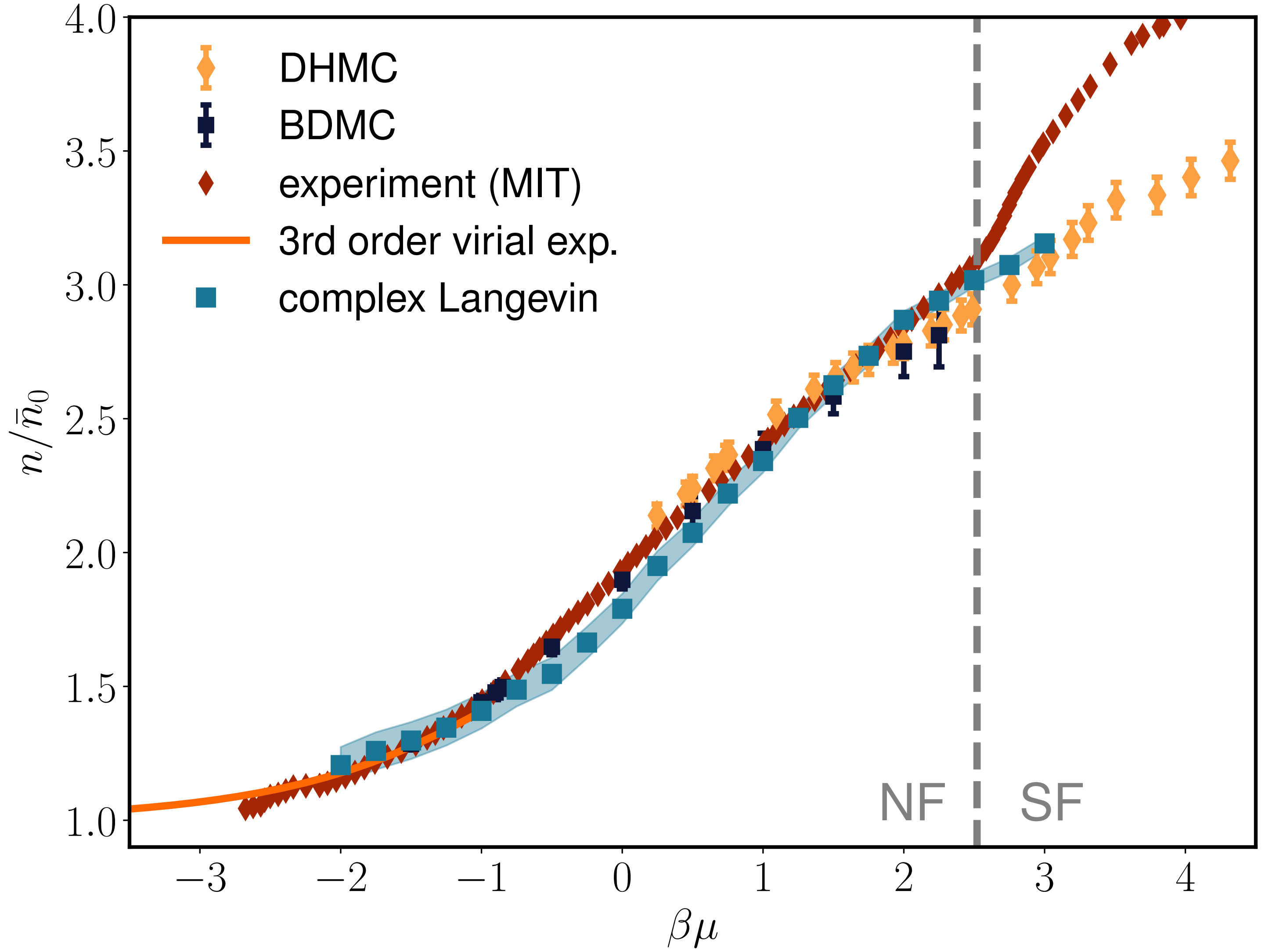


[experiment/BDMC: van Houcke et al. '12]
[DHMC: Drut, Lähde, Wlazlowski, Magierski '12]

UFG at finite T: equation of state

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

$T_C \sim 0.17\, T_F$



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UFG at finite T: equation of state

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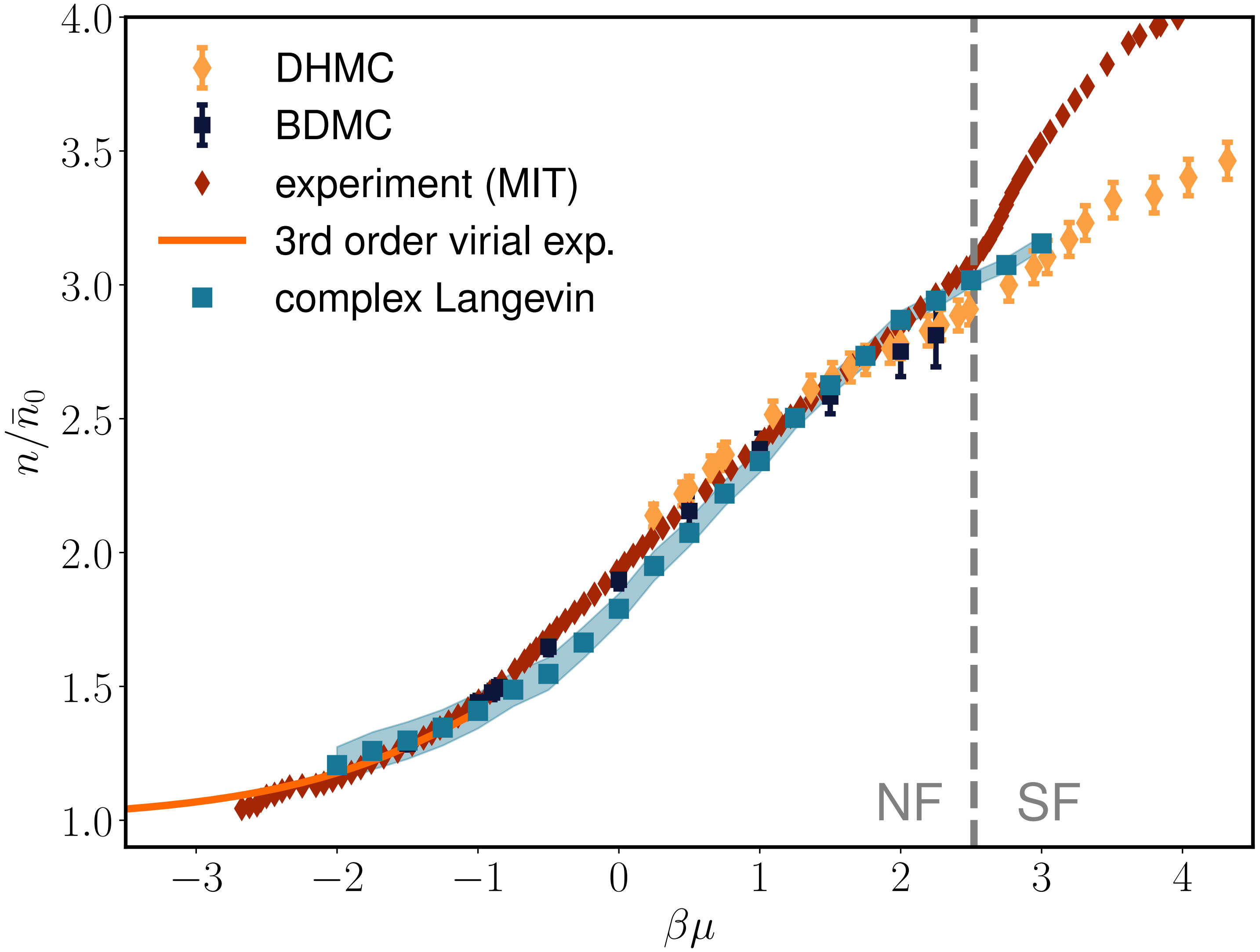


CL results:
finite lattice!
$(V = 9^3)$

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

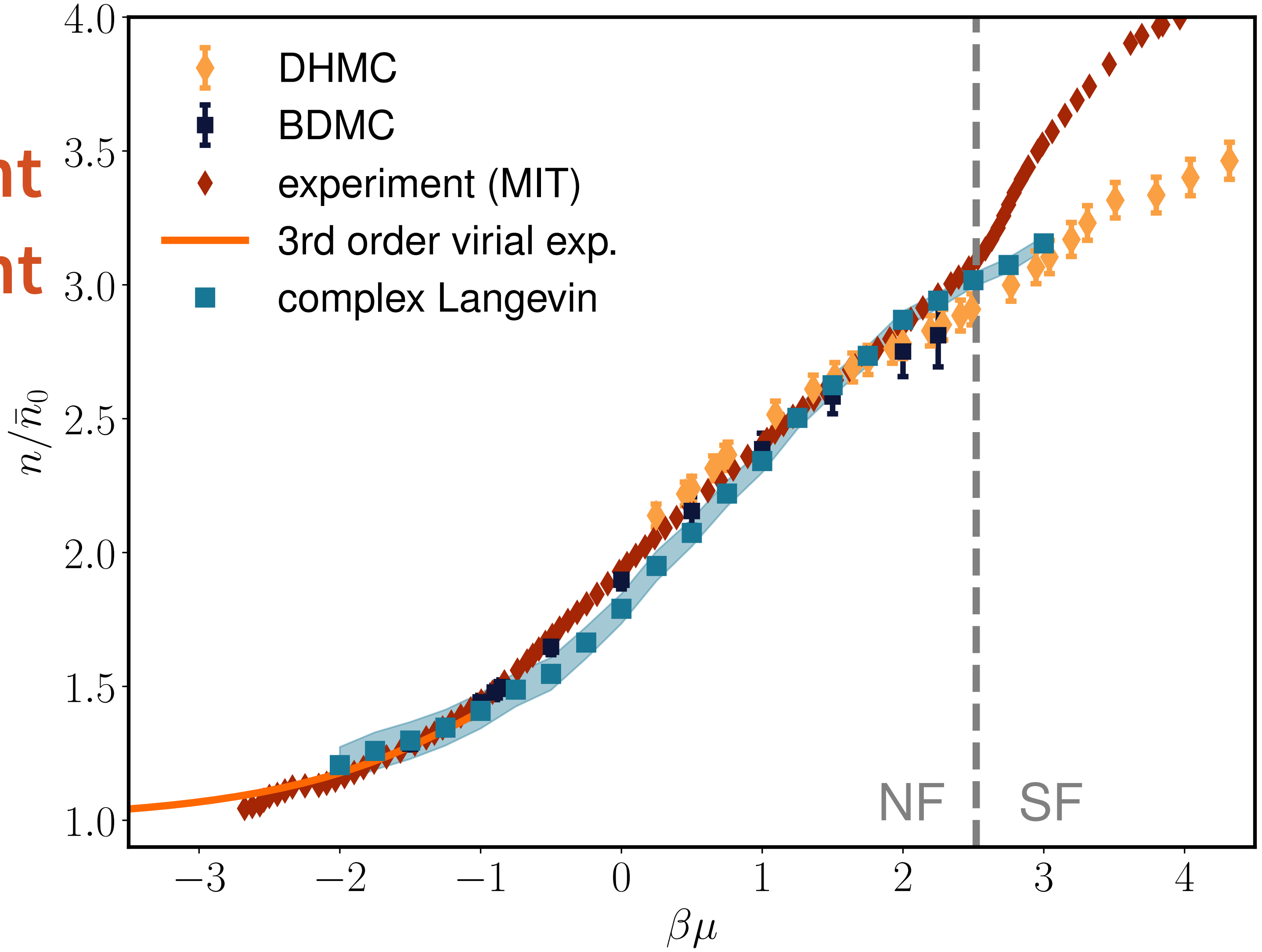
[experiment/BDMC: van Houcke et al. '12]
[DHMC: Drut, Lähde, Wlazlowski, Magierski '12]

UFG at finite T: equation of state

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

$T_C \sim 0.17\,T_F$

good agreement with experiment and other methods!



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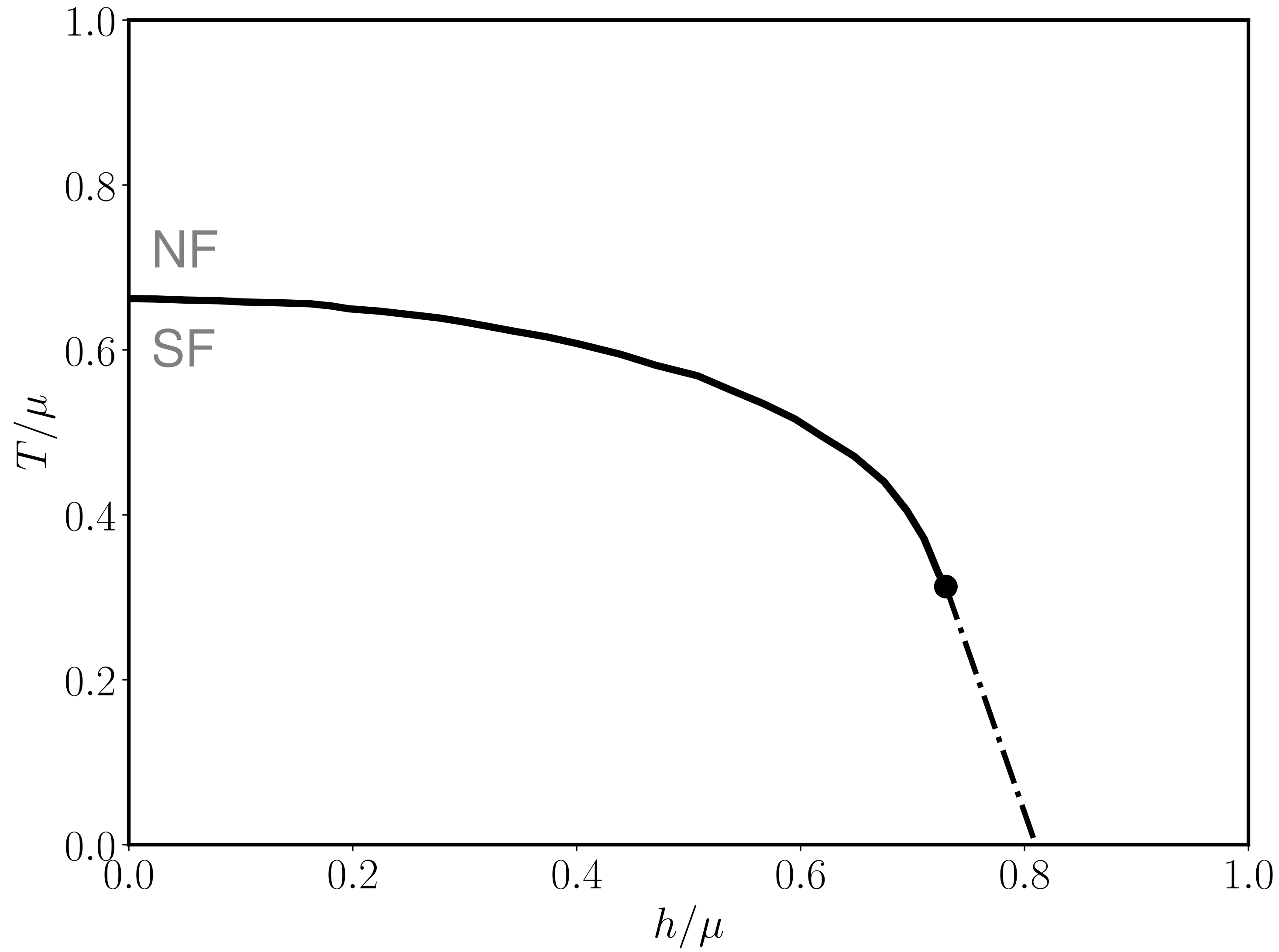
[experiment/BDMC: van Houcke et al. '12]
[DHMC: Drut, Lähde, Wlazlowski, Magierski '12]

UFG at finite T: phase diagram (mean field)

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

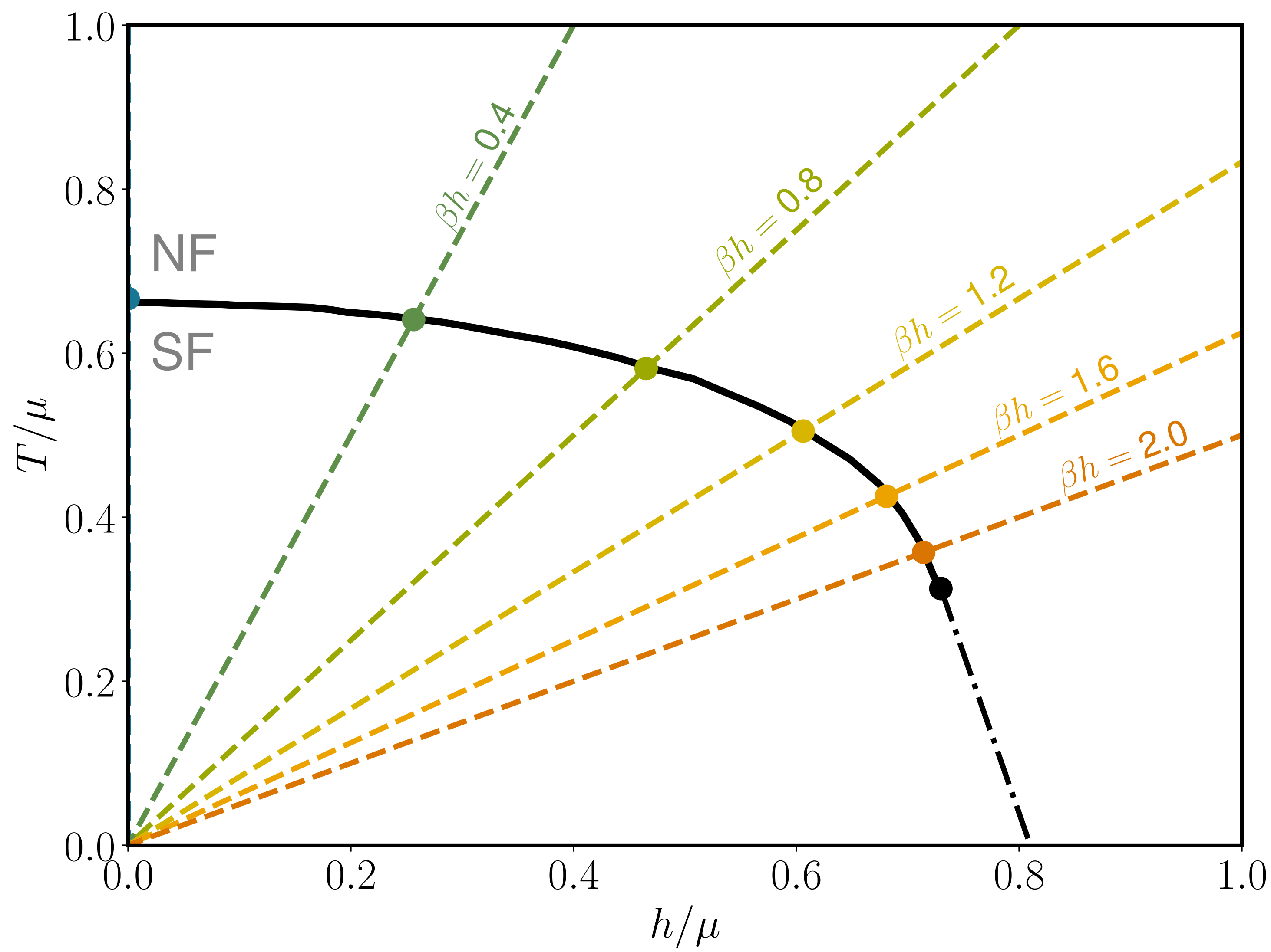


$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

[mean-field phase diagram: e.g. Chevy, Mora '10; Braun et al. '13]
[beyond mean-field:: e.g. Boettcher et al. '14; Roscher, Braun, Drut '15]

UFG at finite T: phase diagram (mean field)

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



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

[mean-field phase diagram: e.g. Chevy, Mora '10; Braun et al. '13]
[beyond mean-field:: e.g. Boettcher et al. '14; Roscher, Braun, Drut '15]

UFG at finite T: equation of state

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

$\beta h = 2.0$

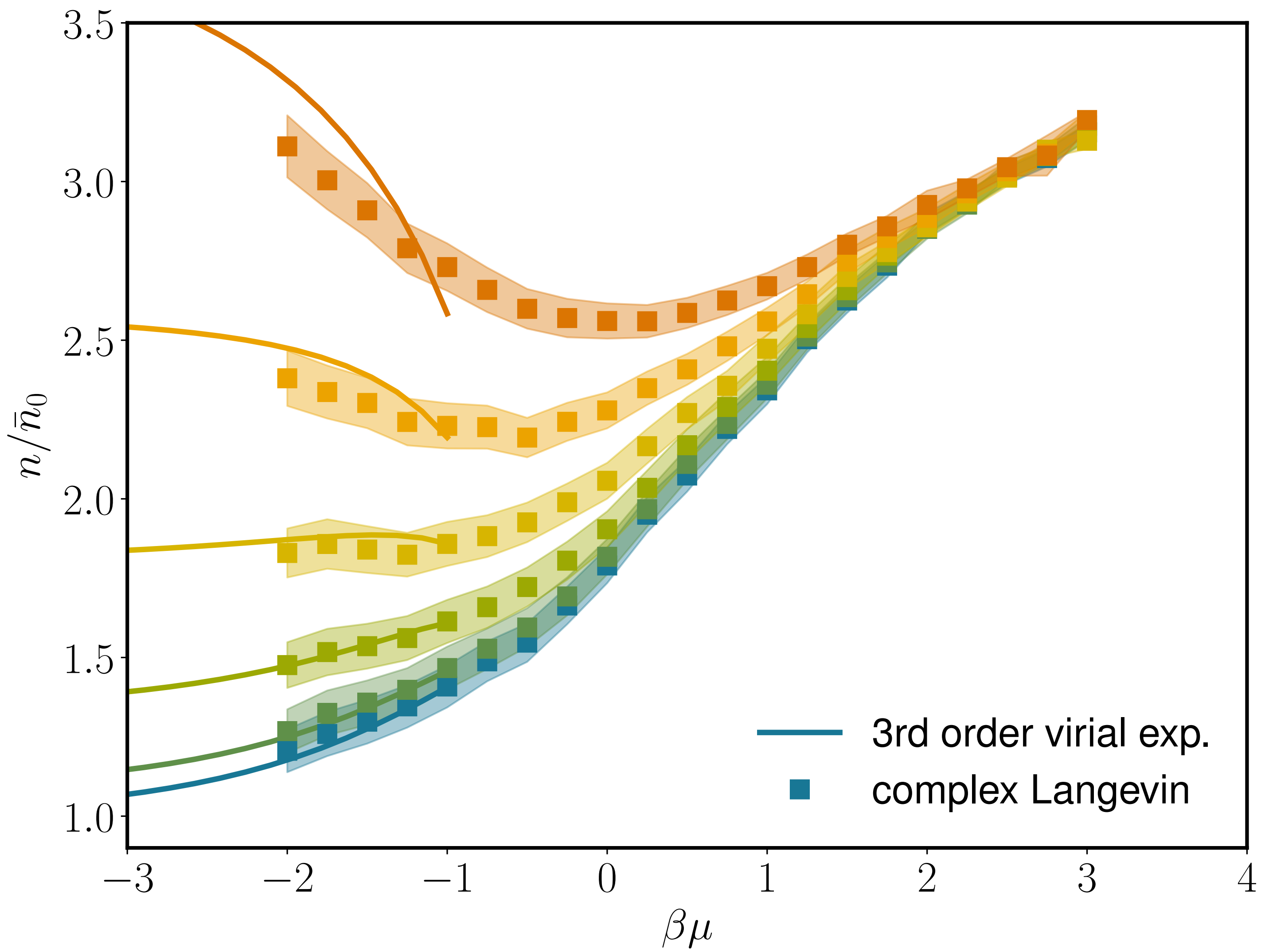
$\beta h = 1.6$

$\beta h = 1.2$

$\beta h = 0.8$

$\beta h = 0.4$

$\beta h = 0.0$



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

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

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 $T > 0$

WHERE TO GO?

investigation of **pair correlations in $d > 1$**

mass imbalance at finite temperature

search for inhomogeneous phases in 2D/3D

ultimately: **phase diagram for mass- and spin-imbalanced 2D and 3D fermions**