STOCHASTIC QUANTIZATION AND SPIN-POLARIZED FERMI GASES

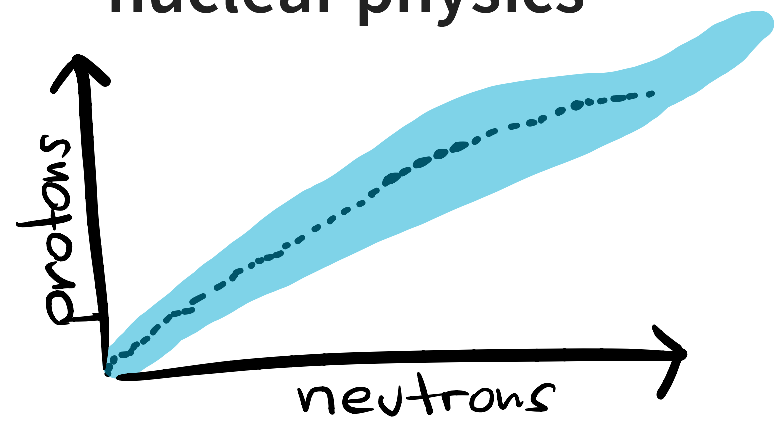
Lukas Rammelmüller, TU Darmstadt

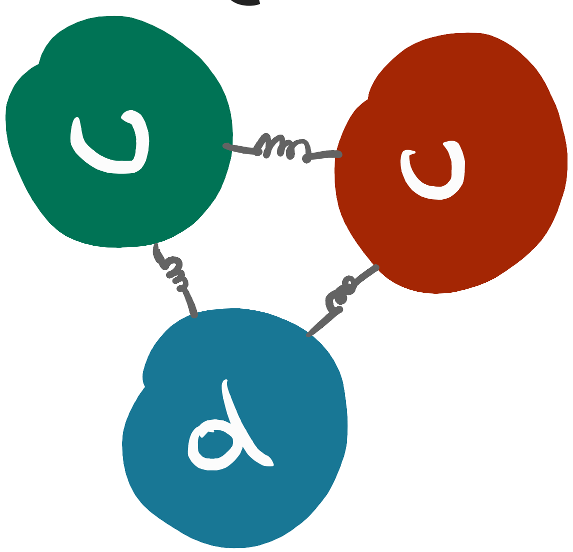
March 26, 2019

[LR, Drut, Braun *in preparation*]
[Berger, Loheac, LR, Ehmann, Braun, Drut *in preparation*]
[LR, Loheac, Drut, Braun *Phys. Rev. Lett.* 121, 173001, 2018]
[LR, Porter, Drut, Braun *Phys. Rev. D* 96, 094506, 2017]

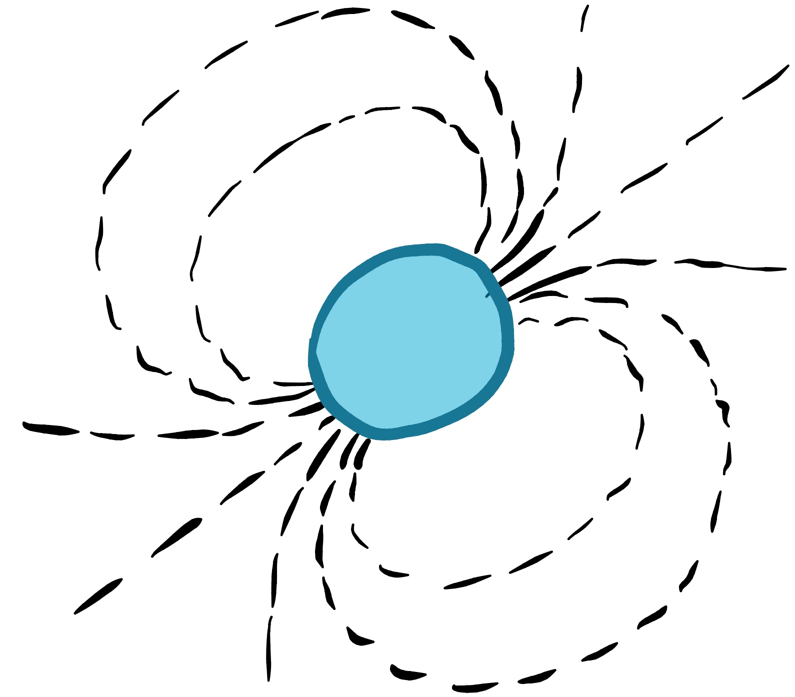
HGS-HIRe for FAIR
Helmholtz Graduate School for Hadron and Ion Research
Center for Scientific Computing Frankfurt
HIC for FAIR
Helmholtz International Center
TECHNISCHE UNIVERSITÄT DARMSTADT

nuclear physics



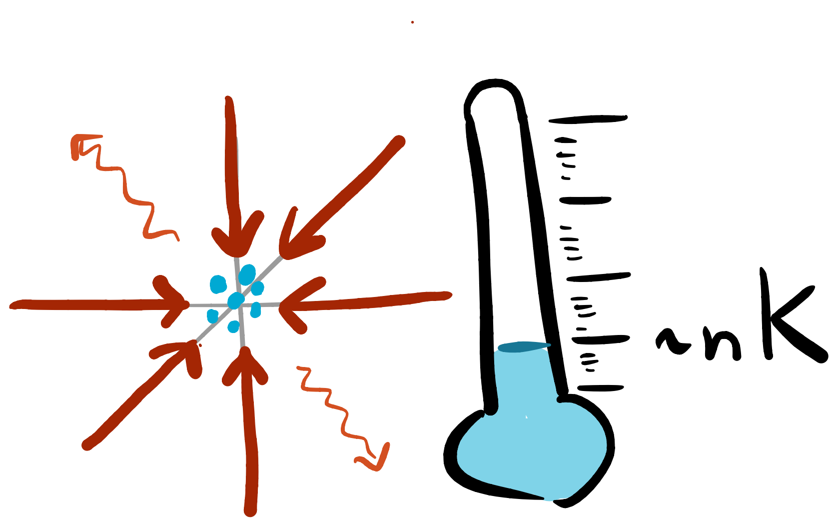


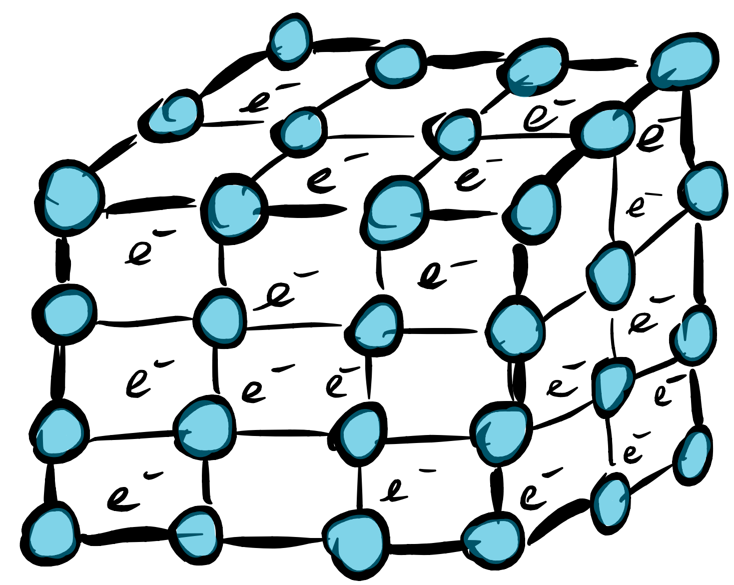
QCD

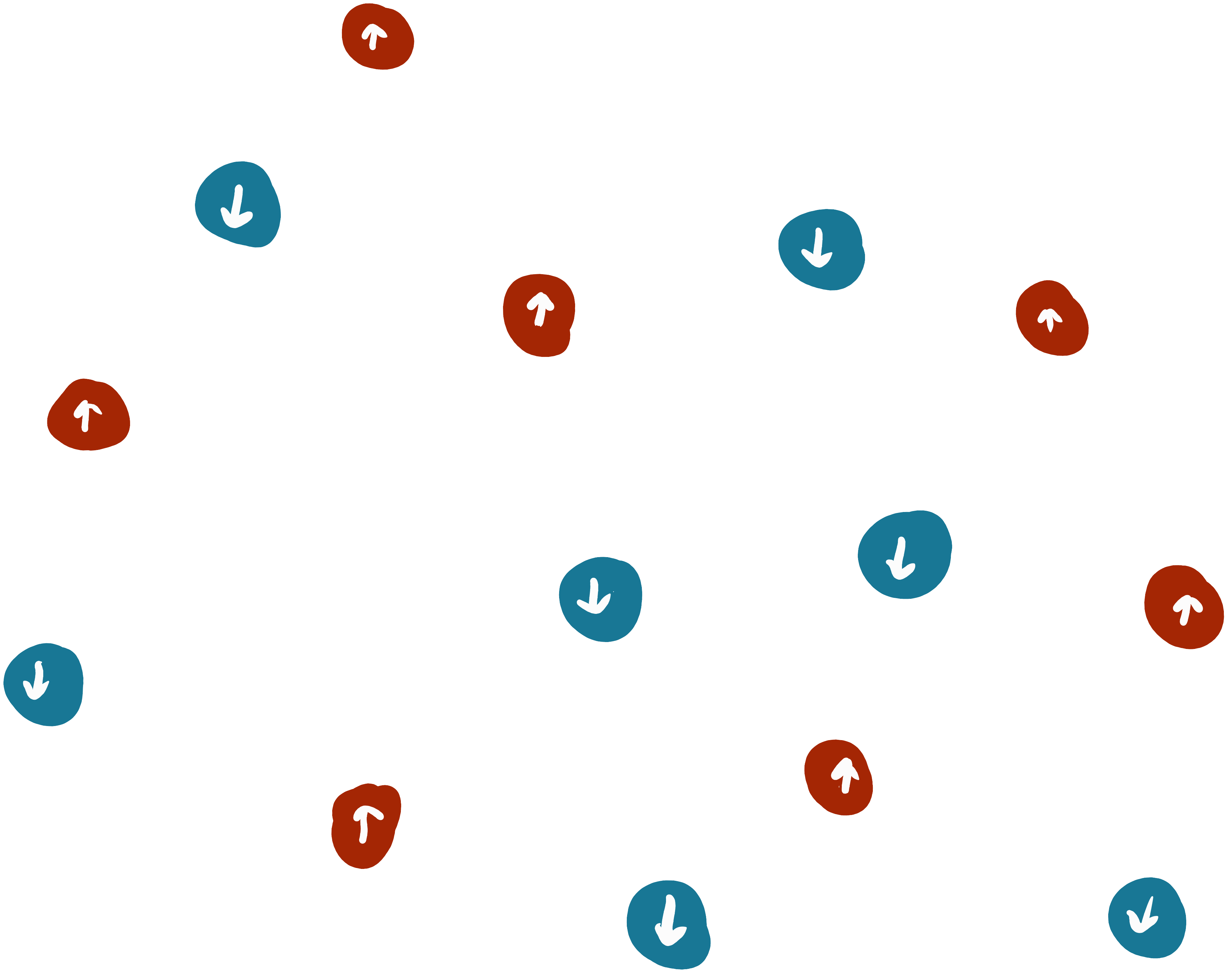


neutron stars

FERMI GASES ARE EVERYWHERE

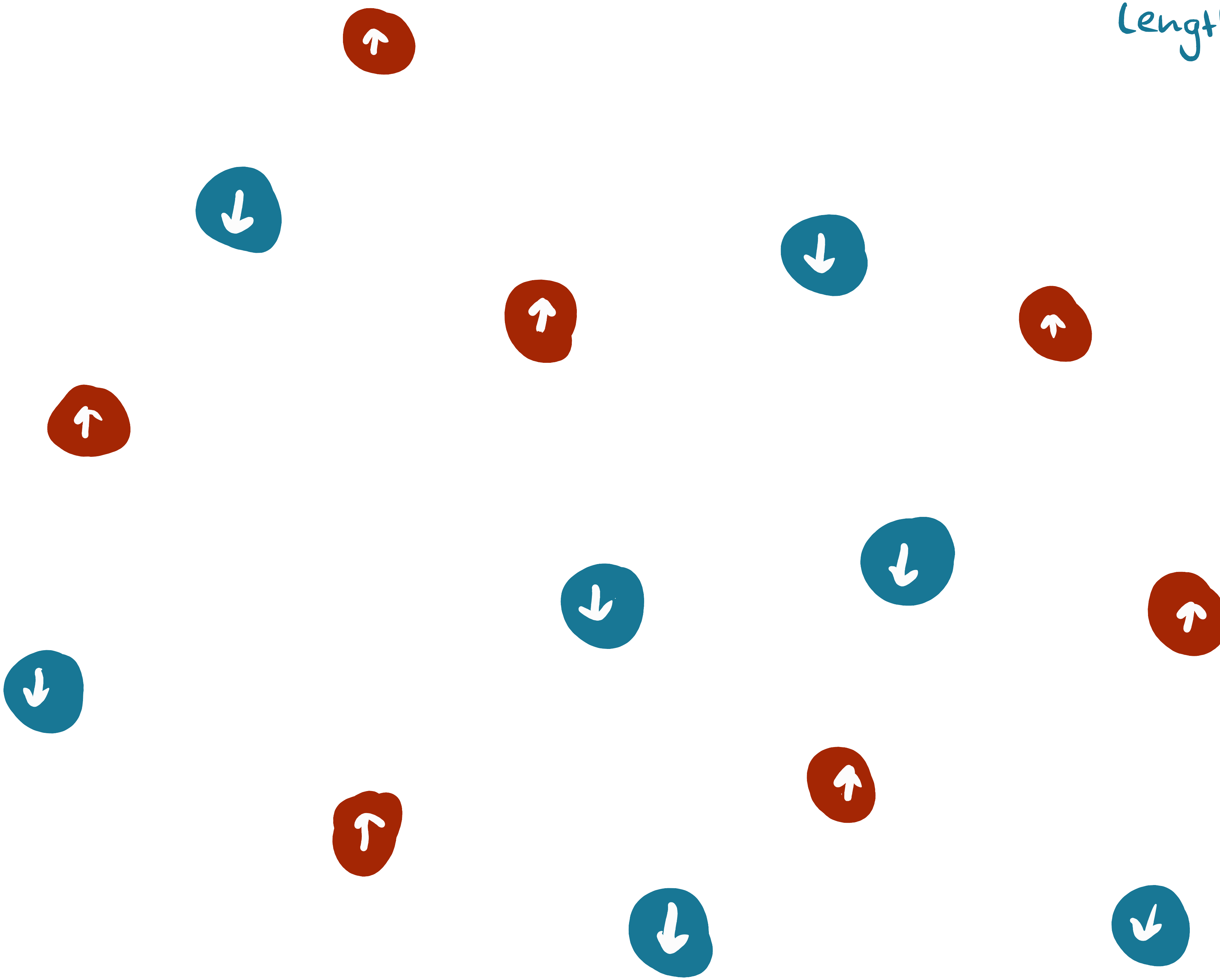


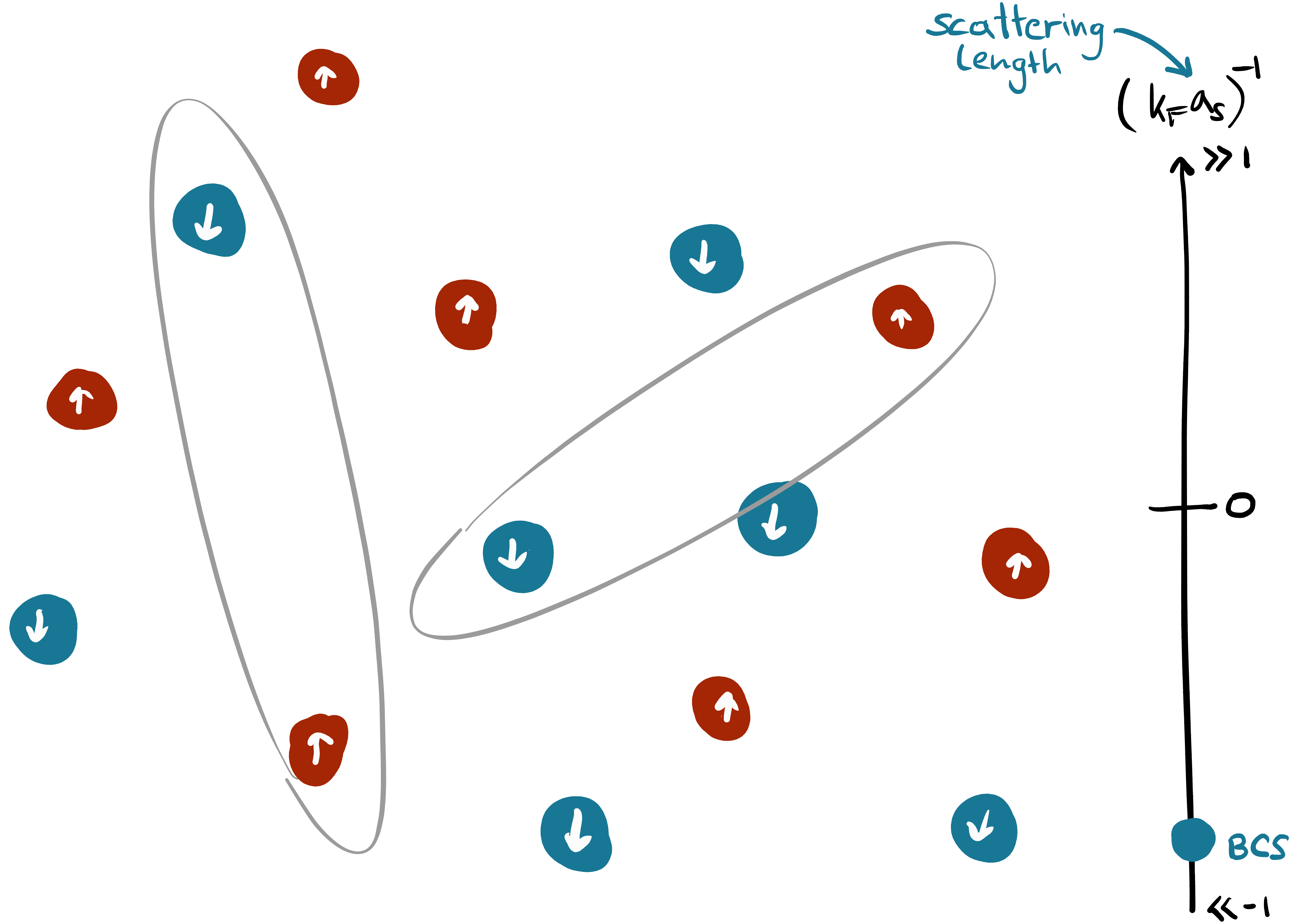




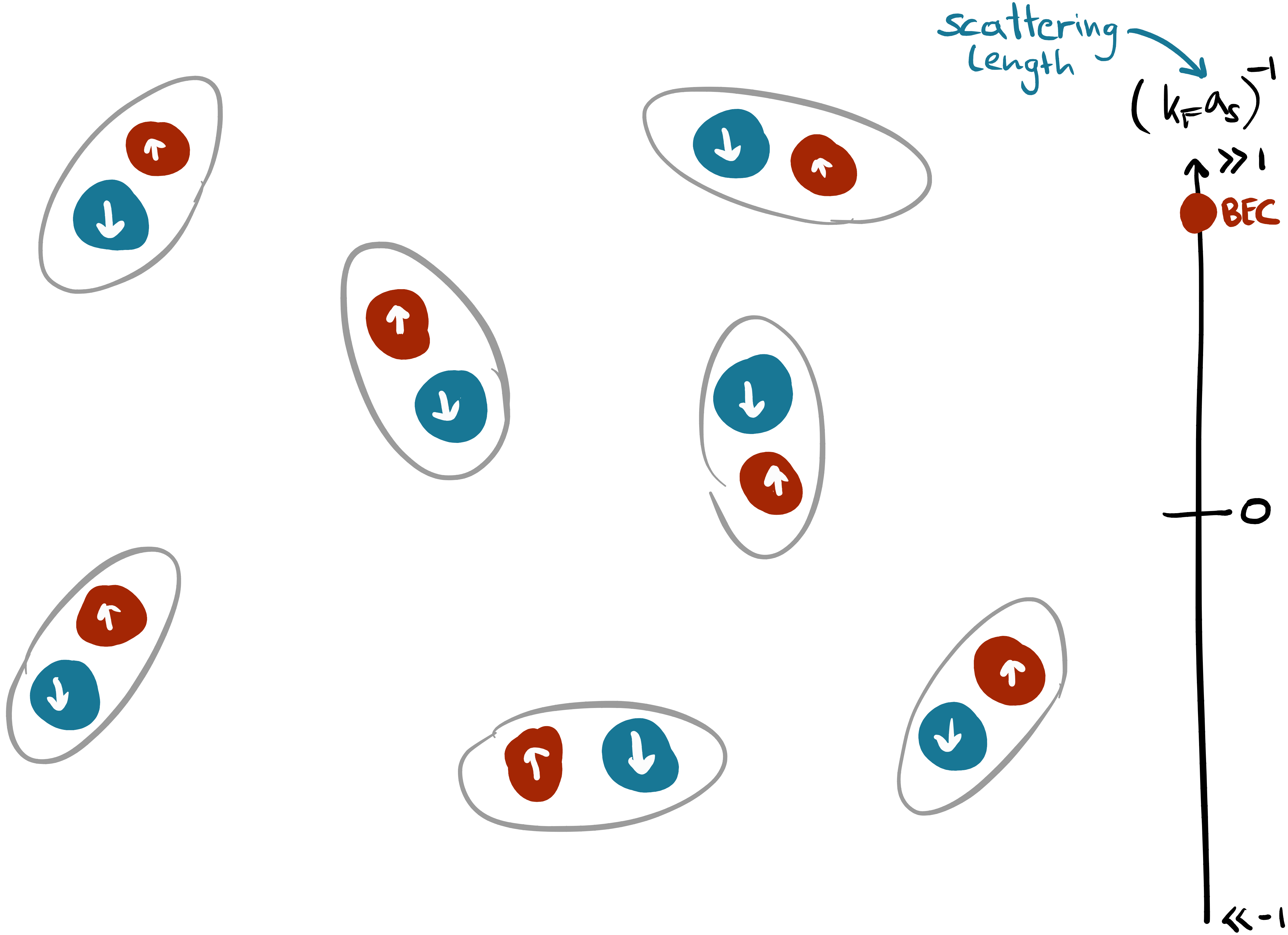
scattering length

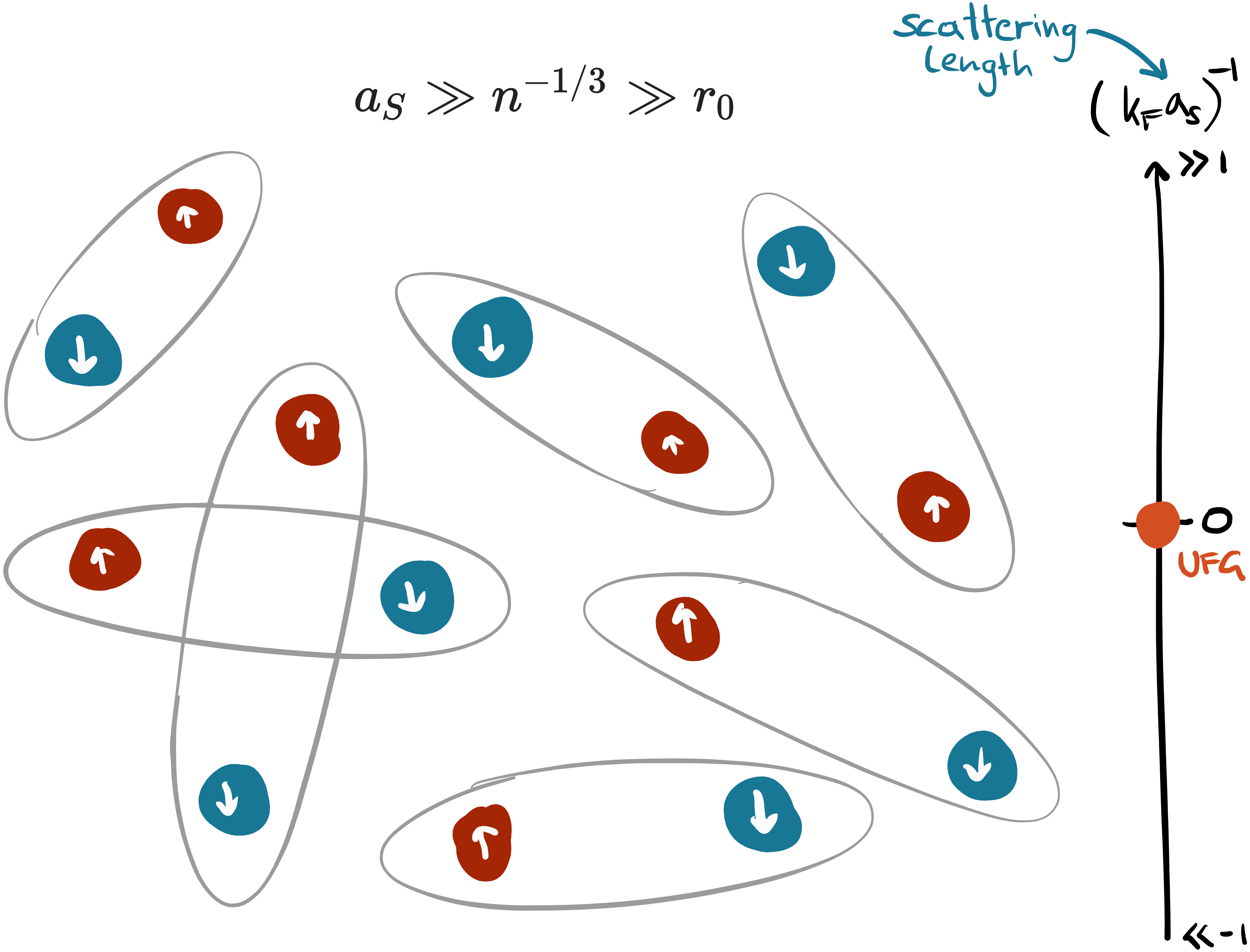
$$(k_F a_s)^{-1}$$





scattering length
$(k_F a_s)^{-1}$
$\gg 1$
0
BCS
$\ll -1$


scattering length
$(k_F a_s)^{-1}$
$\gg 1$
BEC
0
$\ll -1$



$a_S \gg n^{-1/3} \gg r_0$
scattering length
$(k_F a_s)^{-1}$
$\gg 1$
0
UFG
$\ll -1$

the unitary Fermi gas (UFG)

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

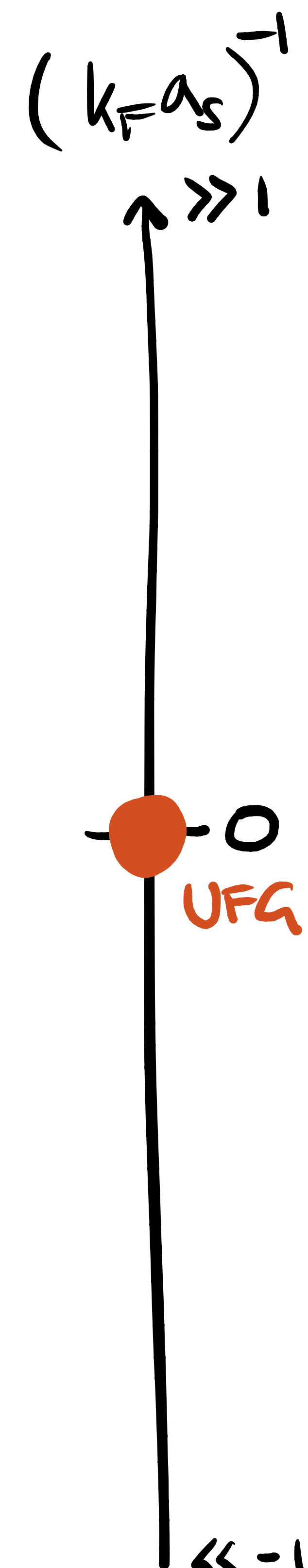
density & temperature are the only dimensionful scales in the system

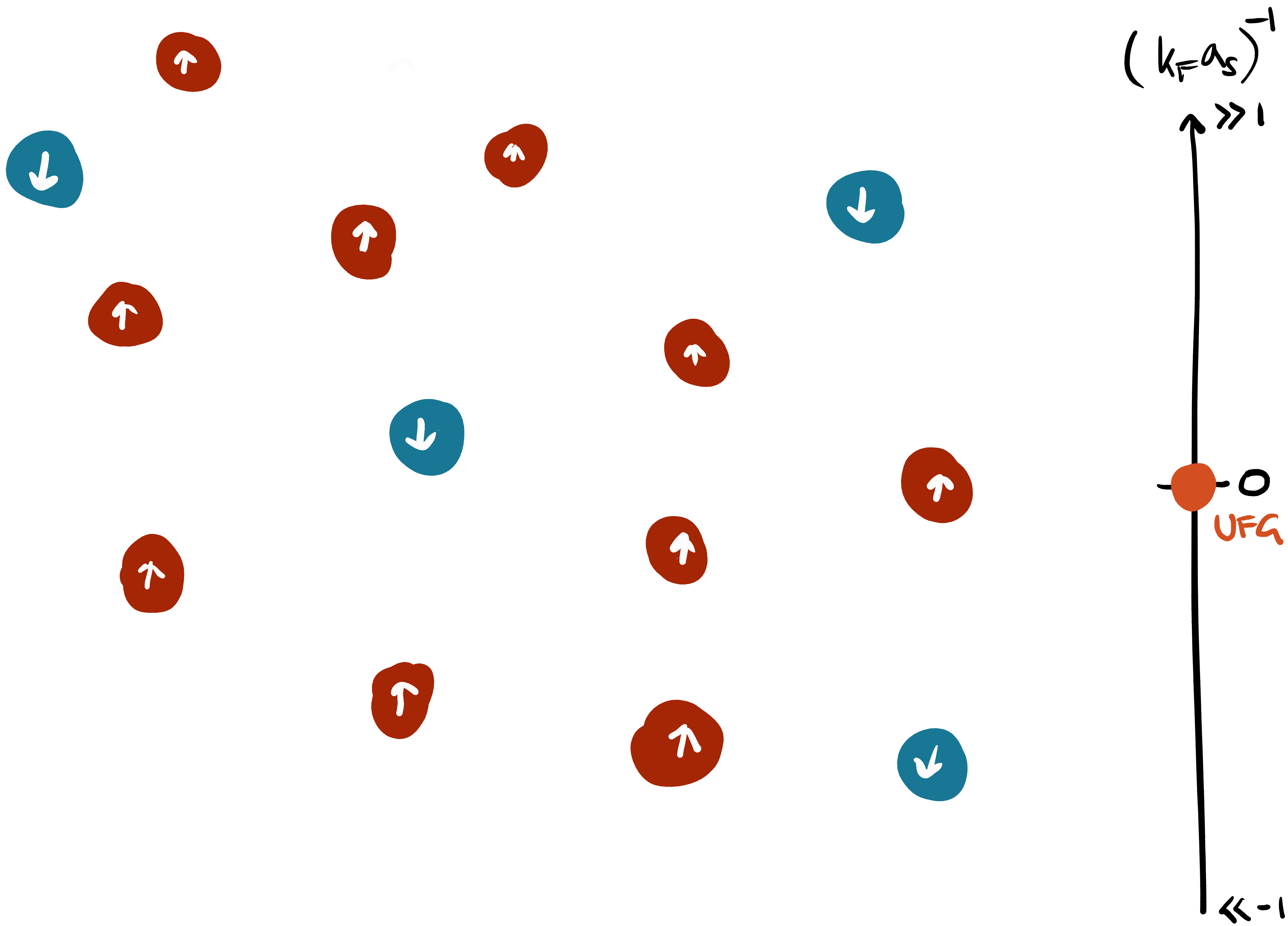
universal scaling functions:

$$
\begin{aligned}
E &= E_{FG}\; f_E(\beta\mu) \\
P &= P_{FG}\; f_P(\beta\mu) \\
&\cdots
\end{aligned}
$$

numerous experiments:

- first realizations of unitary fermions [Regal,Greiner,Jin '04; Zwierlein et al. '04; Kinast et al. '04]
- universal behavior & thermodynamics [Thomas,Kinast,Turpalov '05; Horikoshi et al. '10]
- temperature vs. polarization phase-diagram [Shin,Schunck,Schirotzek,Ketterle '08]
- measurement of equation of state [Nascimbène et al. '10; van Houcke et al. '12]
- superfluid transition [Ku,Sommer,Cheuck,Zwierlein '12]
- temperature dependence of Tan's contact [Carcy et al. '19; Mukherjee et al. '19]
- and many more...





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

THE PLAN

ab initio treatment of imbalanced Fermi gases

KEY QUESTIONS

how can we construct an efficient method
that can deal with those systems?

can we get the EOS for polarized Fermi gases?

how does T_C of the UFG change with polarization?

stochastic quantization

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

$$\mathcal{Z} = \int \mathcal{D}\phi \, e^{-S[\phi]}$$

(partition function)

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

(expectation values)

$$P[\phi] = \frac{1}{\mathcal{Z}} e^{-S[\phi]}$$

(probability measure)

stochastic quantization

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

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(probability measure)

KEY IDEA:

probability measure of a **d-dimensional Euclidean path integral** as equilibrium distribution of a **d+1-dimensional random process**

stochastic quantization

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

random walk governed by

Langevin equation (Brownian motion):

$$\frac{\partial \phi}{\partial t_L} = -\frac{\delta S[\phi]}{\delta \phi} + \eta$$

stochastic quantization

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

random walk governed by

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$$\frac{\partial \phi}{\partial t_L} = -\frac{\delta S[\phi]}{\delta \phi} + \eta$$

ficticous Langevin time
(not physical)

stochastic quantization

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

random walk governed by

Langevin equation (Brownian motion):

$$\frac{\partial \phi}{\partial t_L} = -\frac{\delta S[\phi]}{\delta \phi} + \eta$$

noise term

$$\langle \eta \rangle = 0$$

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

ficticous Langevin time
(not physical)

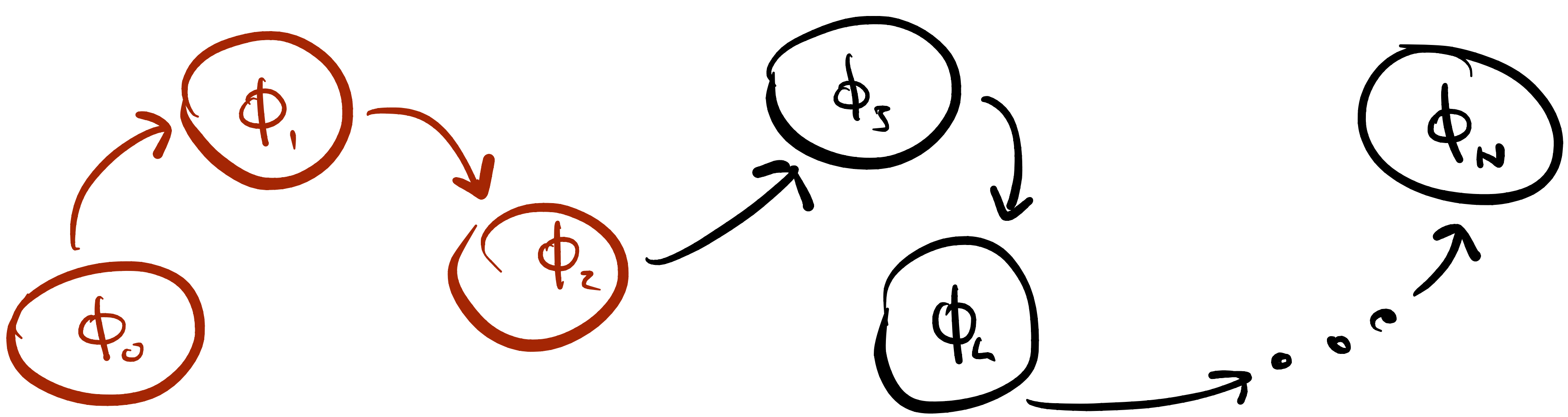
the Langevin method

$$\frac{\partial \phi}{\partial t_L} = -\frac{\delta S[\phi]}{\delta \phi} + \eta$$

discretize

$$\phi^{(n+1)} = \phi^{(n)} - \frac{\delta S[\phi]}{\delta \phi}\bigg|_{\phi^{(n)}} \Delta t_L + \sqrt{2\Delta t_L}\,\tilde{\eta}$$

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{N}\sum_{i=1}^{N} \mathcal{O}[\phi_i]$$



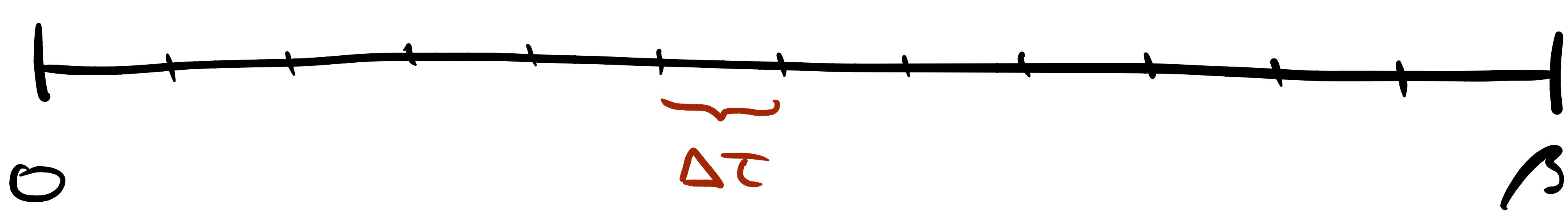
toy problem: the harmonic oscillator

action with harmonic potential:

$$S[x] = \int_0^\beta d\tau \left[\frac{1}{2} \left(\frac{\partial x}{\partial \tau} \right)^2 + \frac{1}{2} \omega^2 x^2 \right]$$

discretization of Euclidean time into $N_\tau = \frac{\beta}{\Delta\tau}$ slices:

$$S[x] = \sum_{k=1}^{N_\tau} \Delta\tau \left[\frac{1}{2} \left(\frac{x_k - x_{k-1}}{\Delta\tau} \right)^2 + \frac{1}{2} \omega^2 x_k^2 \right]$$



discrete Langevin equation for the HO

coupled set of stochastic differential equations:

$$x_k^{(n+1)} = x_k^{(n)} - \left[\frac{2x_k^{(n)} - x_{k+1}^{(n)} - x_{k-1}^{(n)}}{\Delta\tau} + \Delta\tau\omega^2 x_k^{(n)} \right] \Delta t_L + \sqrt{2\Delta t_L}\eta_k$$

calculation of ground-state energy:

$$E = \langle \hat{H} \rangle = \omega^2 \langle x^2 \rangle$$

square of the wavefunction:

$$\langle x \rangle = \int dx \; x \; P[x] = \int dx \; x \; |\psi(x)|^2$$

RECAP:
STOCHASTIC QUANTIZATION

interpret Euclidean field theories
as equilibrium limit of a ficticious random process

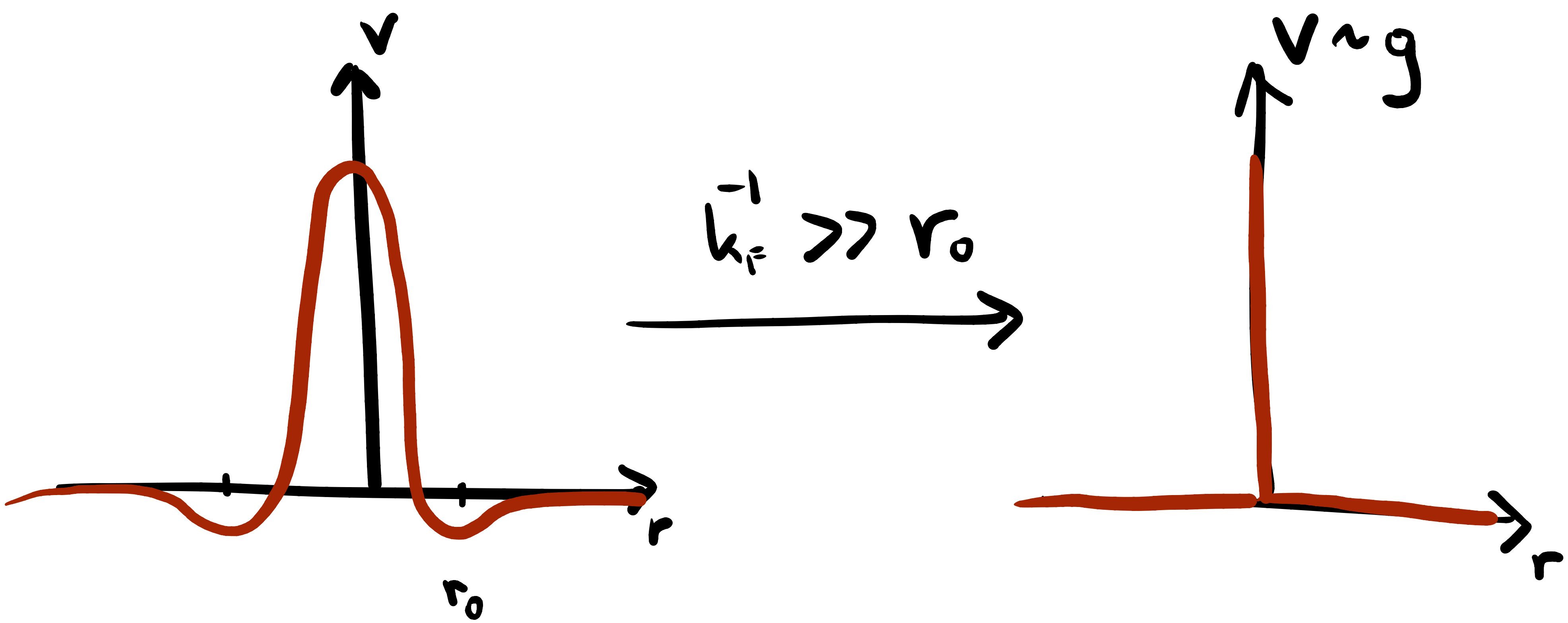
we can use this to construct a numerical method
based on Markov chains

simple toy problem: QM harmonic oscillator
as 0+1-dimensional QFT

fermions with 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?

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

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

what do we need to compute?

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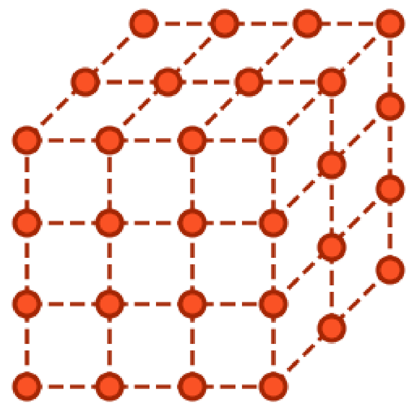

+ Trotter decomposition

+ 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]

the path integral

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

discrete Langevin equation:

$$\phi^{(n+1)} = \phi^{(n)} + \Delta\phi^{(n)}$$

$$\Delta\phi^{(n)} = -\frac{\delta S[\phi]}{\delta\phi}\bigg|_{\phi^{(n)}} \Delta t_L + \sqrt{2\Delta t_L}\,\eta$$

the path integral & complex actions

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

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

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

discrete Langevin equation:

$$\phi^{(n+1)} = \phi^{(n)} + \Delta\phi^{(n)}$$

$$\Delta\phi^{(n)} = -\frac{\delta S[\phi]}{\delta\phi}\bigg|_{\phi^{(n)}} \Delta t_L + \sqrt{2\Delta t_L}\,\eta$$

the path integral & complex actions

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

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

discrete Langevin equation:

$$\phi^{(n+1)} = \phi^{(n)} + \Delta\phi^{(n)}$$

$$\Delta\phi_R^{(n)} = -\mathrm{Re}\left[\frac{\delta S[\phi]}{\delta\phi}\right]_{\phi^{(n)}} \Delta t_L + \sqrt{2\Delta t_L}\,\eta$$

$$\Delta\phi_I^{(n)} = -\mathrm{Im}\left[\frac{\delta S[\phi]}{\delta\phi}\right]_{\phi^{(n)}} \Delta t_L$$

complex action $\longrightarrow$ complex Langevin equation

[Parisi '83; Klauder '84; Koonin,Adami '01; Aarts '08; LR,Porter,Drut,Braun '17; LR,Loheac,Drut,Braun '18]

complex probablities & possible issues

derivation requires **vanishing boundary terms**
(challenging to show rigorously)
[Aarts,Seiler,Stamatescu '10]

sometimes convergence to the wrong
limit has been observed,
some conditions are available
that ensure validity
[Aarts,Seiler,Stamatescu '11; Aarts,Seiler,Sexty,Stamatescu '17]

for many systems CL has been **very successful**, for others **it failed**

careful checks and benchmarks have to be performed

PHYSICAL REVIEW D **81**, 054508 (2010)

Complex Langevin method: When can it be trusted?

Gert Aarts*
Department of Physics, Swansea University, Swansea, United Kingdom

Erhard Seiler†
Max-Planck-Institut für Physik (Werner-Heisenberg-Institut), München, Germany

Ion-Olimpiu Stamatescu‡
Institut für Theoretische Physik, Universität Heidelberg and FEST, Heidelberg, Germany
(Received 18 December 2009; published 22 March 2010)

ELSEVIER

Nuclear Physics A642 (1998) 239c–250c

Complex Langevin: A Numerical Method?

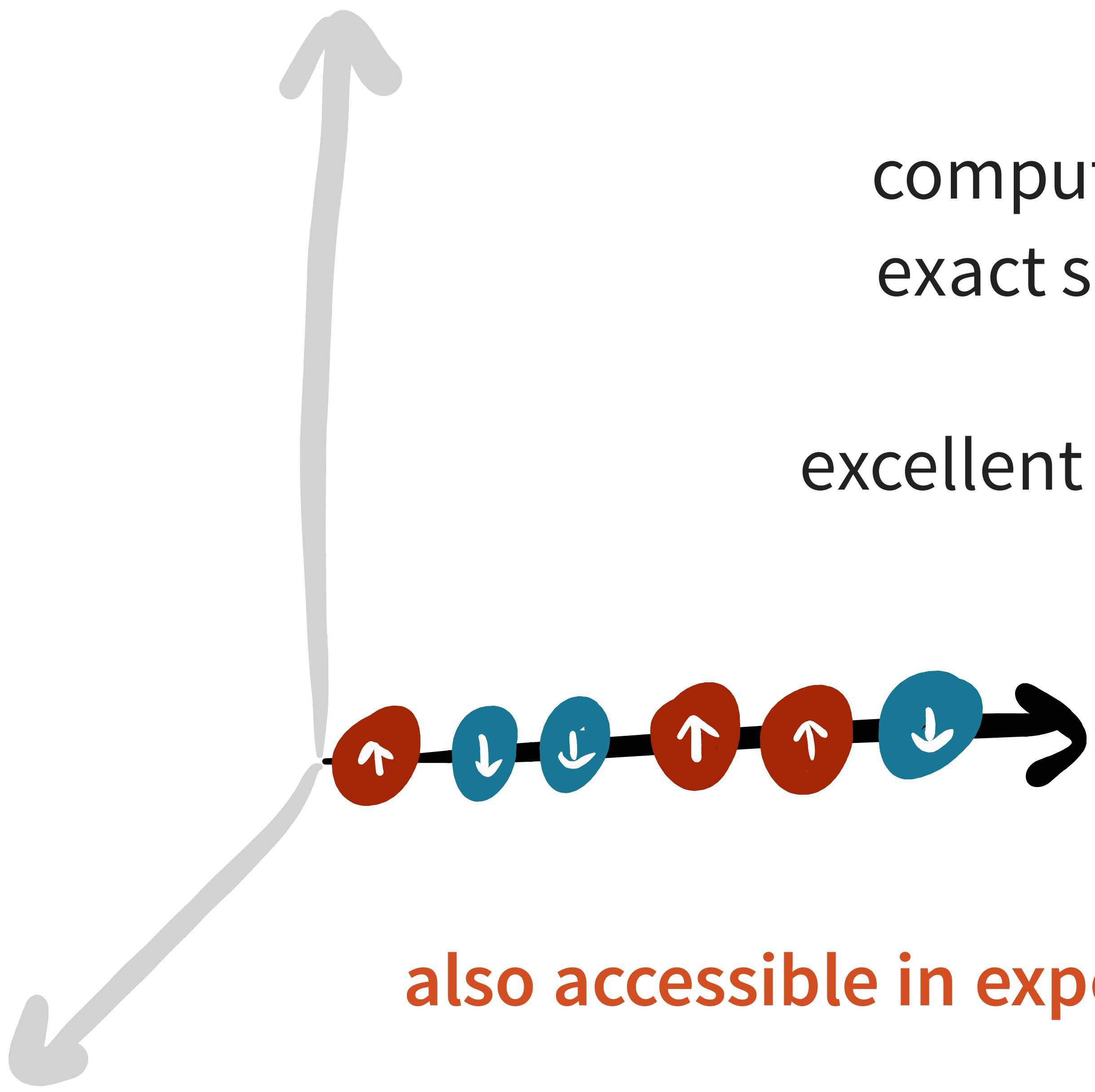
H. Gausterer [a]

[a]Institut für Theoretische Physik,
Universität Graz, A-8010 Graz, AUSTRIA

Does the complex Langevin method give unbiased results?

L.L. Salcedo*
Departamento de Física Atómica, Molecular y Nuclear and
Instituto Carlos I de Física Teórica y Computacional,
Universidad de Granada, E-18071 Granada, Spain.
(Dated: November 22, 2016)

one-dimensional systems

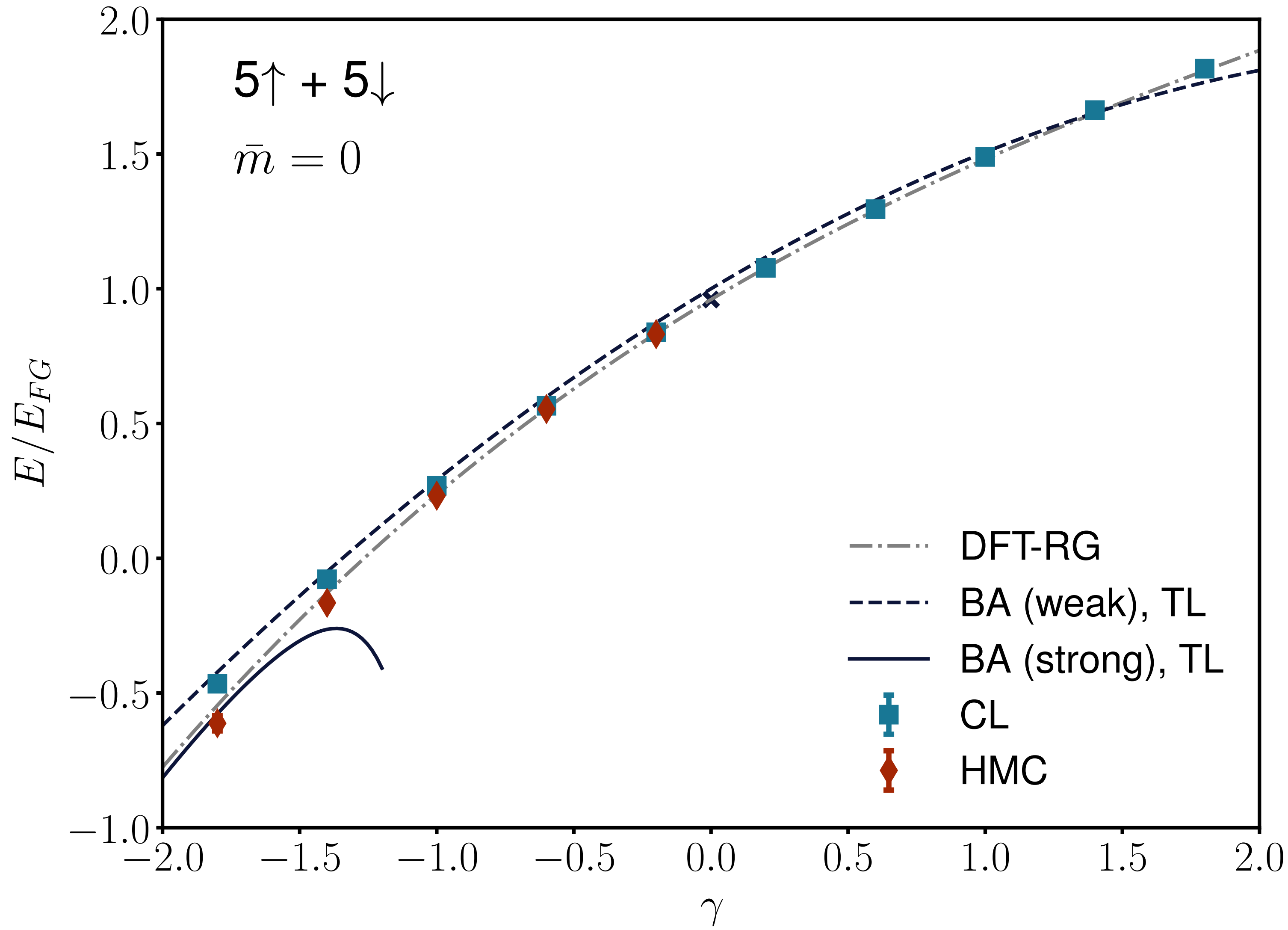


computationally cheap &
exact solutions available
=
excellent benchmark systems

also accessible in experiment

first step: compare to other methods

[LR,Porter,Drut,Braun '17]

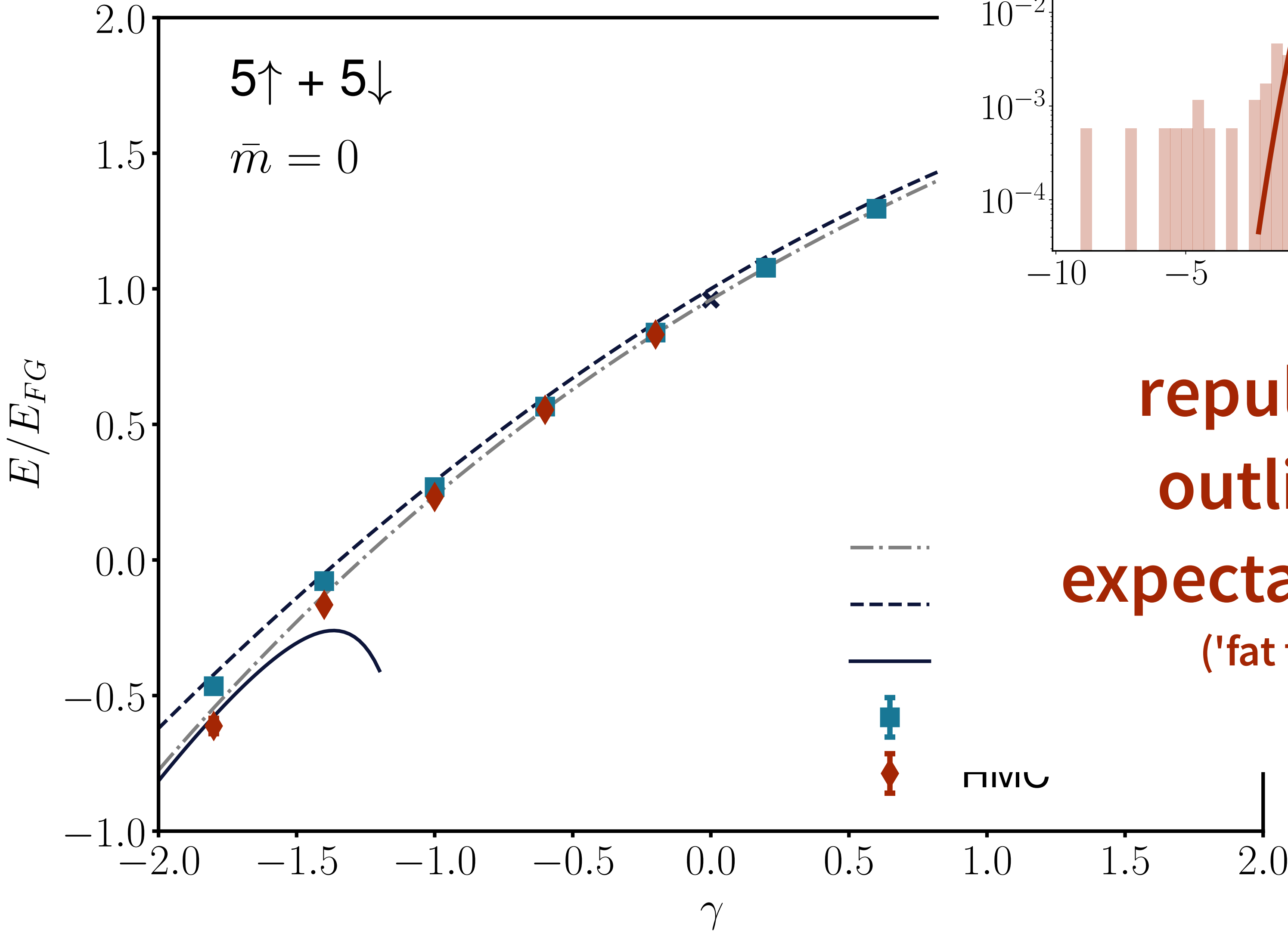


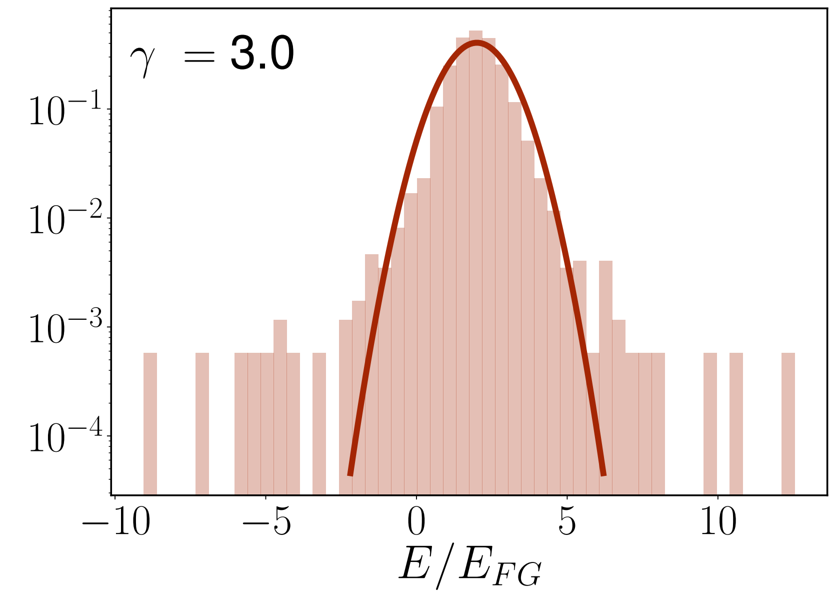
$\gamma = g/n$

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

first step: compare to other methods

[LR,Porter,Drut,Braun '17]





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]
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first step: compare to other methods

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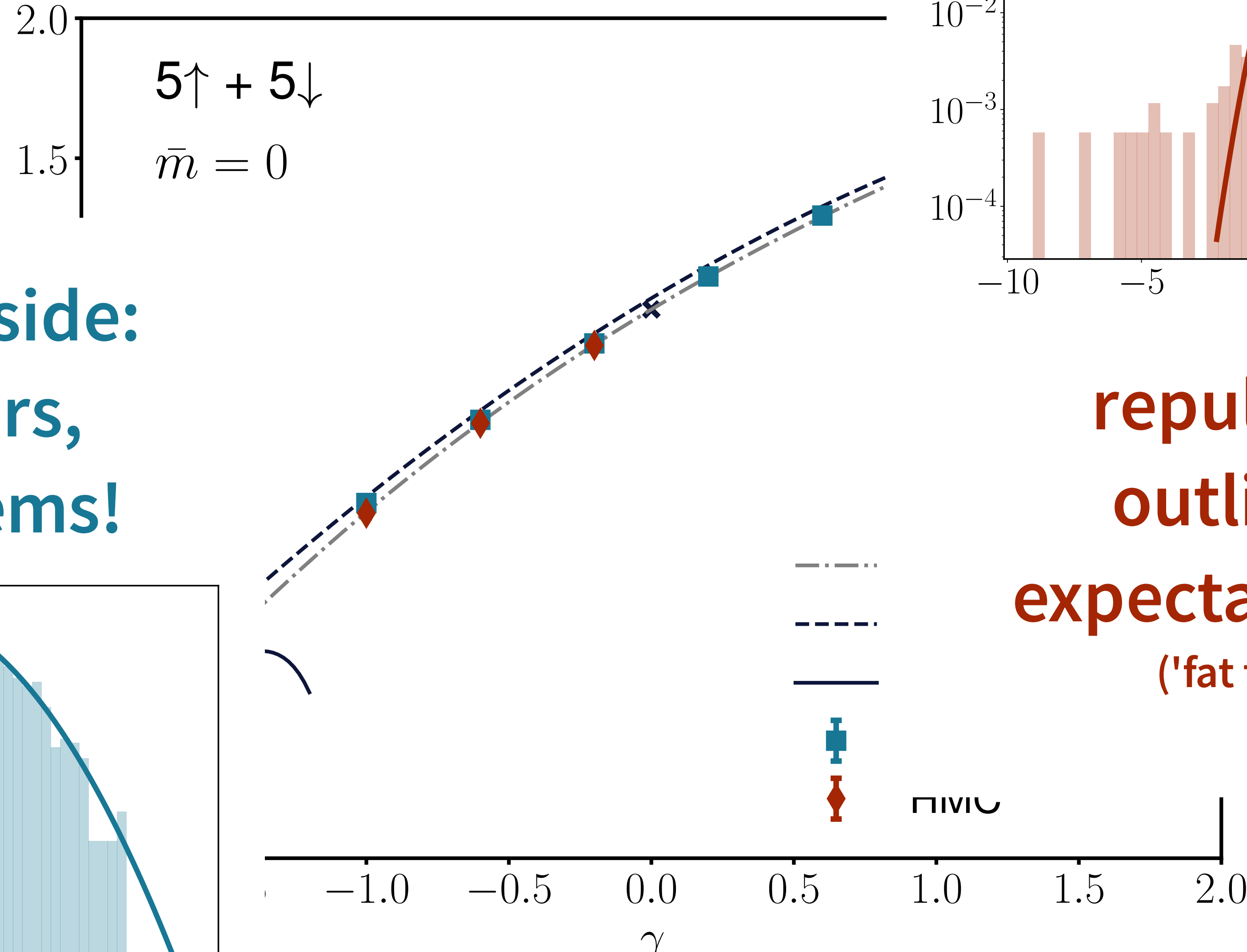
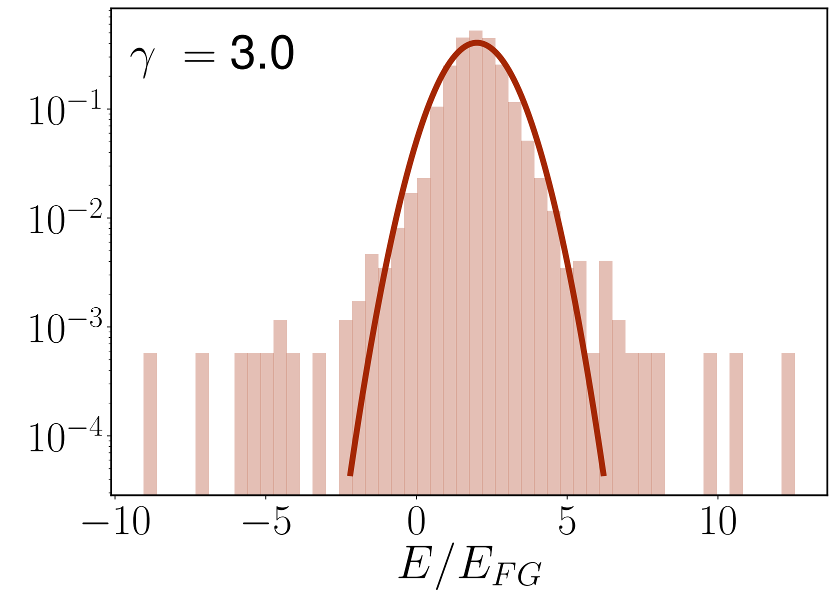
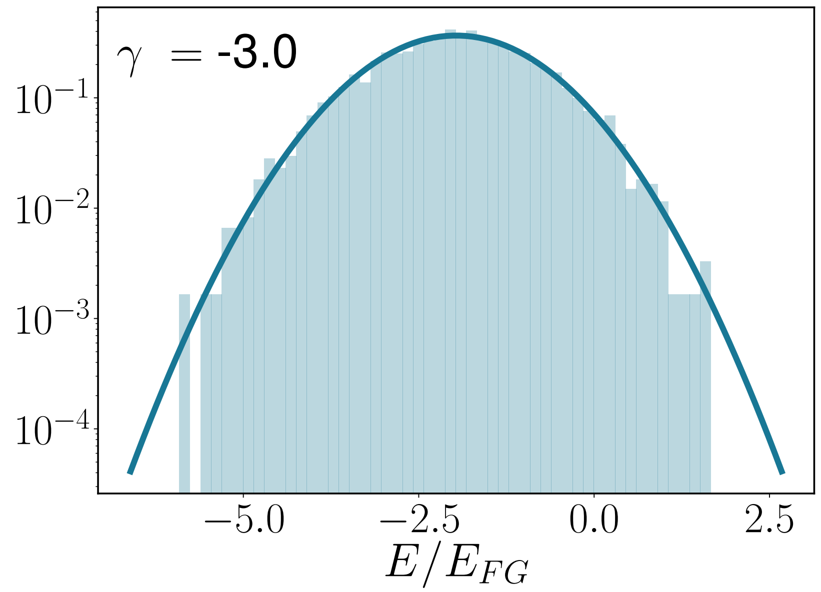




attractive side:
no outliers,
no problems!



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

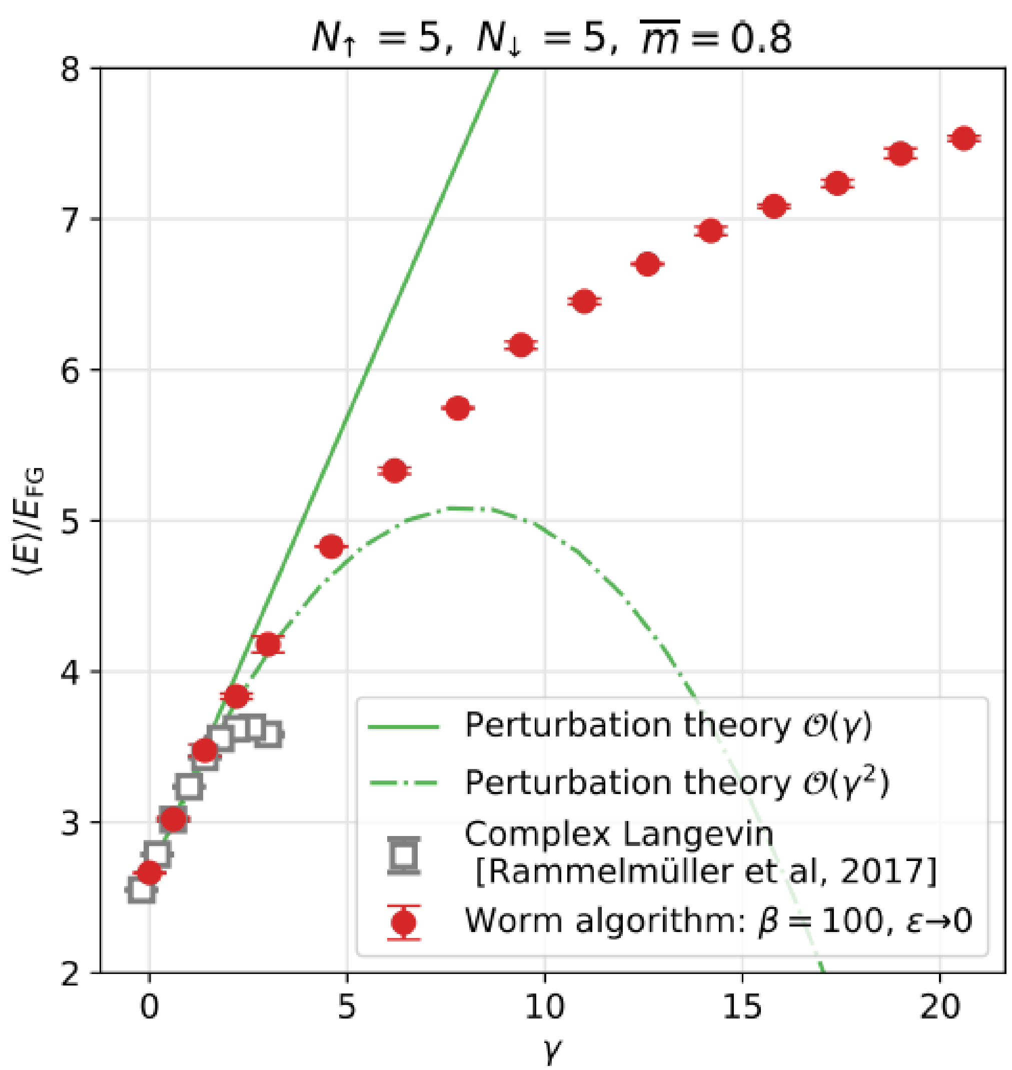
$$\gamma = g/n$$

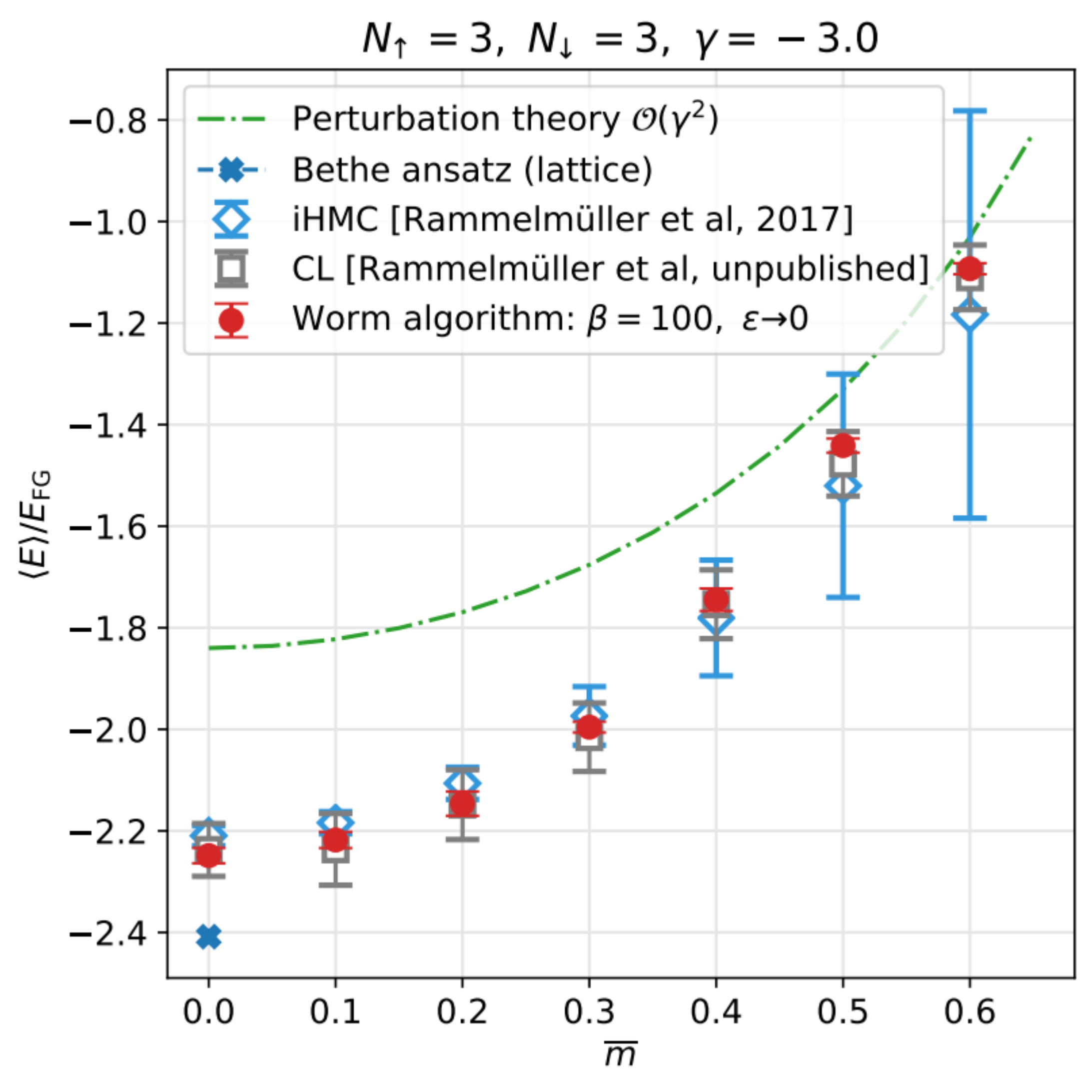
[BA: Iida, Wadati '07; Tracy, Widom '16]
[DFT-RG: Kemler, Pospiech, Braun '17; Kemler '17]
[HMC: LR, Porter, Loheac, Drut '15]

more comparisons: mass-imbalance

[wordline: Singh,Chandrasekharan '18]
[CL/iHMC: LR,Porter,Drut,Braun '17]

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

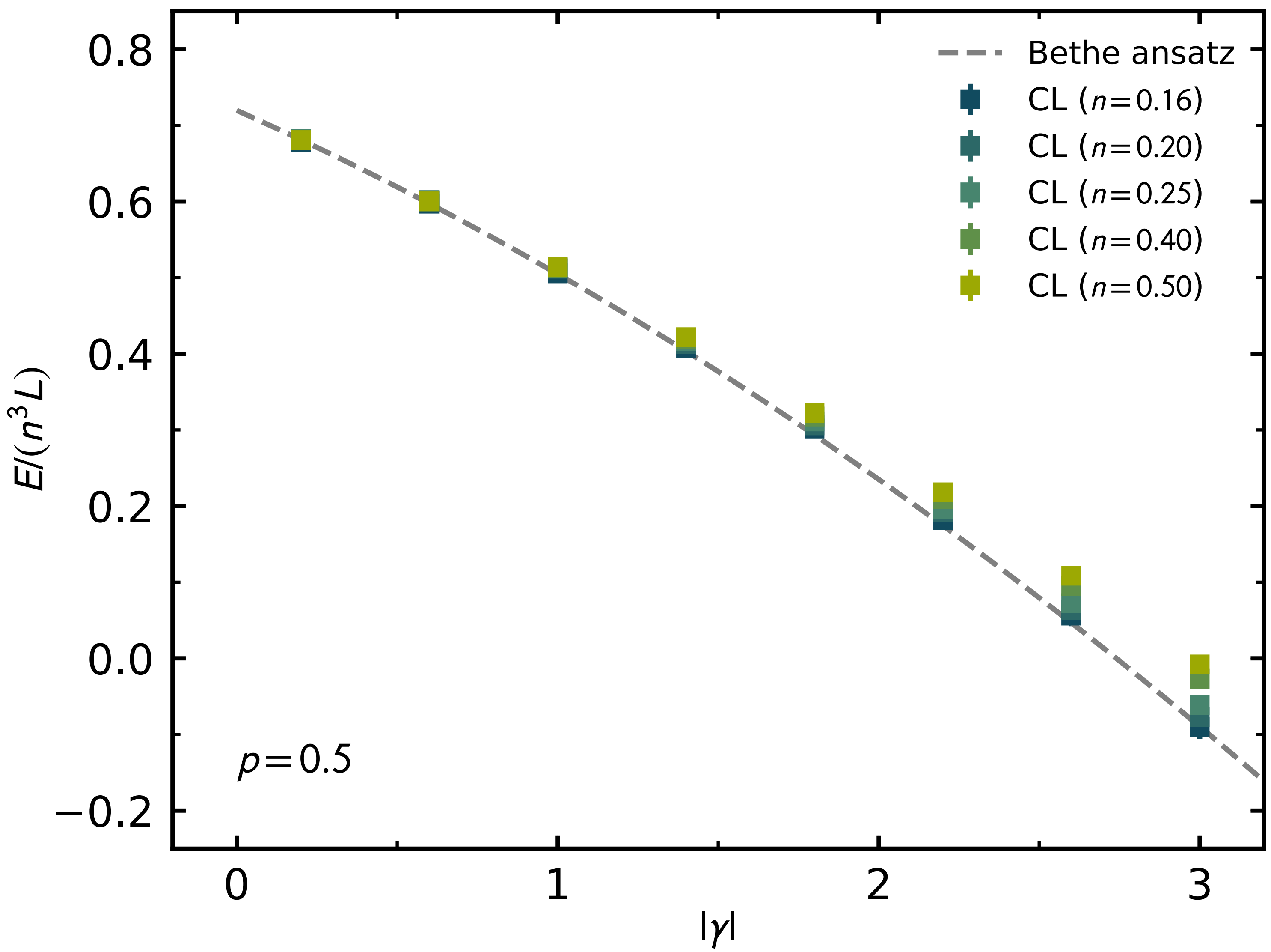




discrepancy with worldline methods for **repulsive interaction**

polarized 1D fermions: equation of state

[LR, Drut, Braun in preparation]



excellent agreement at low densities (zero-range limit)

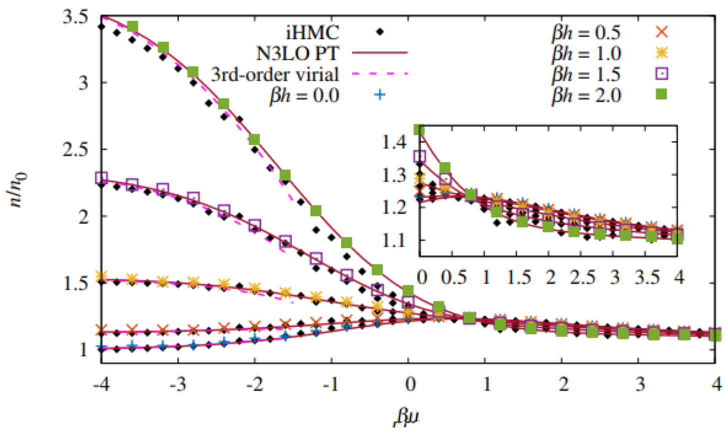
$$\gamma = g/n$$

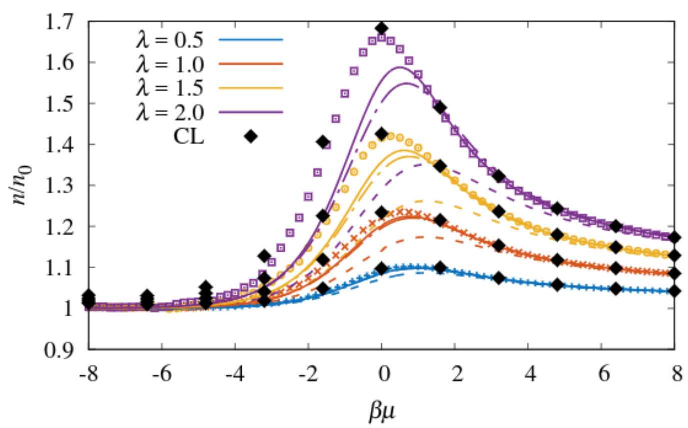
$$p = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

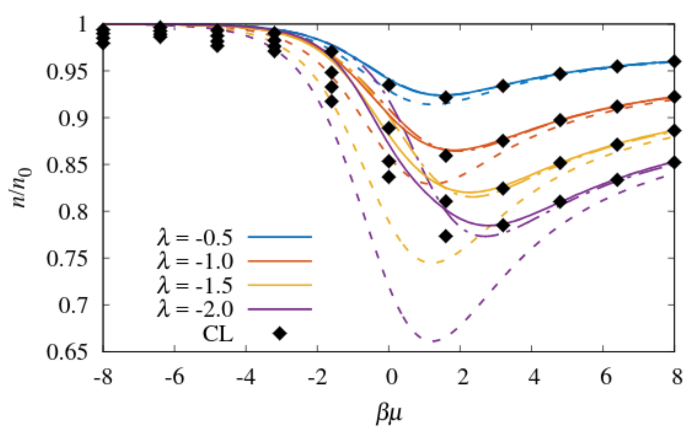
[Iida, Wadati '07; Tracy, Widom '16]

more CL results for 1D

[Loheac,Drut '17]

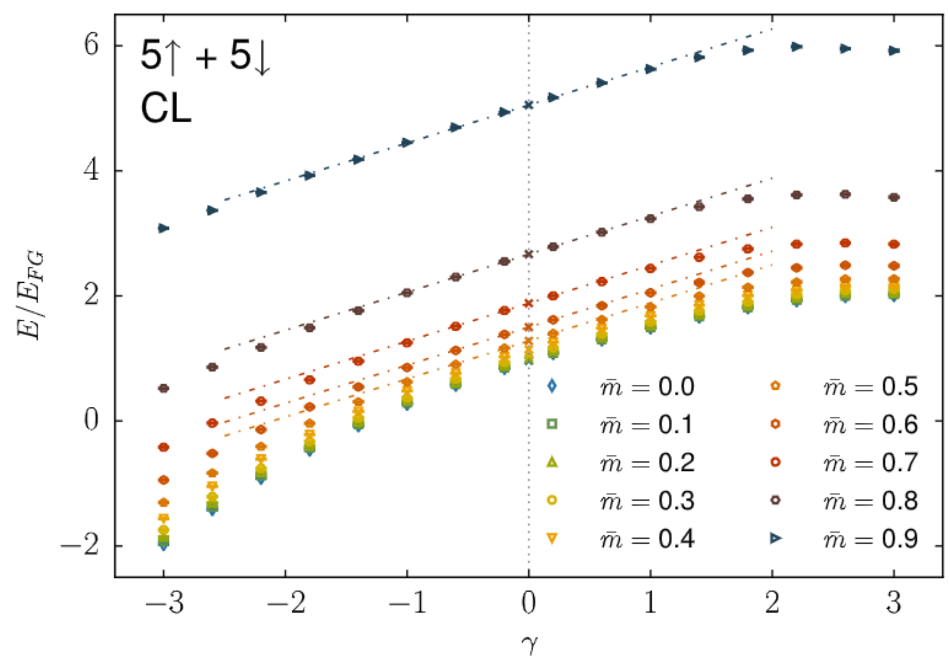


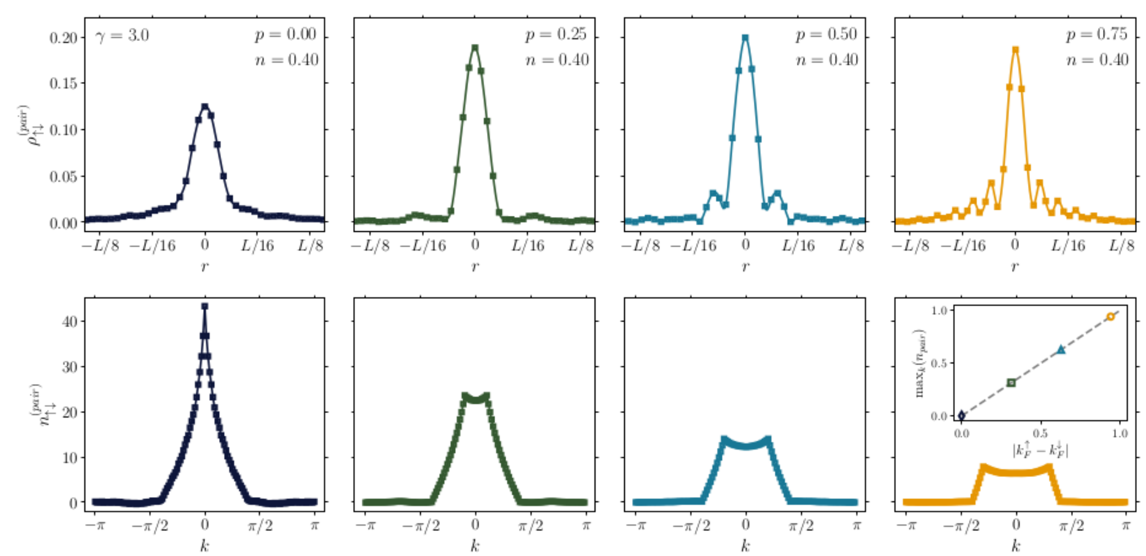




[Loheac,Braun,Drut '18]

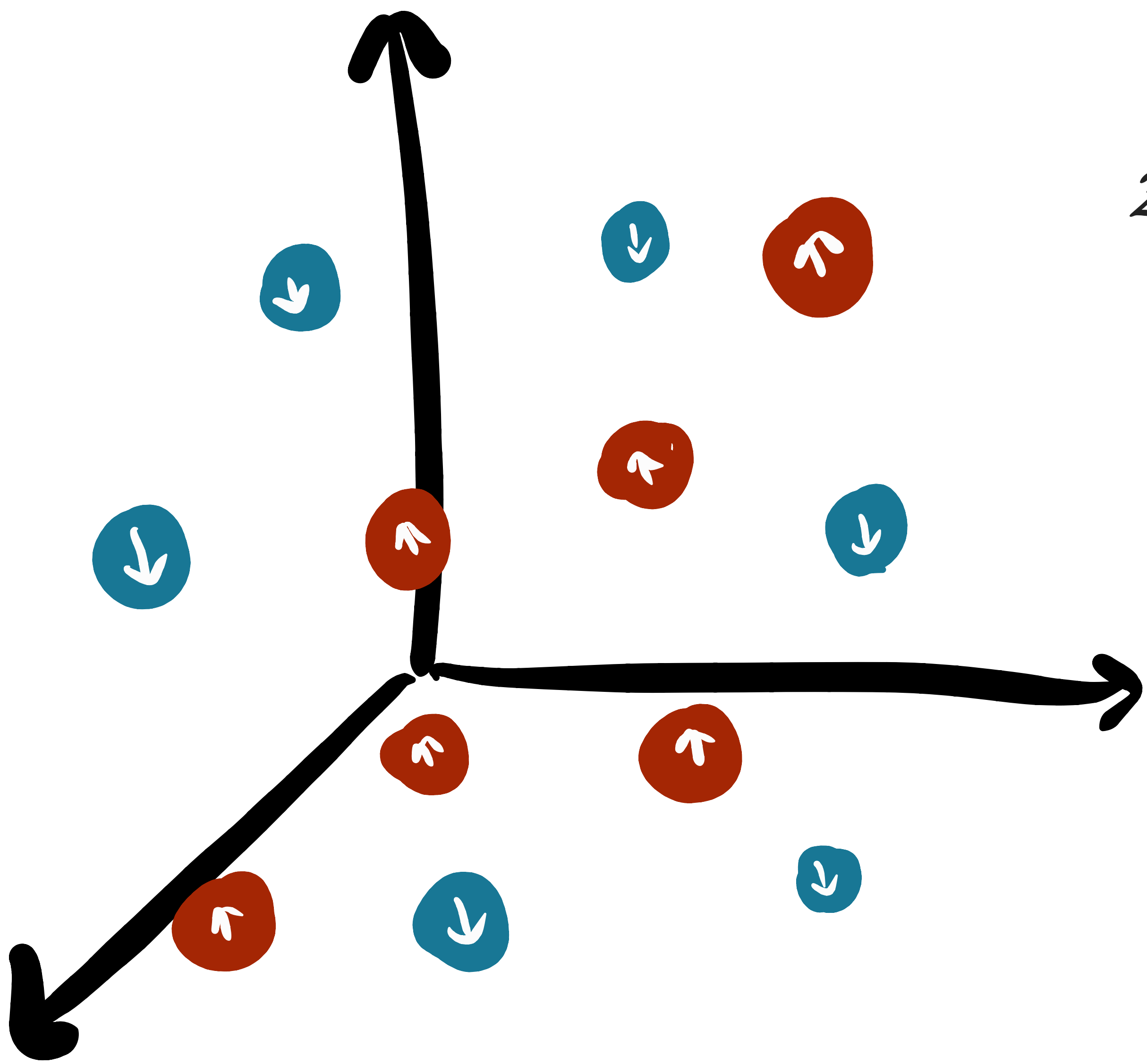
[LR,Porter,Drut,Braun '17]





[LR,Drut,Braun in preparation]

the unitary Fermi gas at finite temperature



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

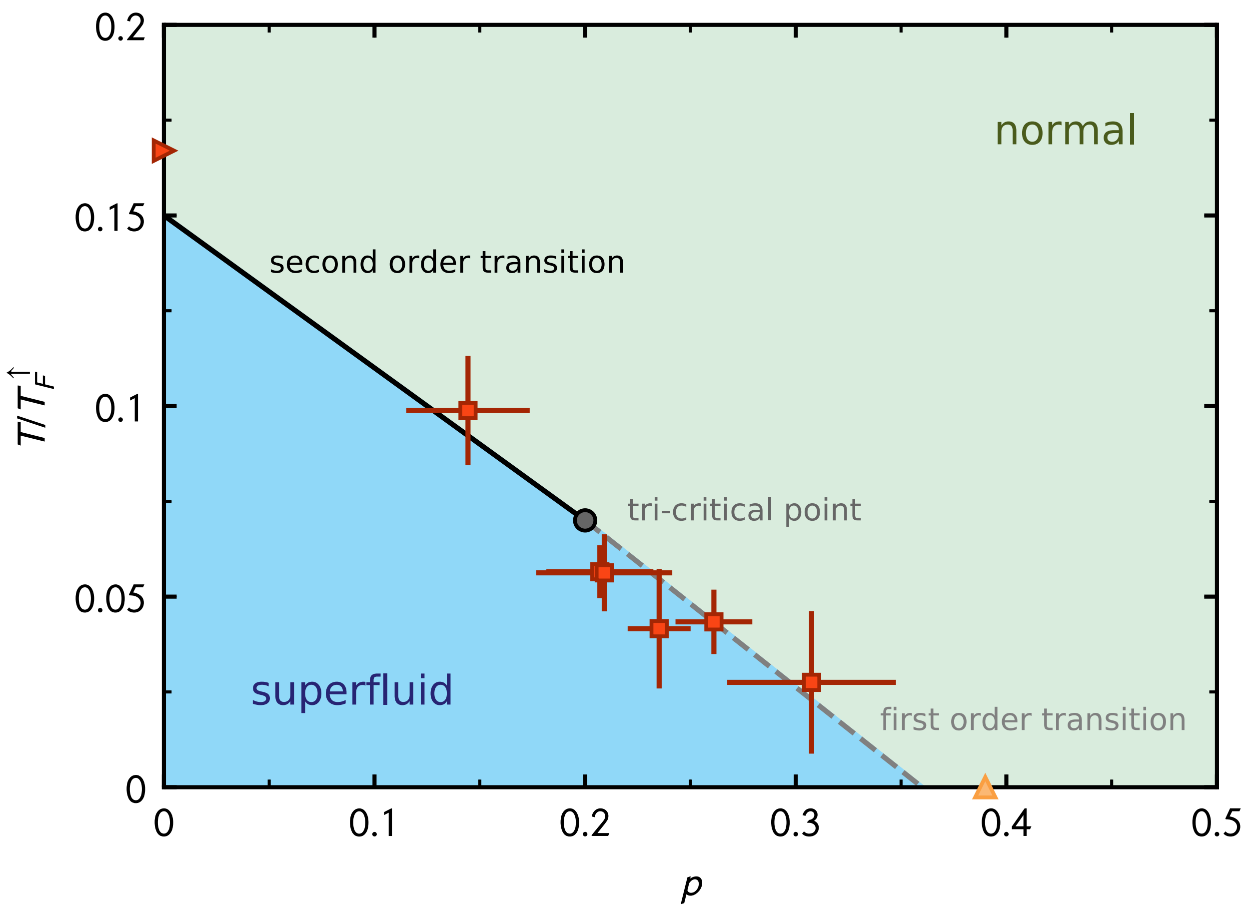
$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$
$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

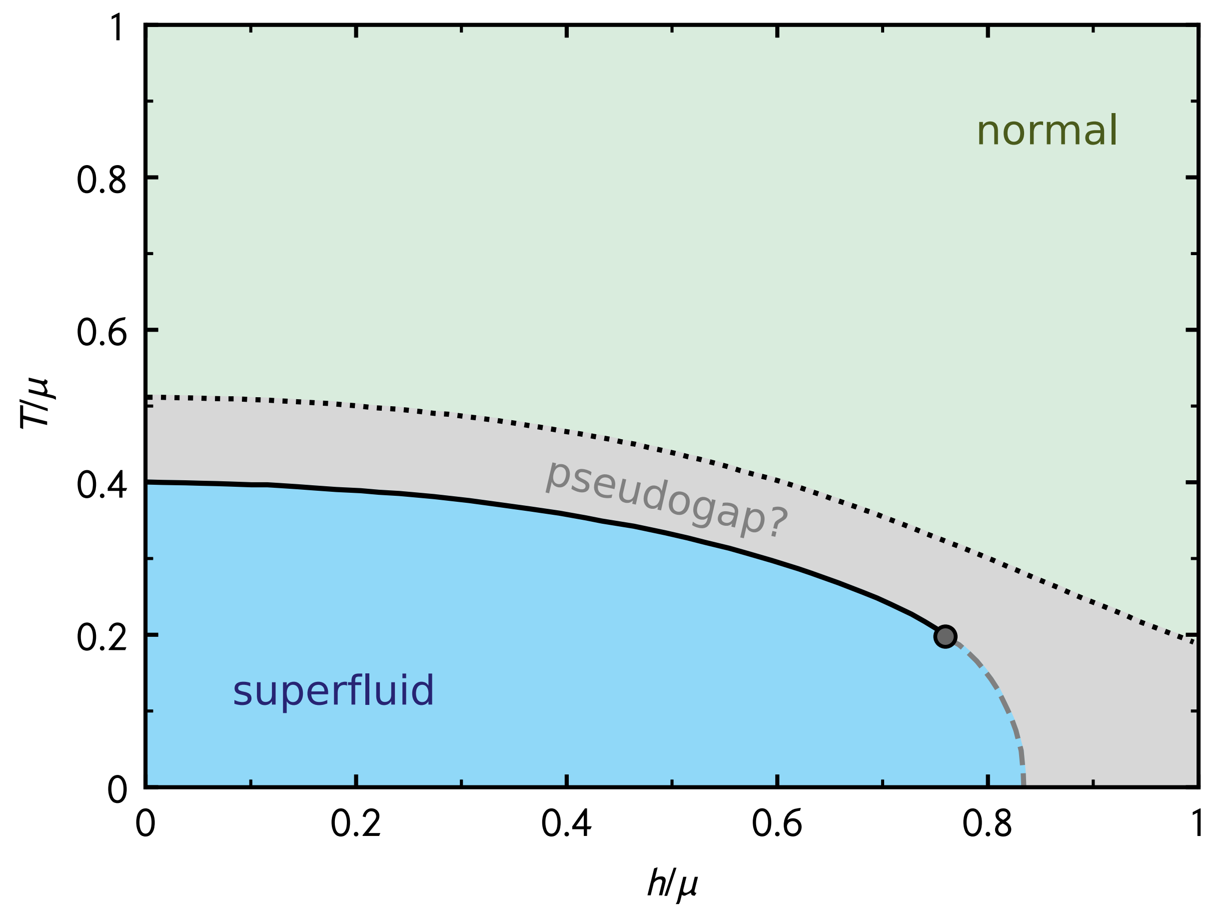
computationally challenging (but feasible)

exploring the phase diagram

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

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



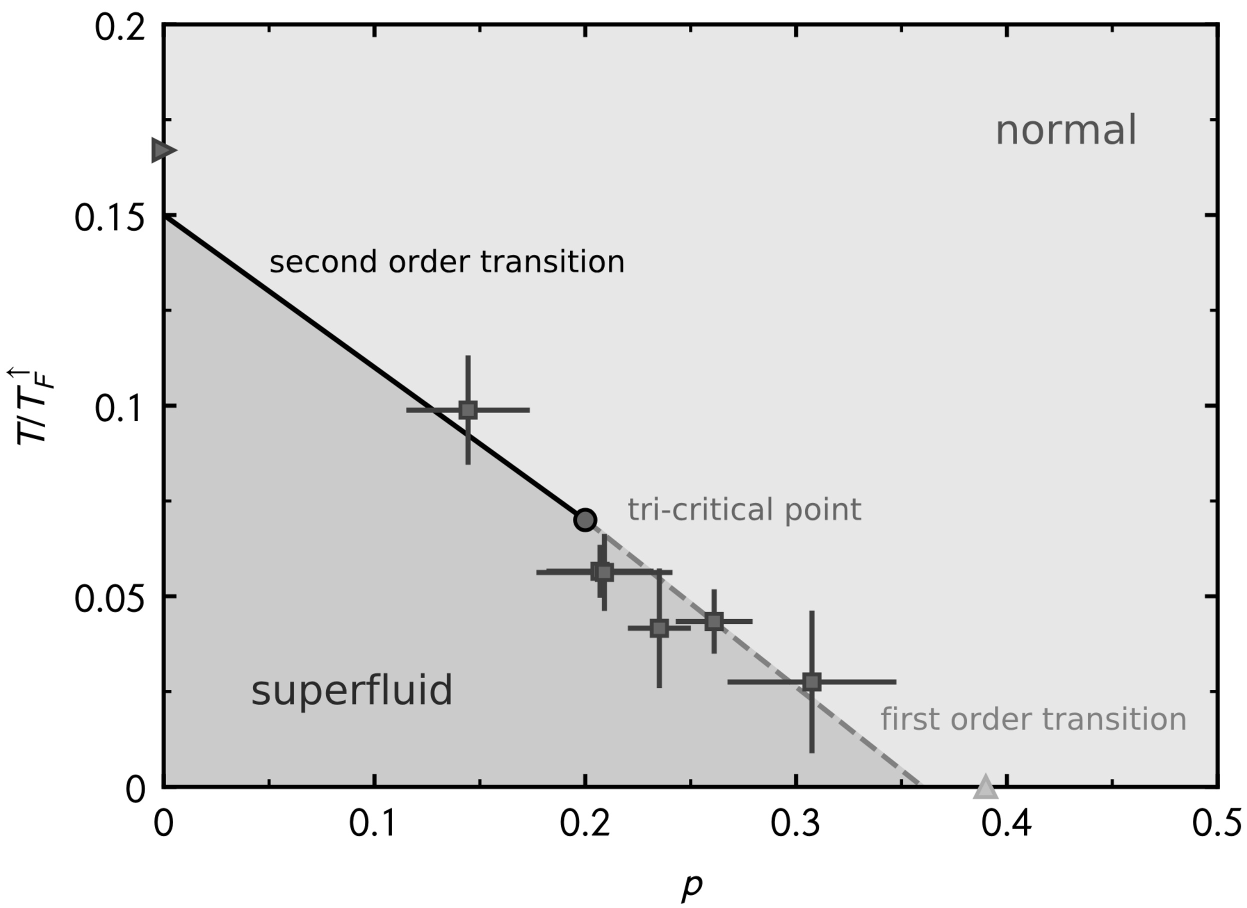


[experiment: Shin,Schunck,Schirotzek,Ketterle '08]
[zero-temperature p_c: Lobo,Recati,Giorgini,Stringari '06]
[balanced T_c: Ku,Sommer,Cheuck,Zwierlein '12]

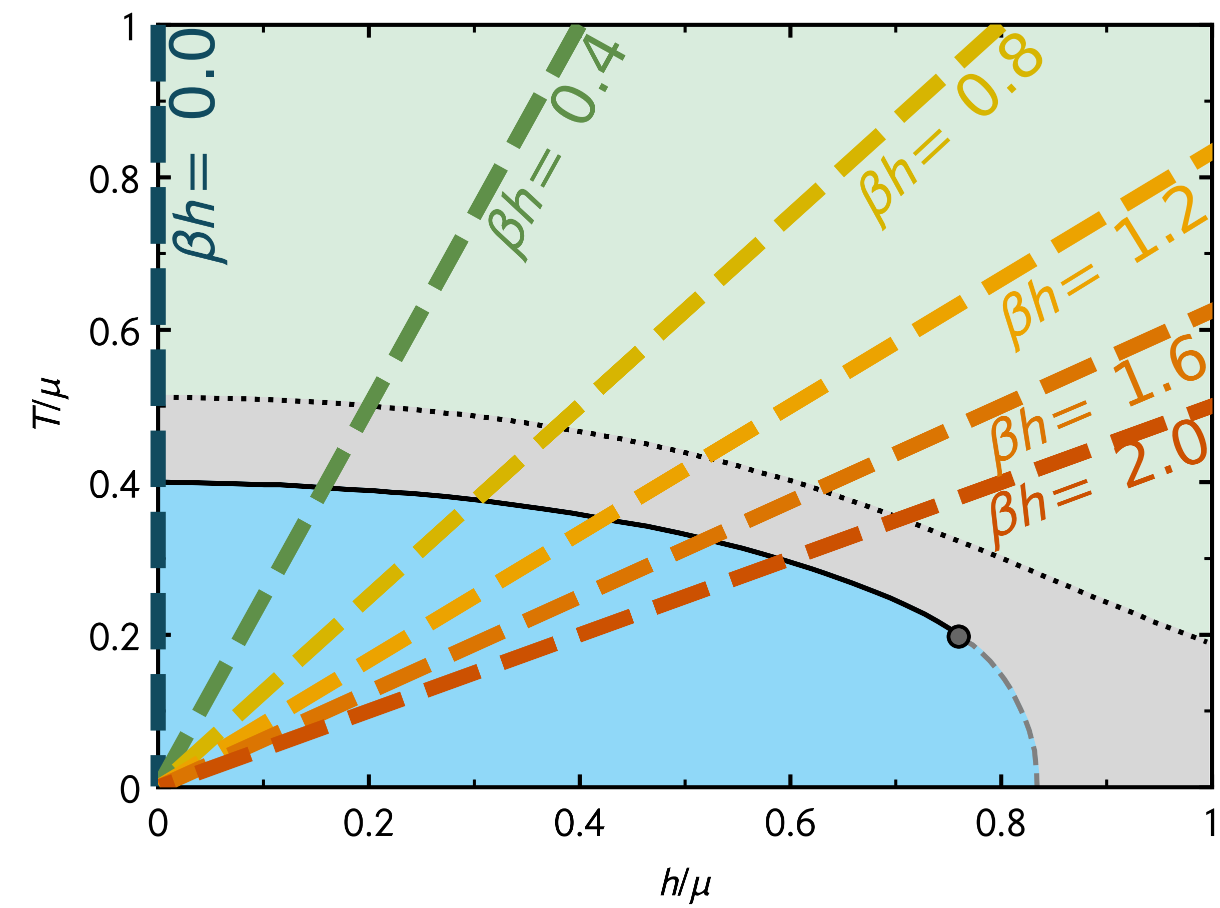
[fRG: Boettcher et. al '15]

exploring the phase diagram

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



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



[experiment: Shin,Schunck,Schirotzek,Ketterle '08]
[zero-temperature p_c: Lobo,Recati,Giorgini,Stringari '06]
[balanced T_c: Ku,Sommer,Cheuck,Zwierlein '12]

[fRG: Boettcher et. al '15]

density equation of state

[LR, Loheac, Drut, Braun '18]

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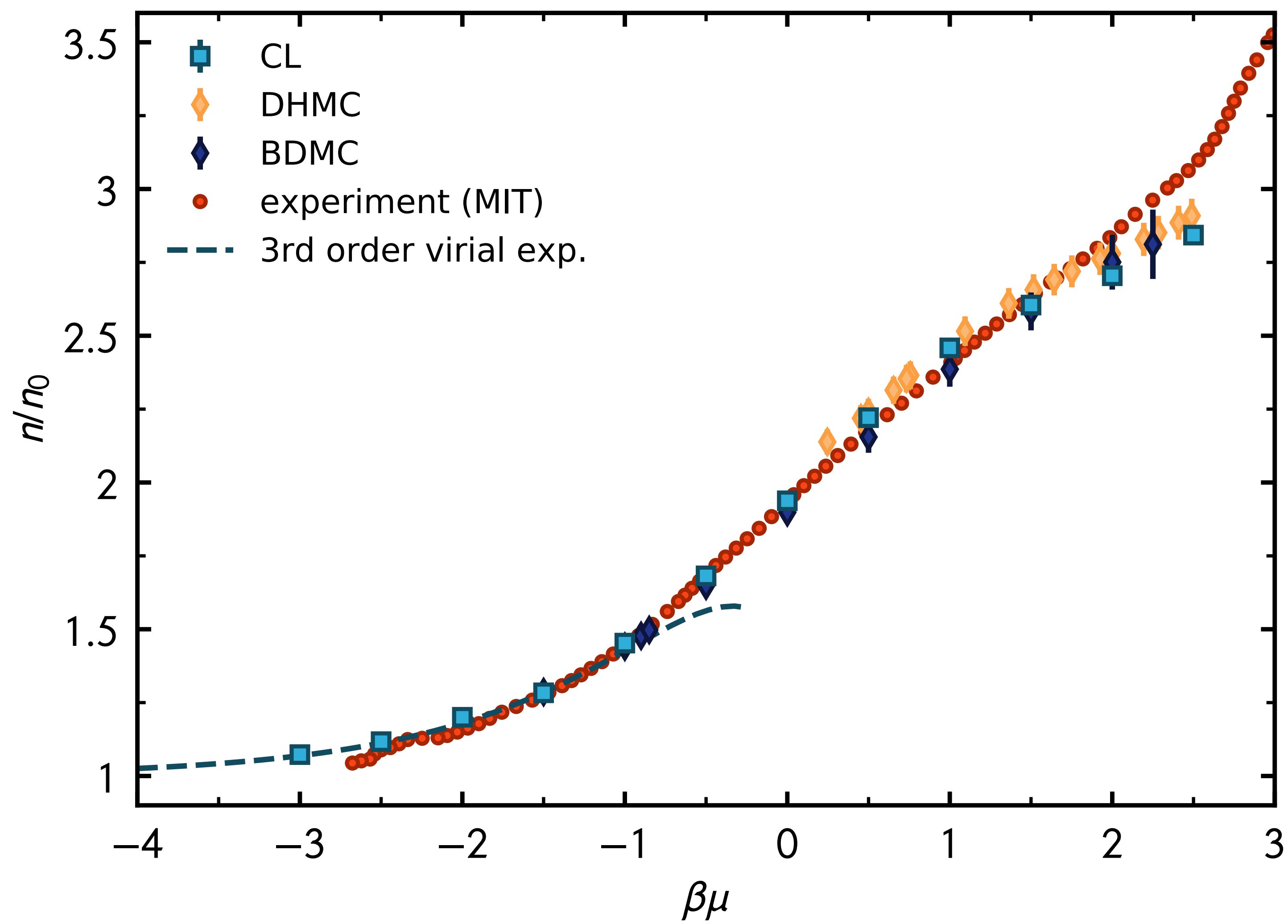

$k_B T$ dominates

E_F dominates

density equation of state

[LR, Loheac, Drut, Braun '18]

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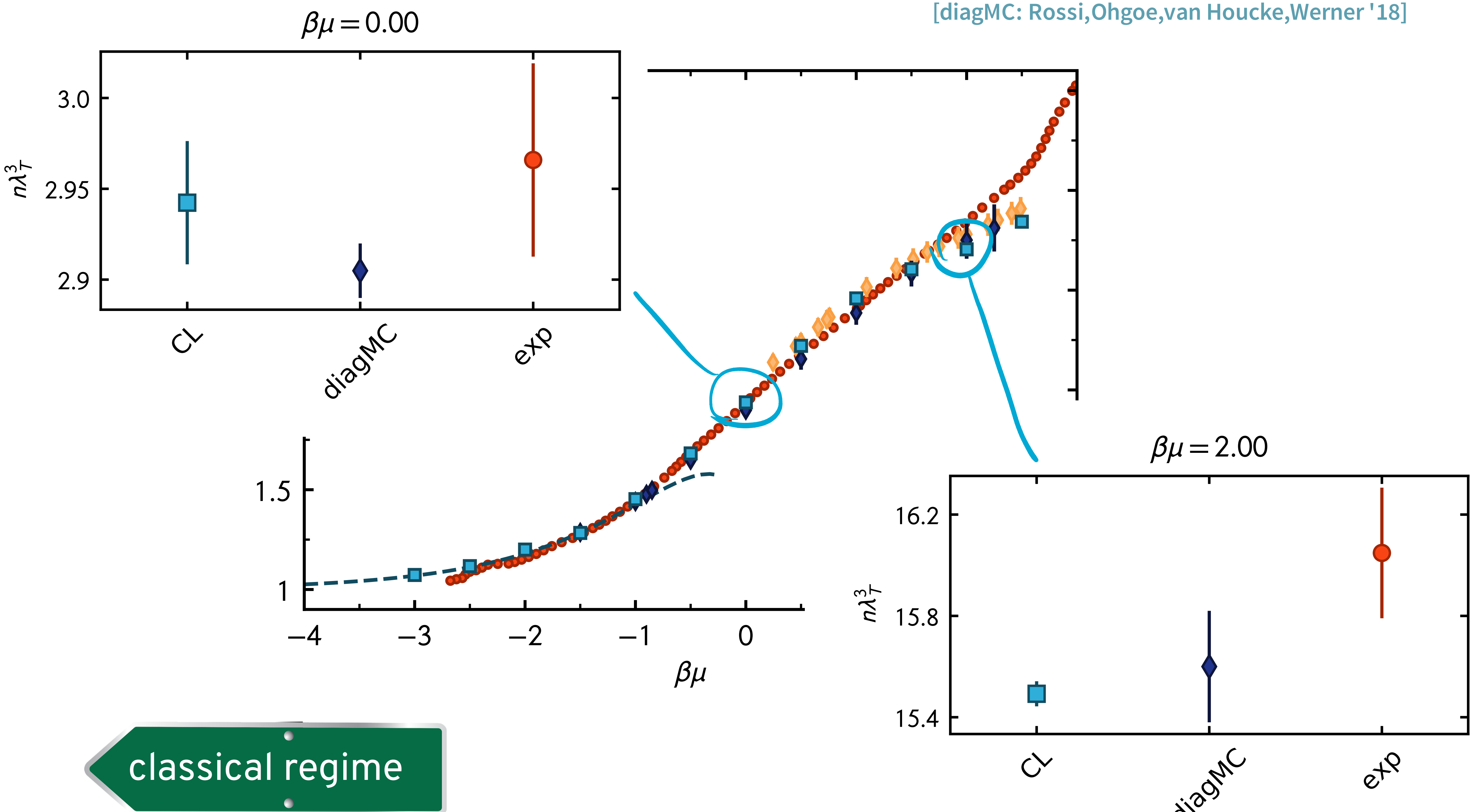

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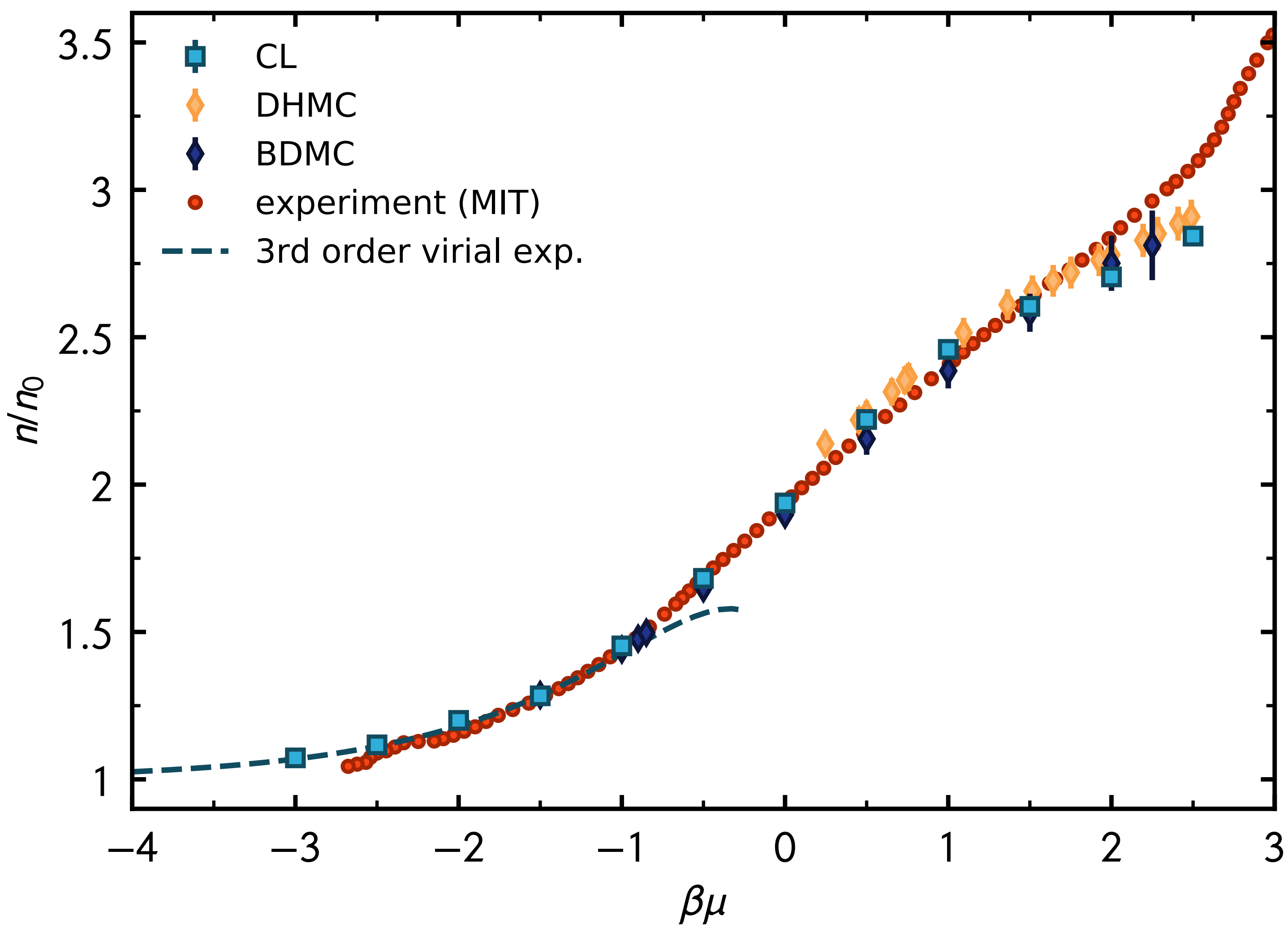
good agreement with experiment and other methods!

CL results:

finite lattice $V = 11^3$



classical regime

quantum regime

$k_B T$ dominates

E_F dominates

density equation of state

[LR, Loheac, Drut, Braun '18]

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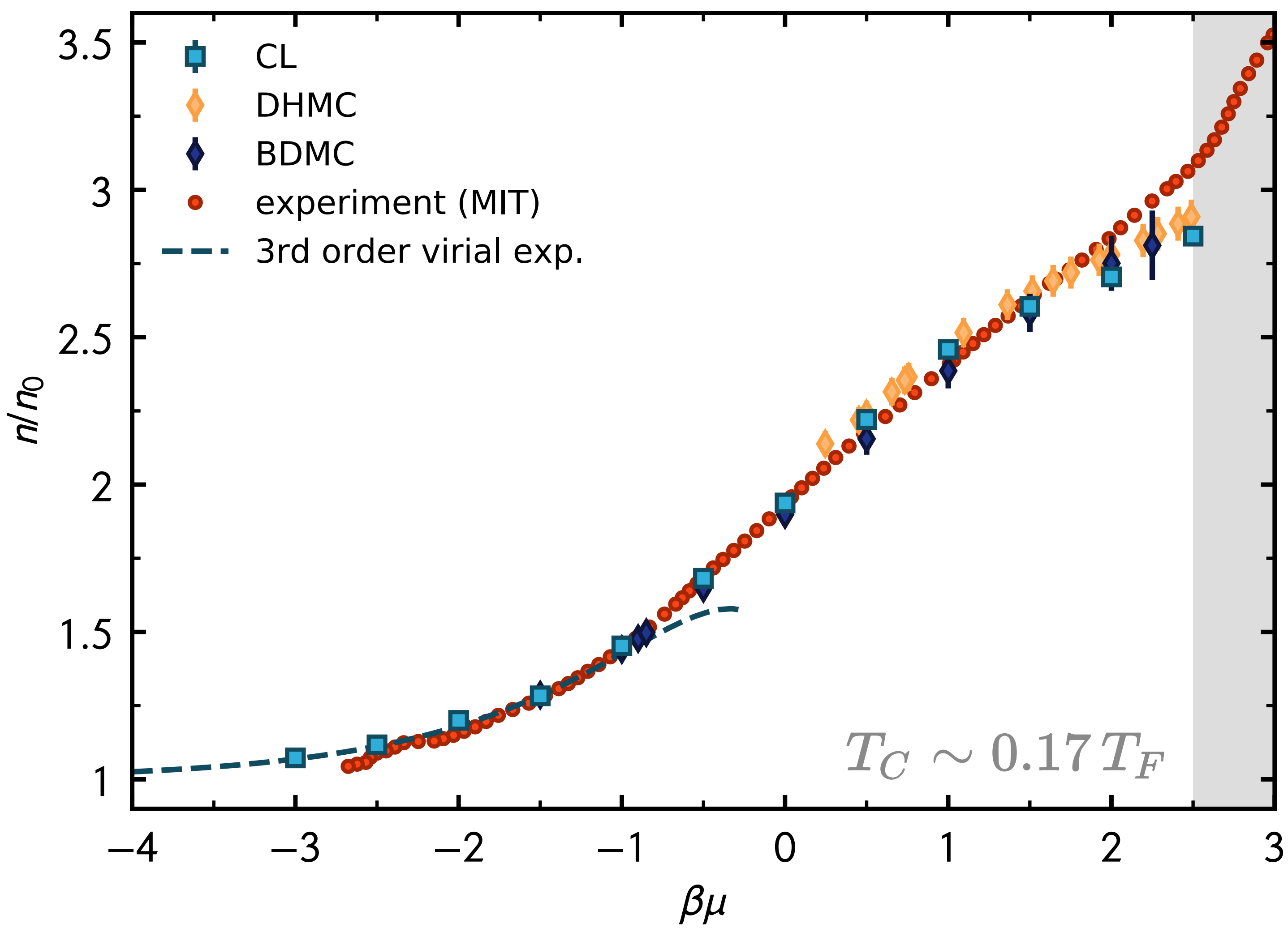


low temperatures: λ_T increases ($\lambda_T \ll V^{1/3}$ must be fulfilled)

classical regime

$k_B T$ dominates

quantum regime

E_F dominates

interlude: the virial expansion

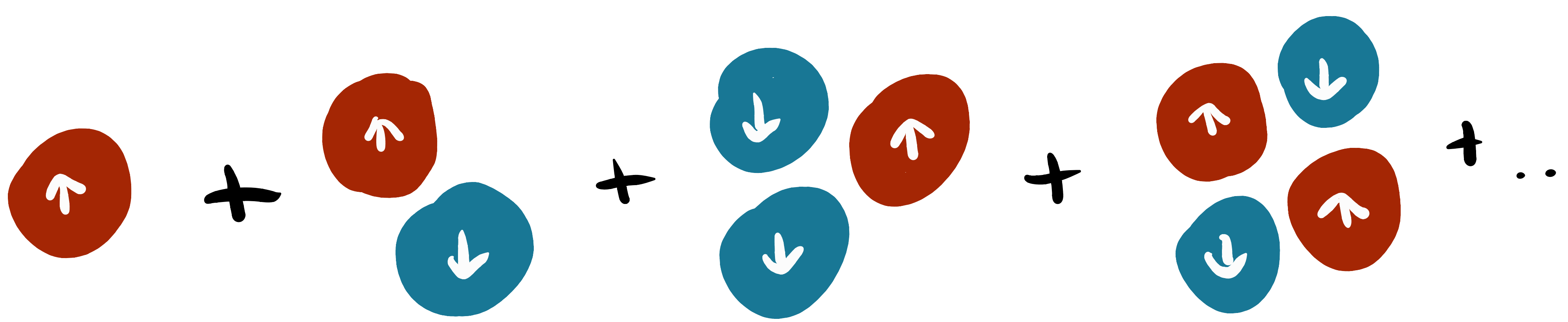
[Liu '13]

dilute gases: few-body correlations dominate

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

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

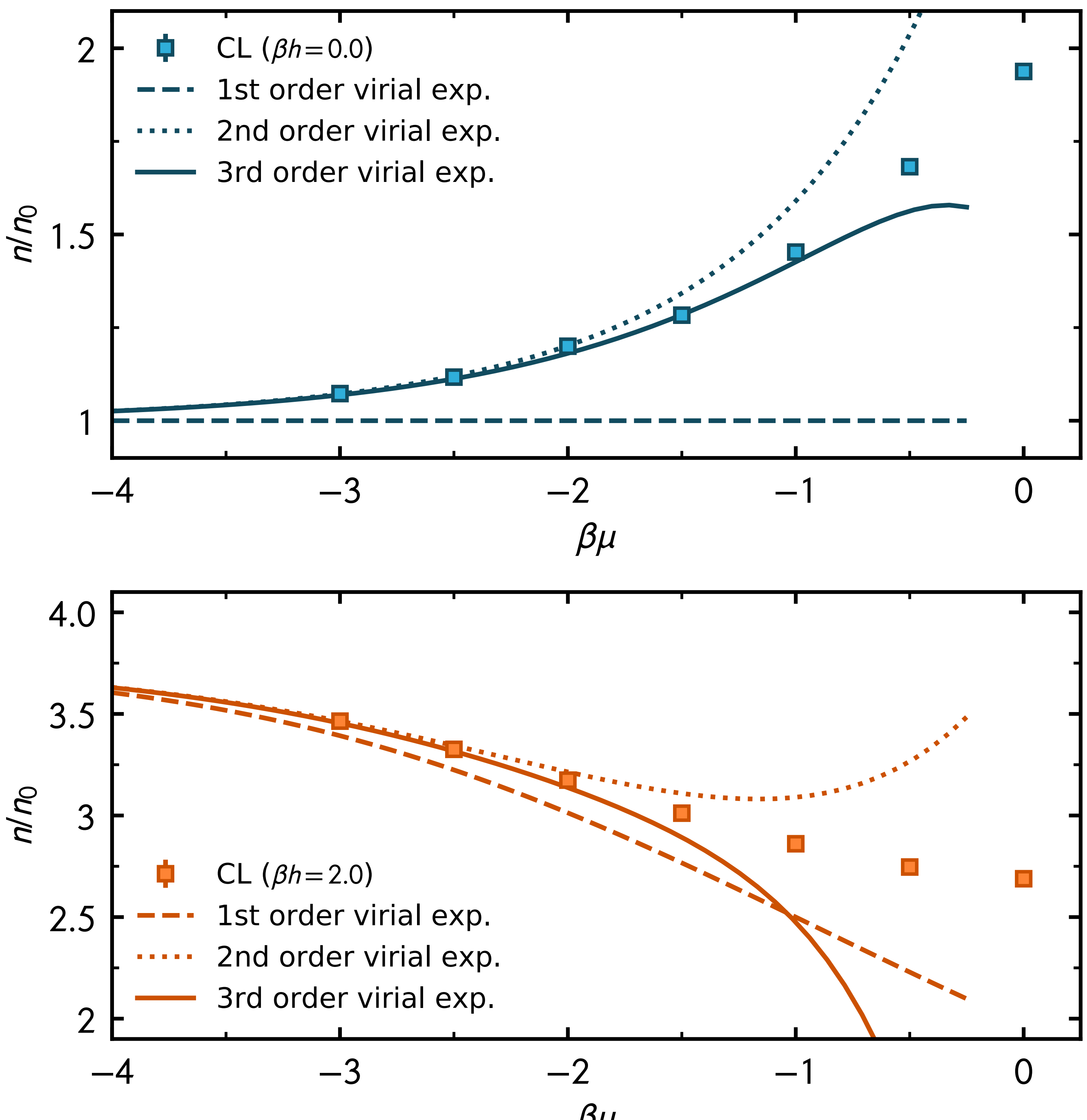
$$\ln \mathcal{Z} = Q_1 \sum_n z^n b_n$$



density EOS (virial regime)

[LR, Loheac, Drut, Braun '18]

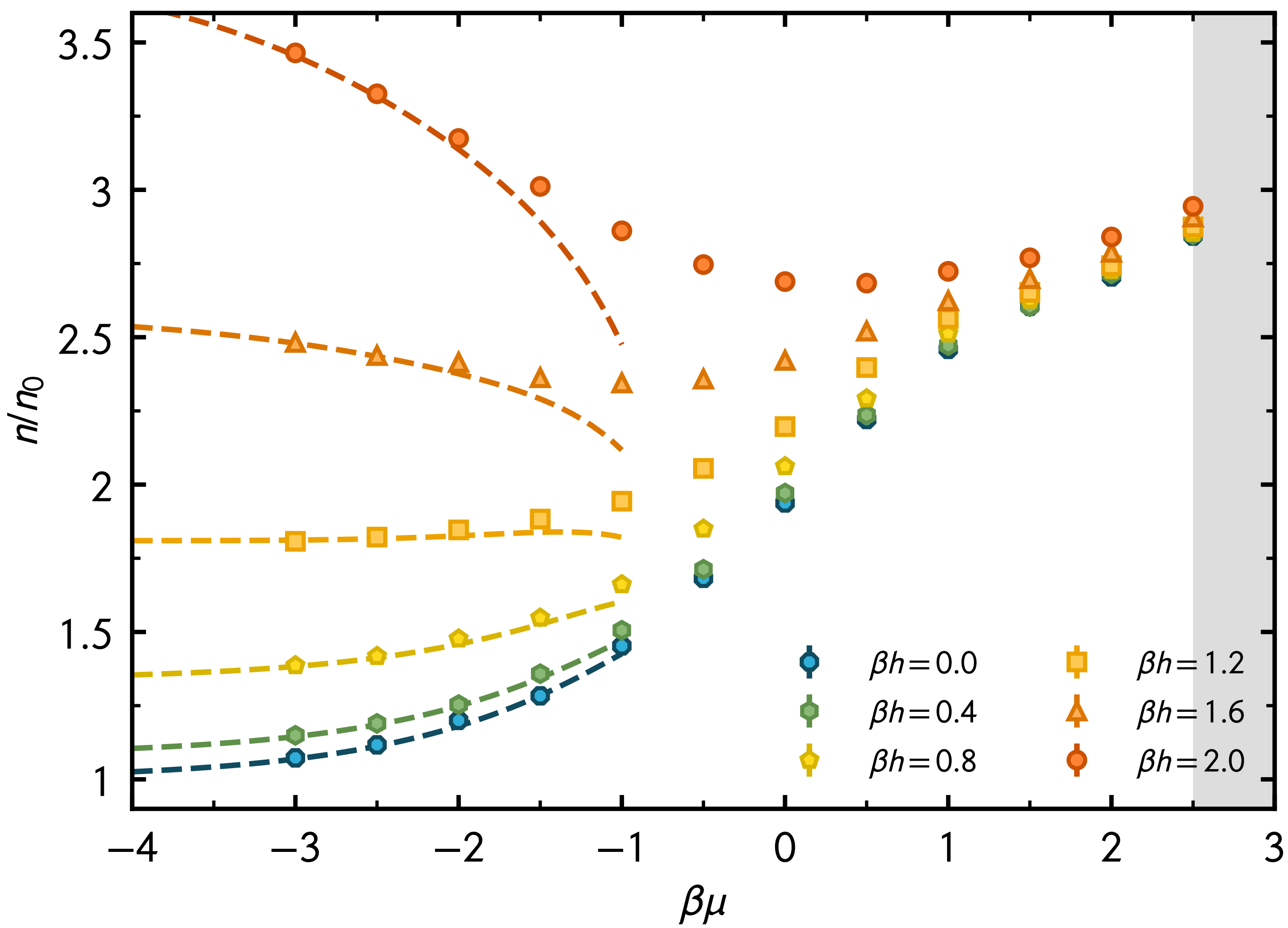
VE approaches the CL results order-by-order



VE deviates earlier for polarized systems

density EOS at finite polarization

[LR, Loheac, Drut, Braun '18]



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

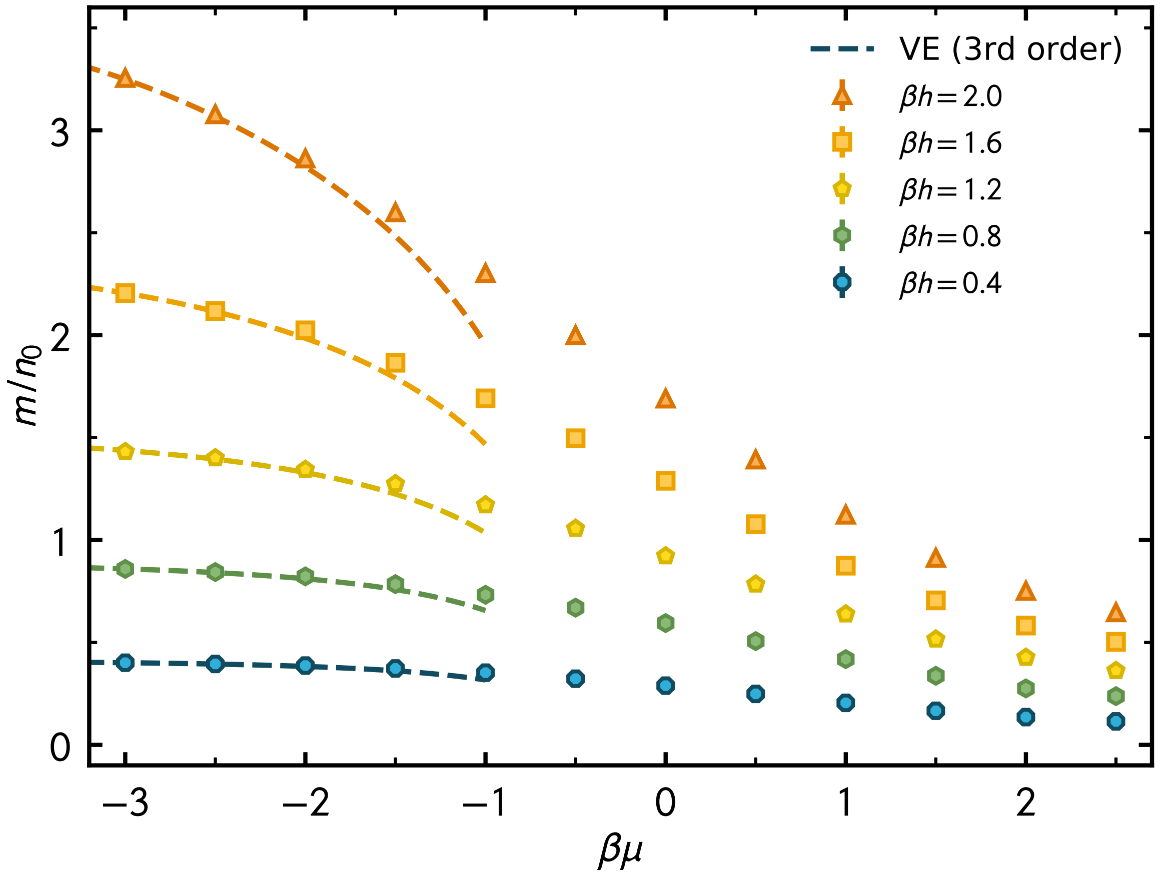
excellent agreement with virial expansion for all polarizations

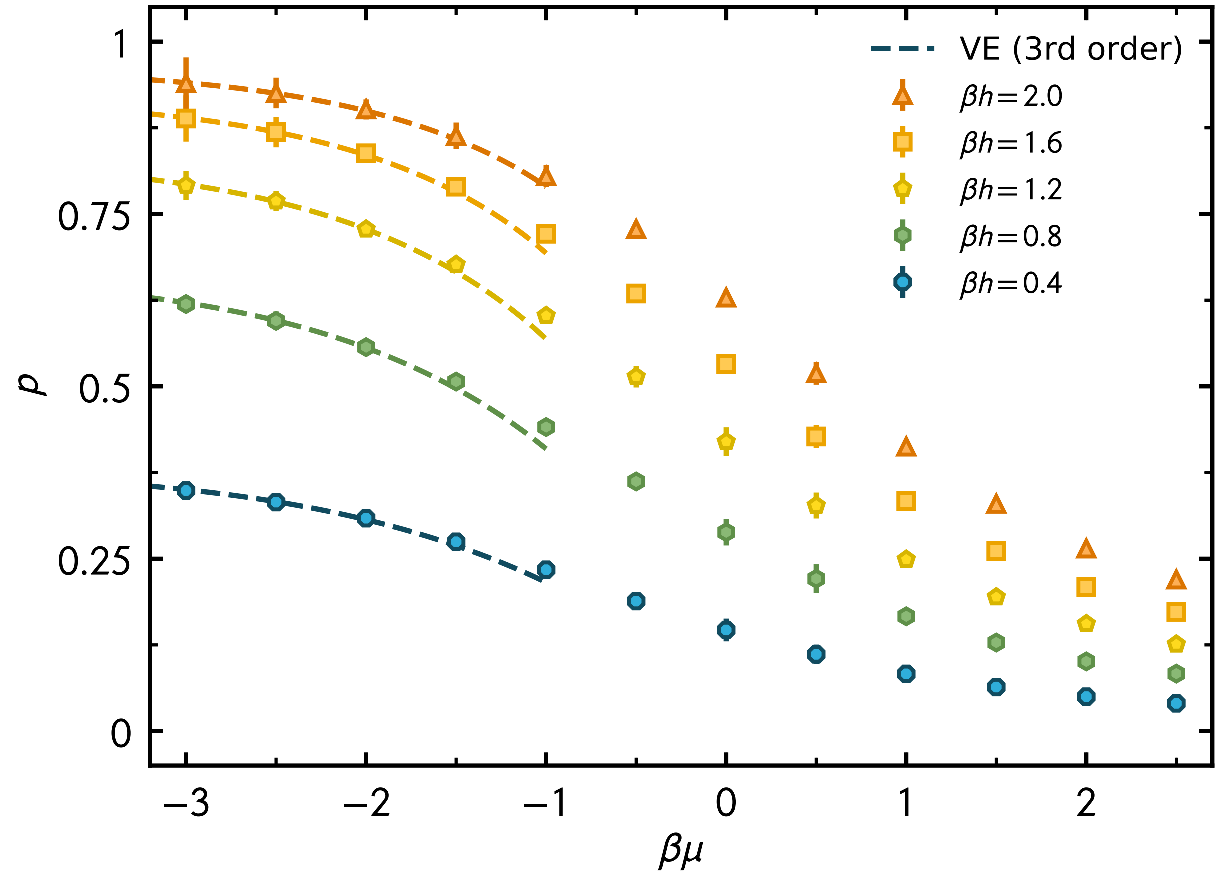
magnetization & polarization

[LR, Loheac, Drut, Braun '18]

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

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

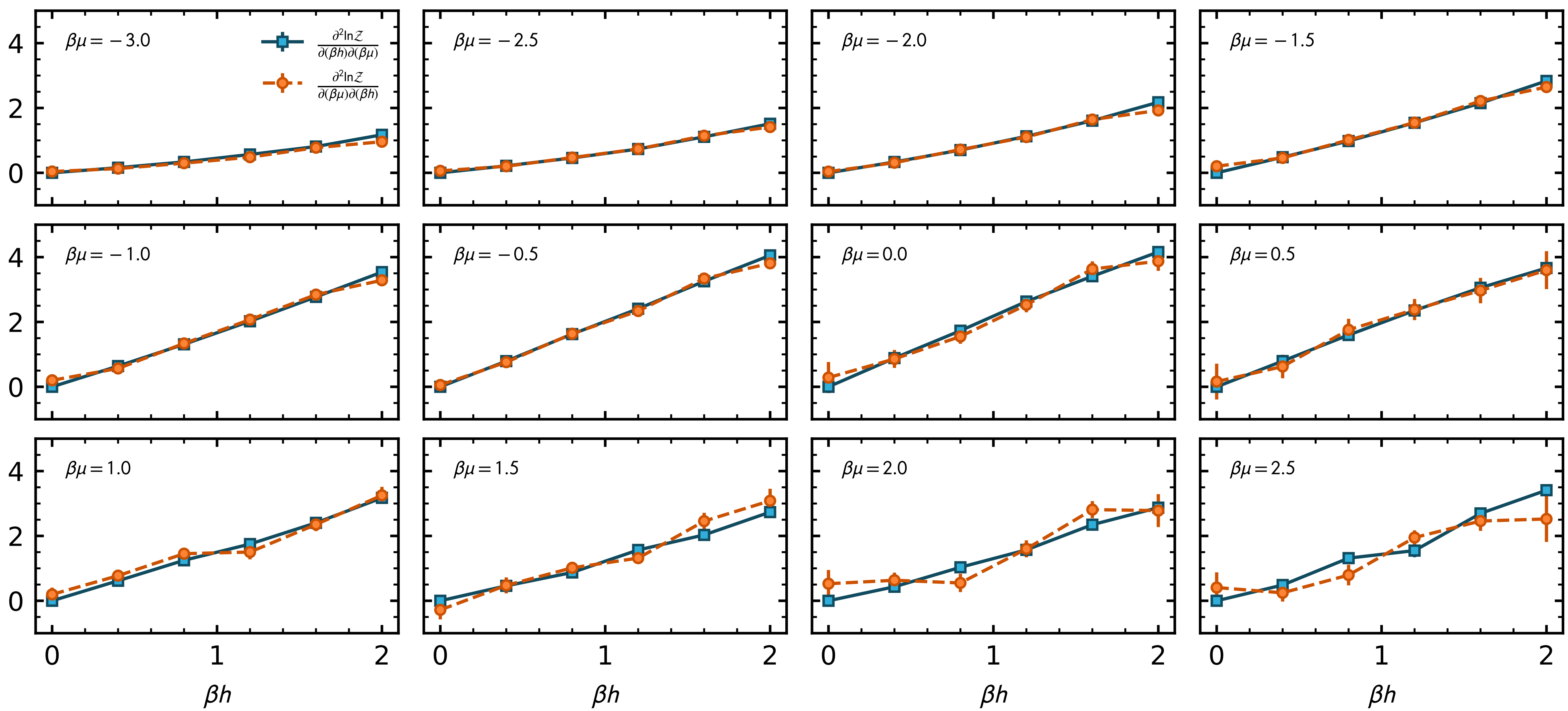




Maxwell relations: consistency check

[LR, Loheac, Drut, Braun '18]

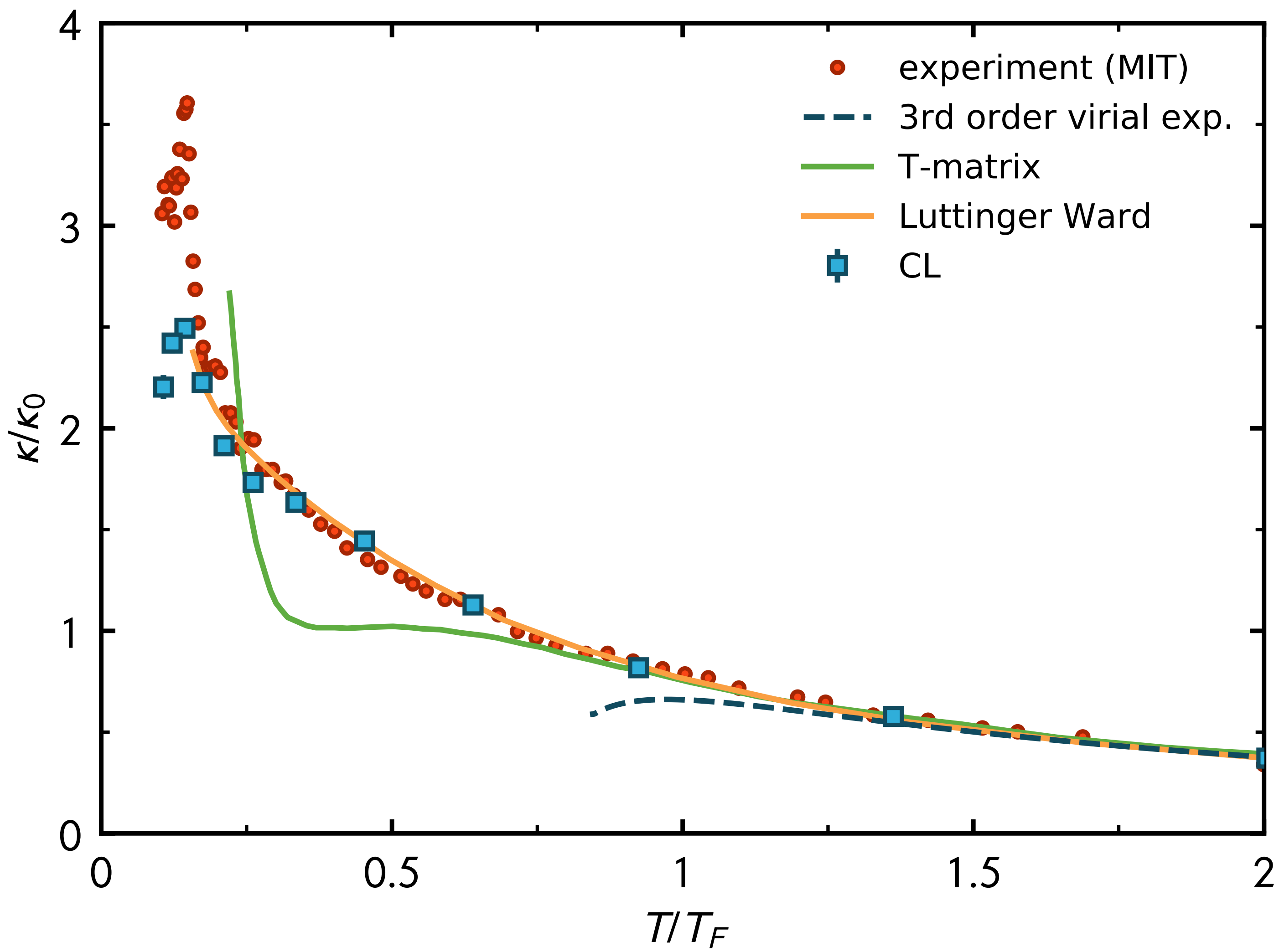
$$\left(\frac{\partial n}{\partial(\beta h)}\right)_{\beta\mu} \stackrel{!}{=} \left(\frac{\partial m}{\partial(\beta\mu)}\right)_{\beta h}$$



compressibility (unpolarized)

[LR, Loheac, Drut, Braun '18]

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



[experiment: Ku,Sommer,Cheuck,Zwierlein '12]
[Luttinger-Ward: Enns,Haussmann '12]

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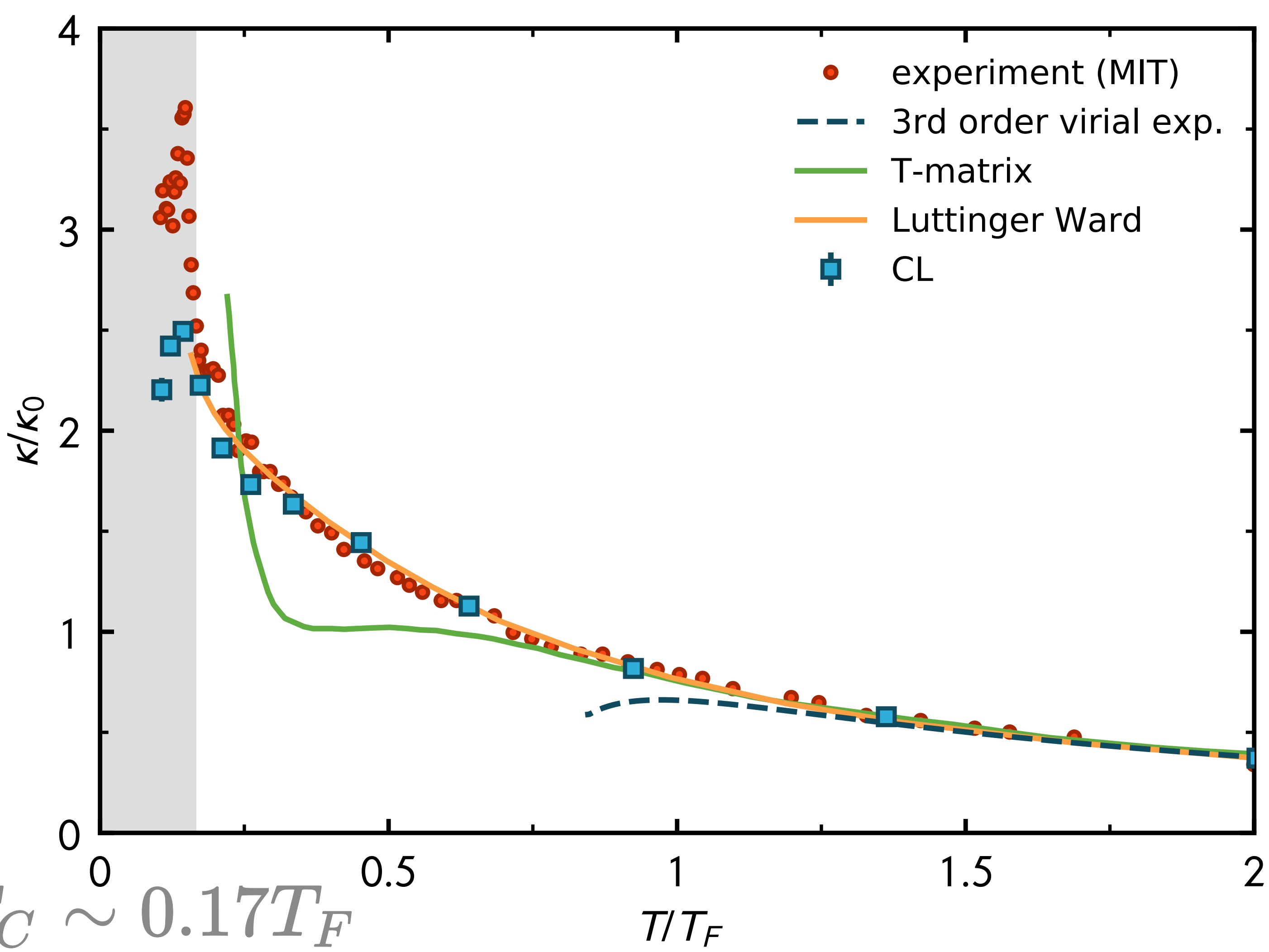
$$\kappa = \frac{1}{n}\left(\frac{\partial n}{\partial P}\right)_{T,V,h} = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_{T,V,h}$$

sudden increase of κ indicates superfluid phase transition



$T_C \sim 0.17 T_F$

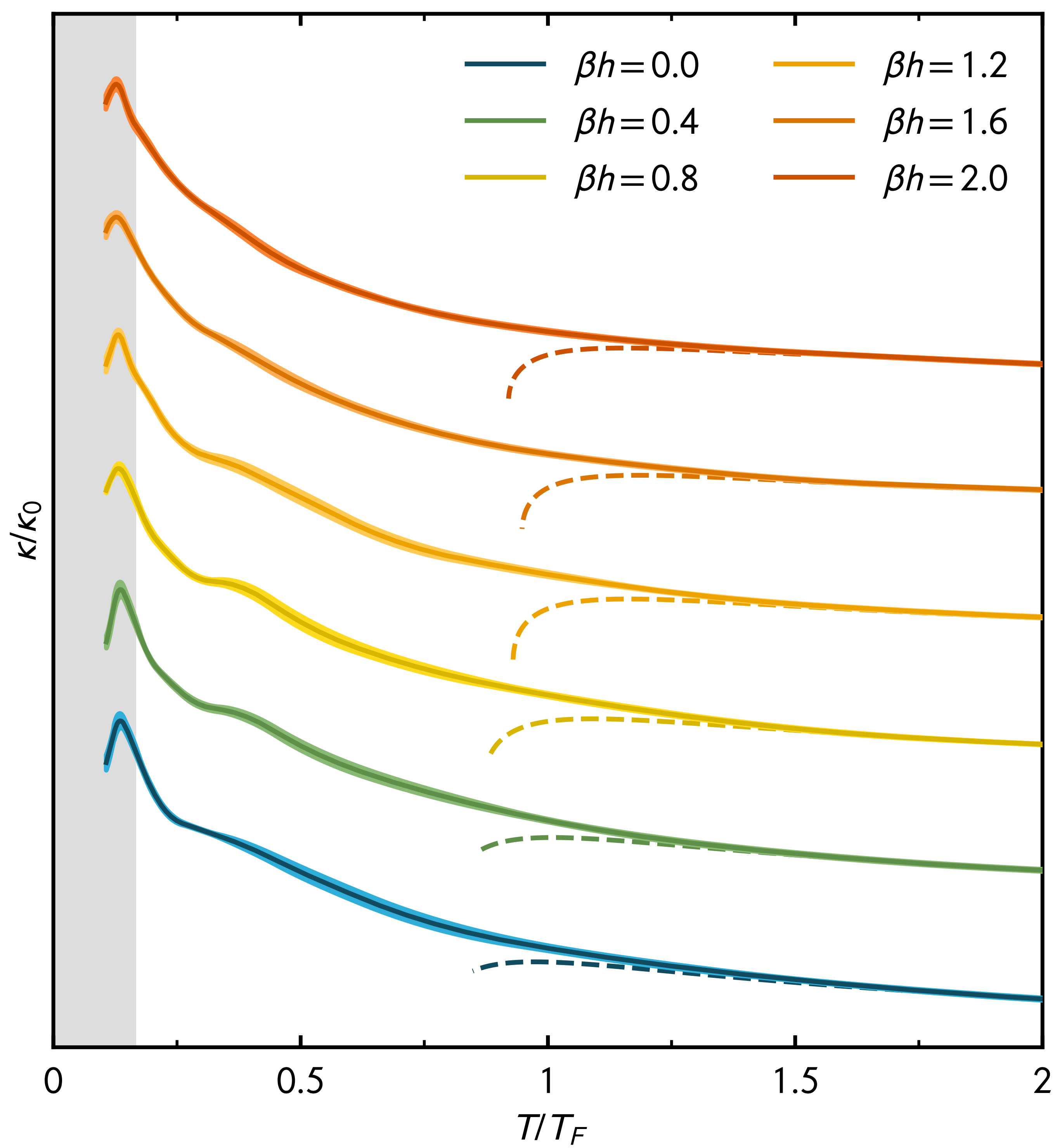
features of curve recovered with CL

quantitative disagreement at low temperatures

[experiment: Ku,Sommer,Cheuck,Zwierlein '12]
[Luttinger-Ward: Enns,Haussmann '12]

compressibility for polarized systems

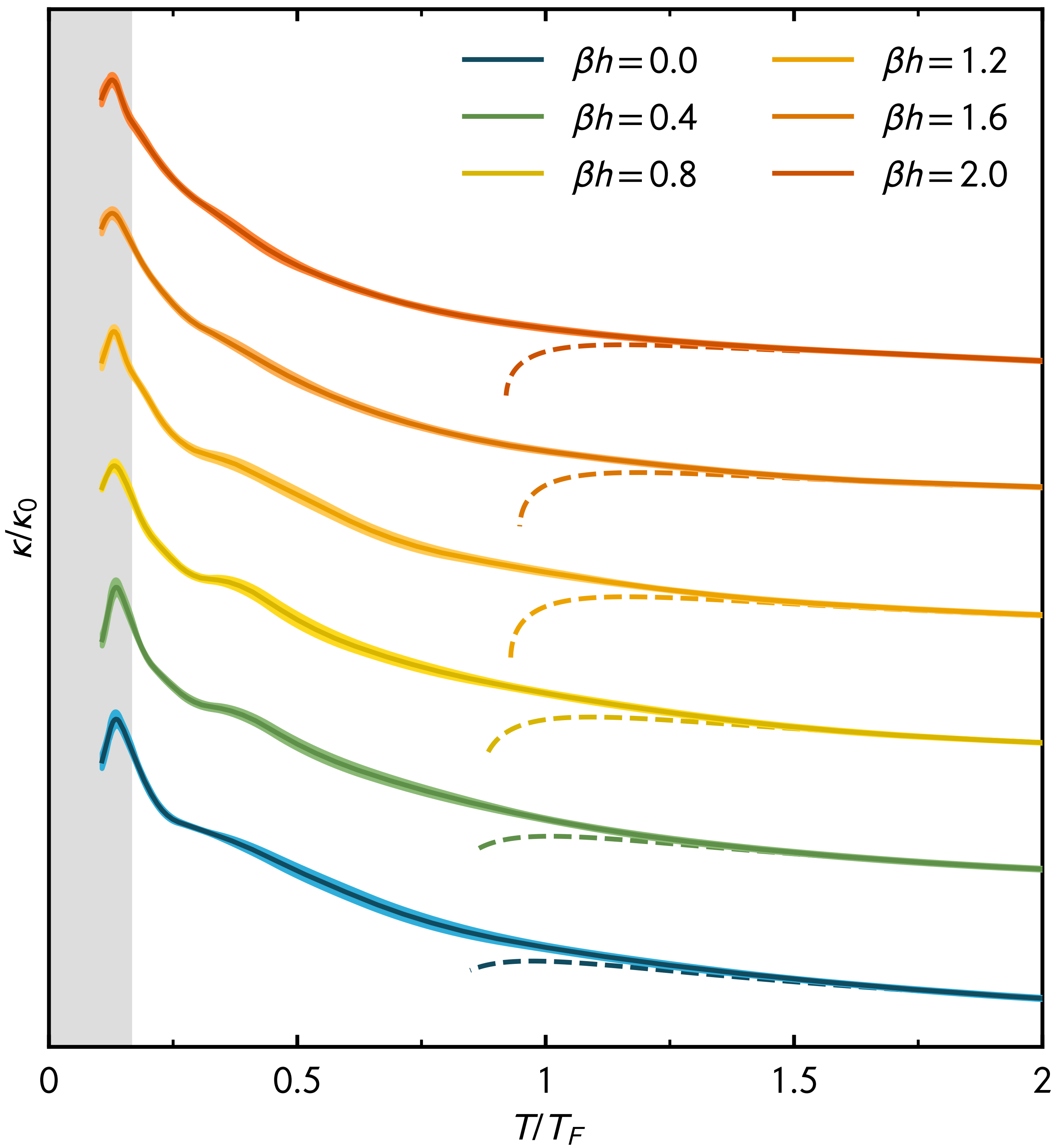
[LR, Loheac, Drut, Braun '18]



compressibility for polarized systems

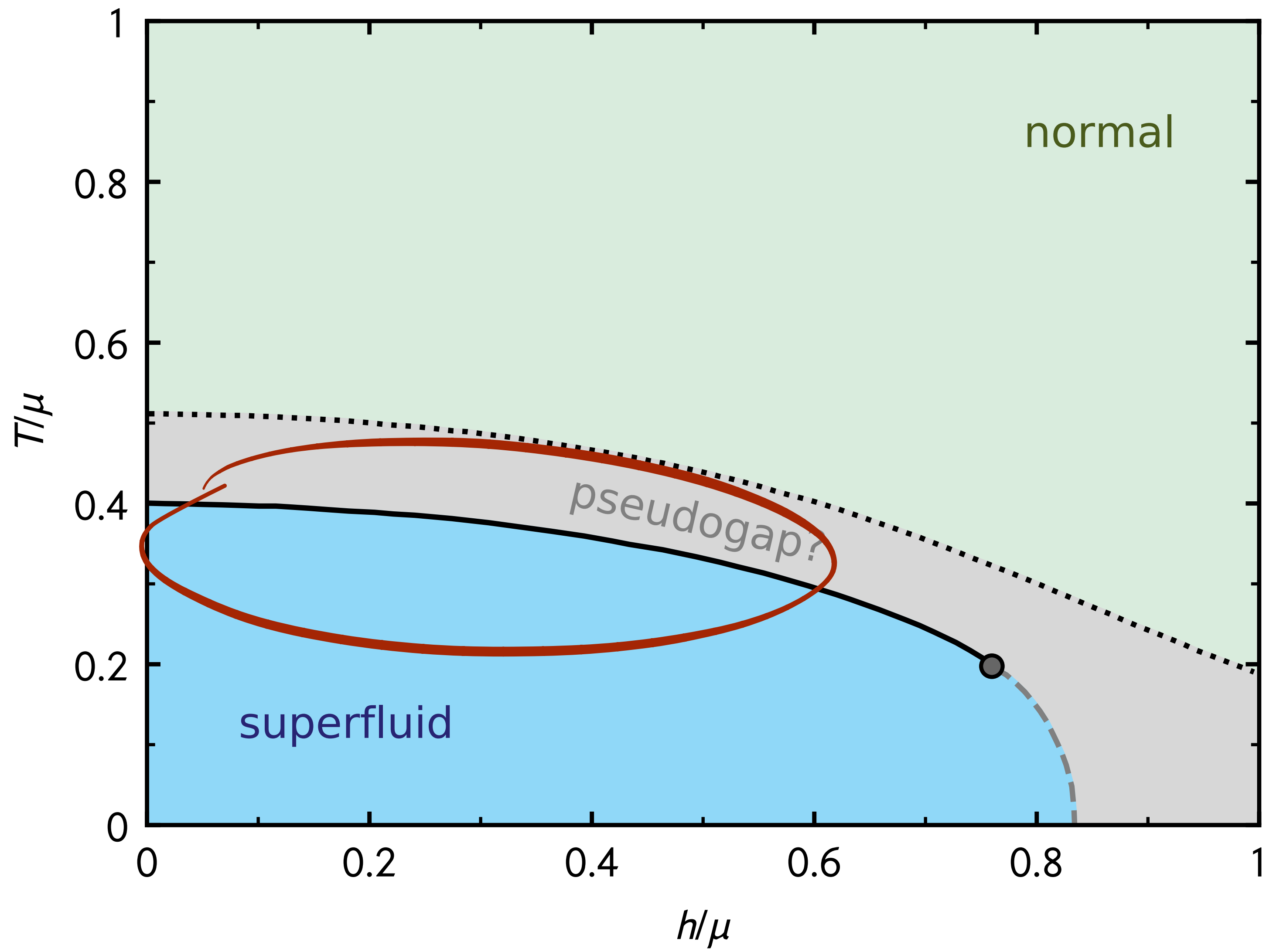
[LR, Loheac, Drut, Braun '18]

weak dependence of the critical temperature on polarization indicated



challenging to extract precise T_C

UFG phase diagram



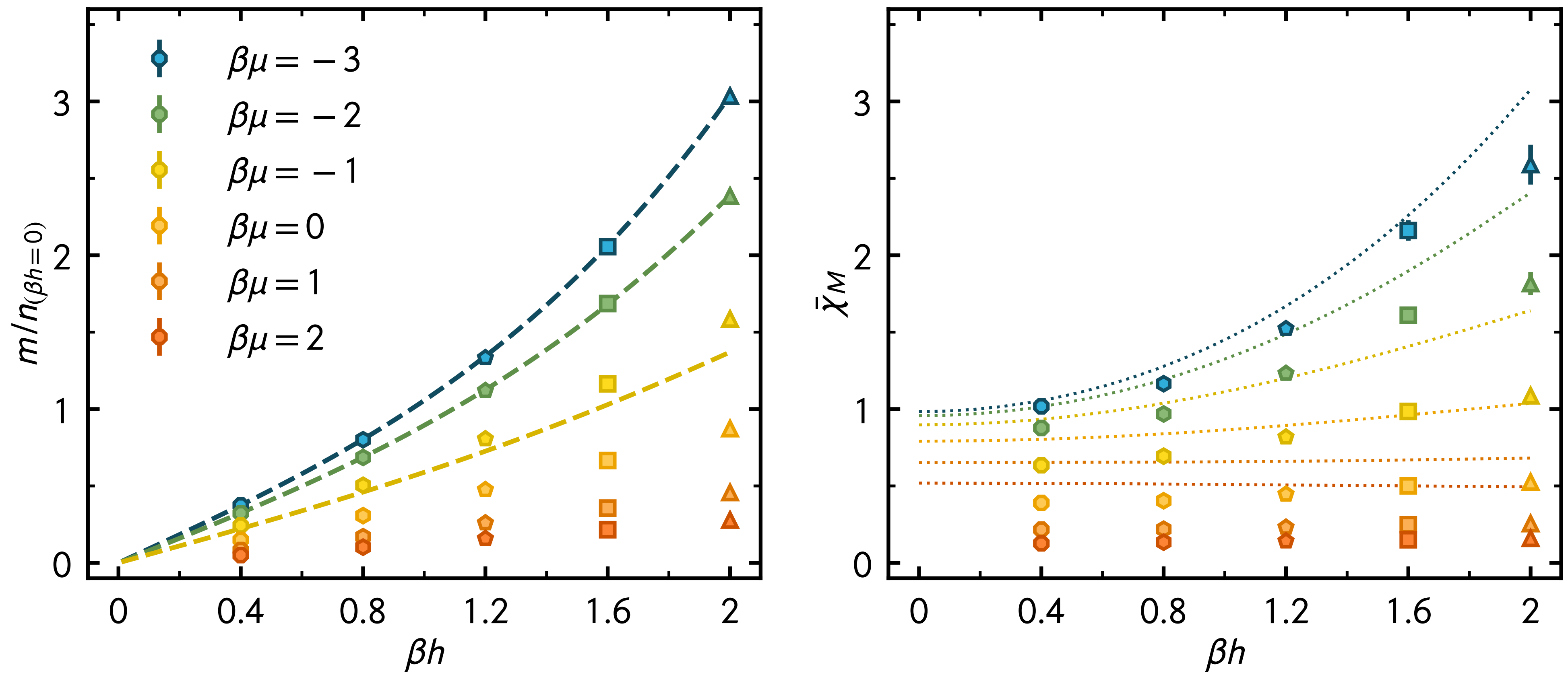
$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$
$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

[fRG: Boettcher et. al '15]

spin susceptibility

[LR, Loheac, Drut, Braun '18]

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



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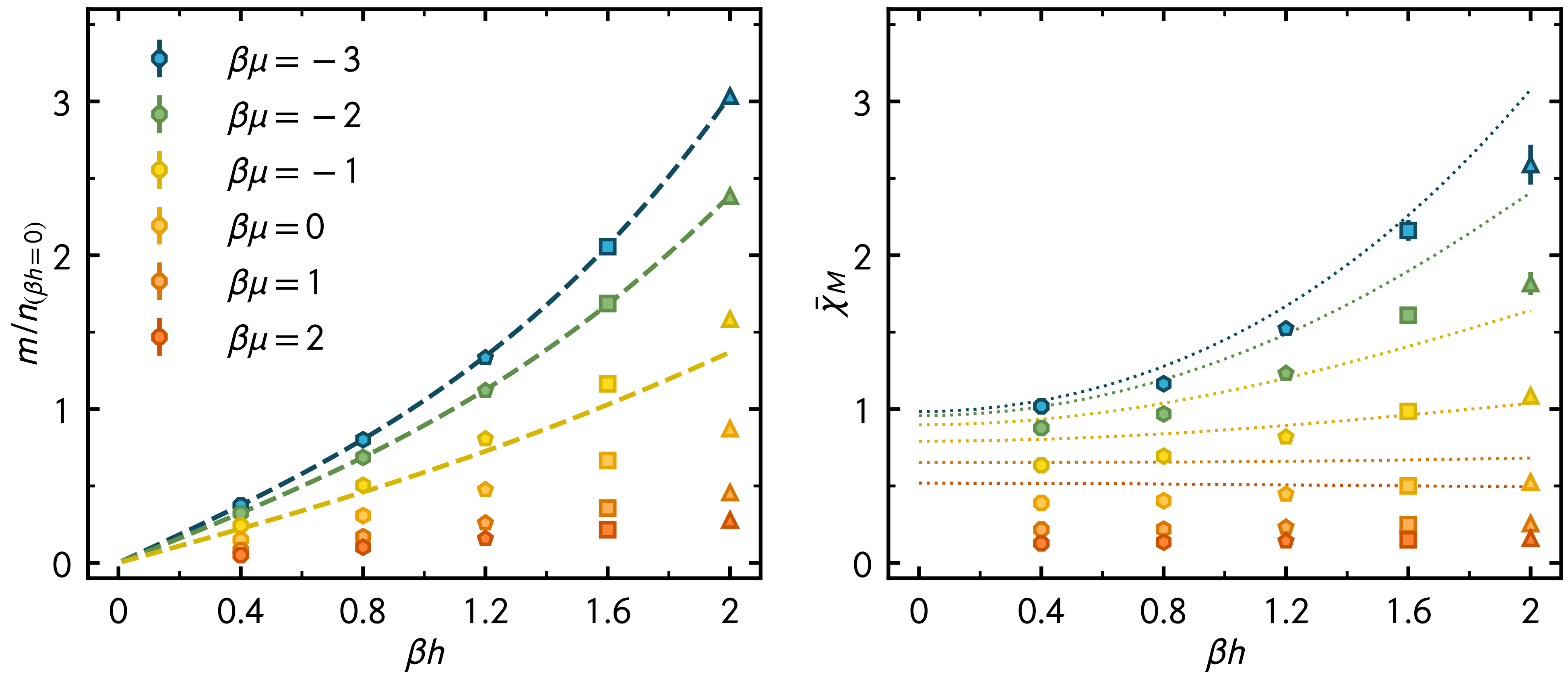
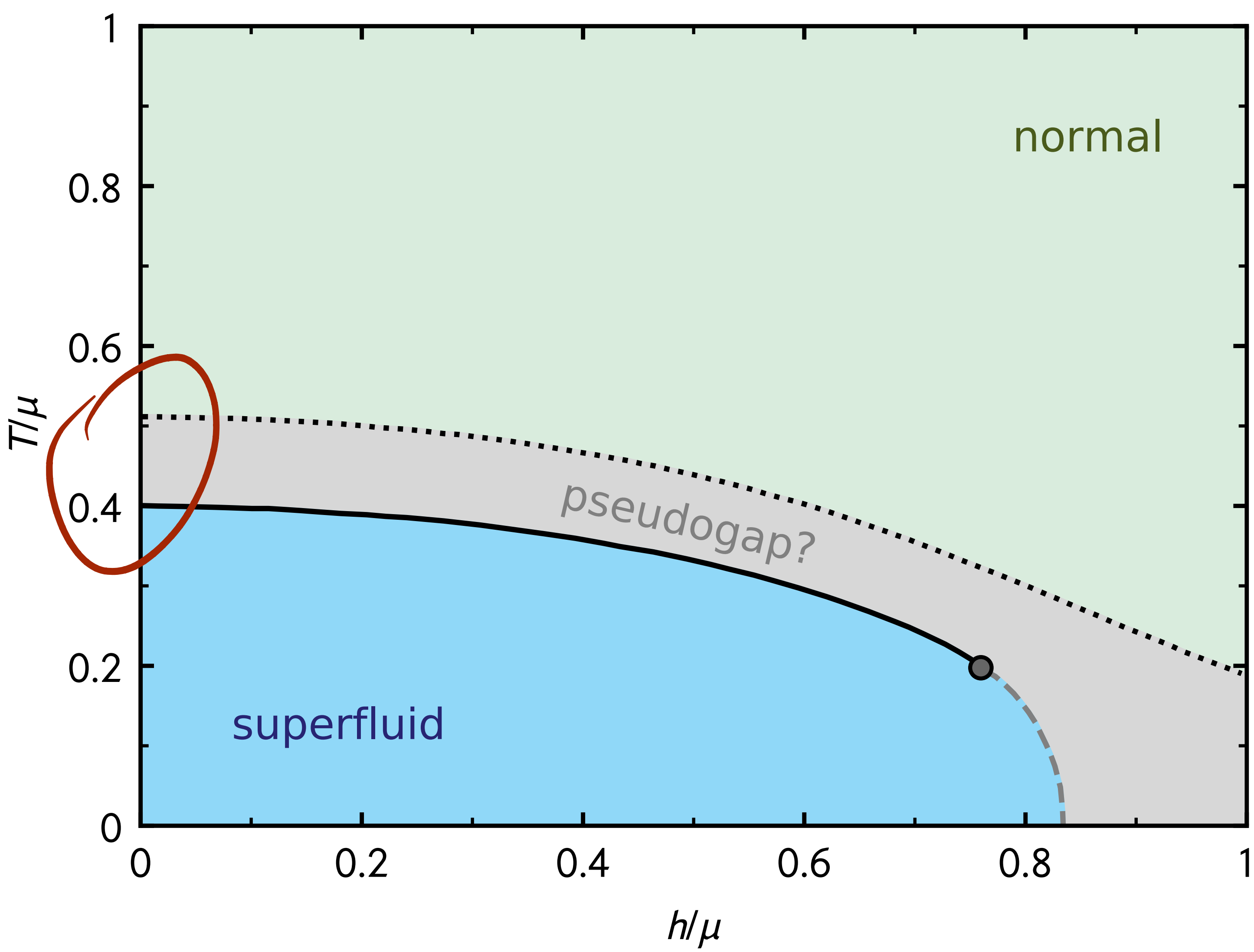


Pauli susceptibility field independent at low field and temperature

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

UFG phase diagram (sketch)



$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$
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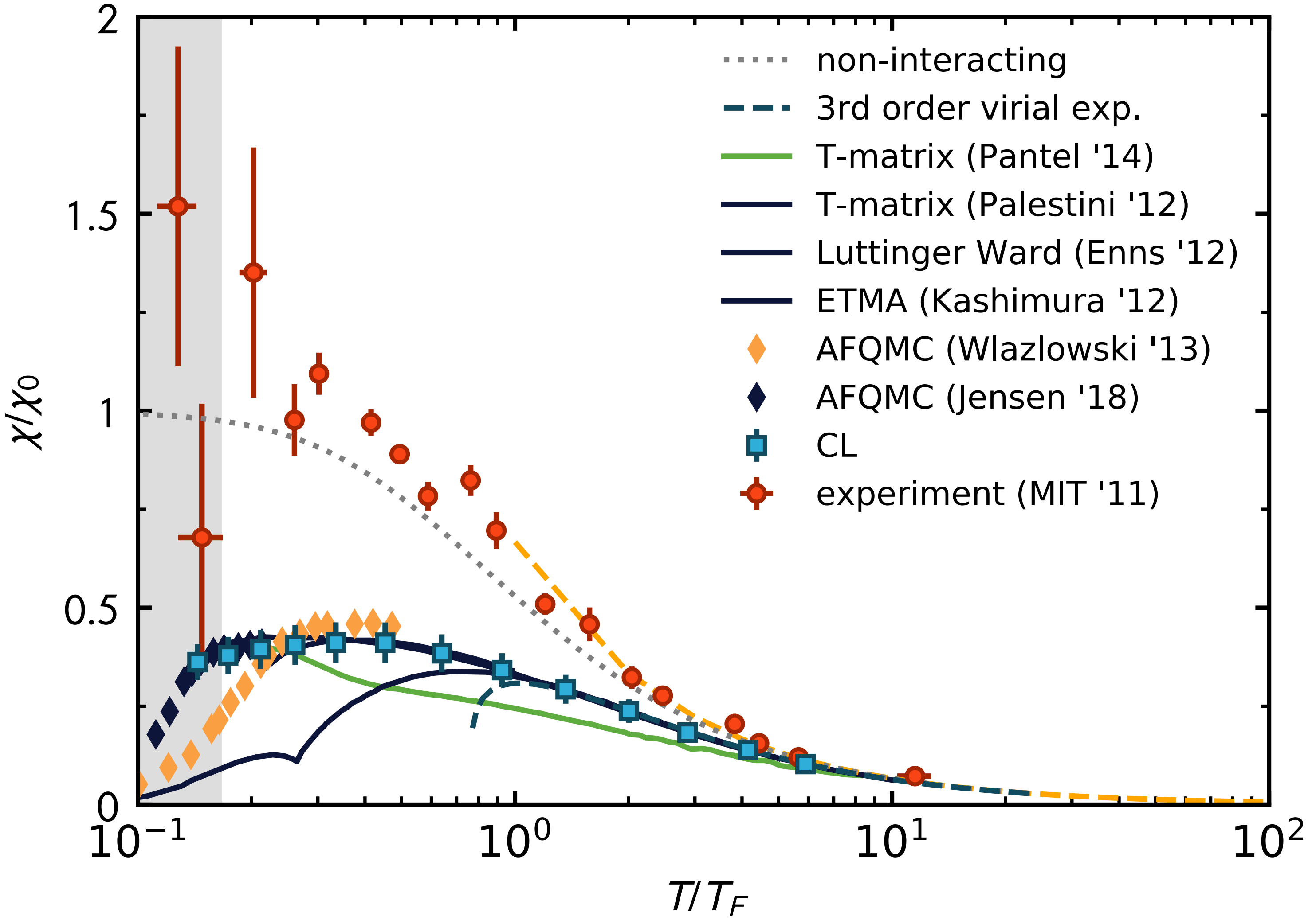
[fRG: Boettcher et. al '15]

magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]



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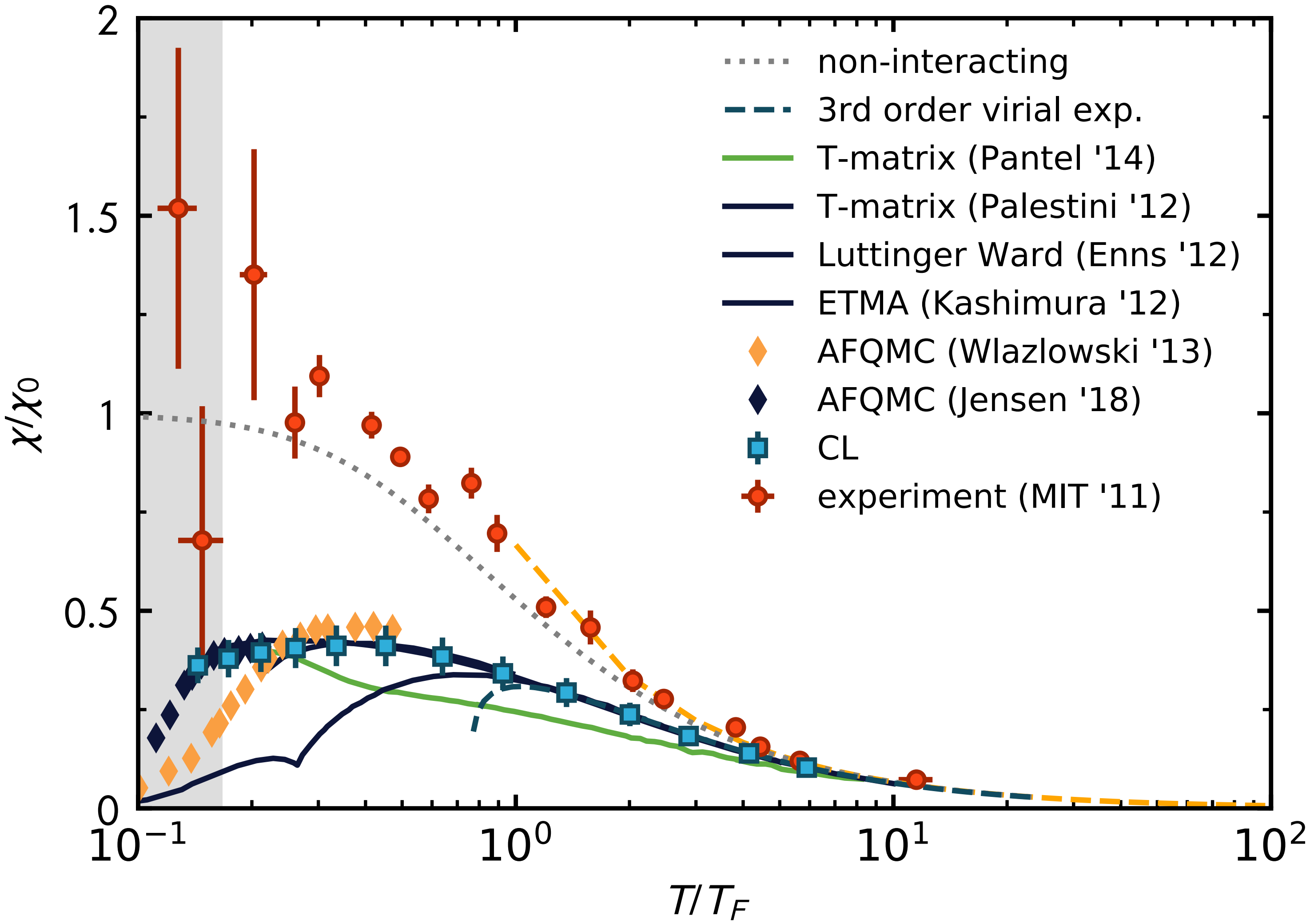


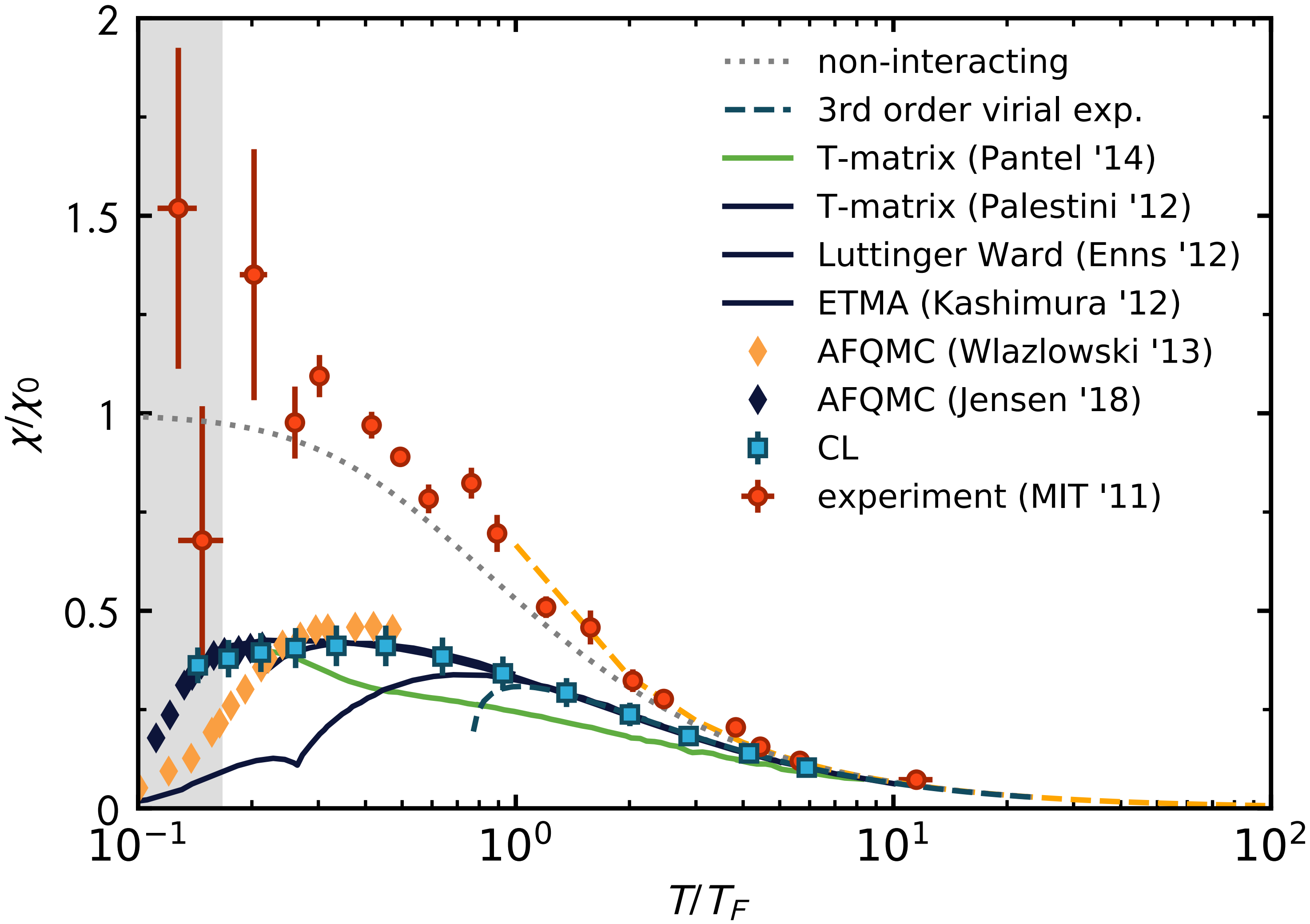
high temperature:
Curie's law
$\chi \propto T^{-1}$

theory & experiment agree at high temperatures

magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]

low temperature: discrepancy between experiment and theory



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Pseudogap: suppression of χ at $T > T_C$

[recent review: Jensen et al. '18]

magnetic susceptibility (unpolarized)

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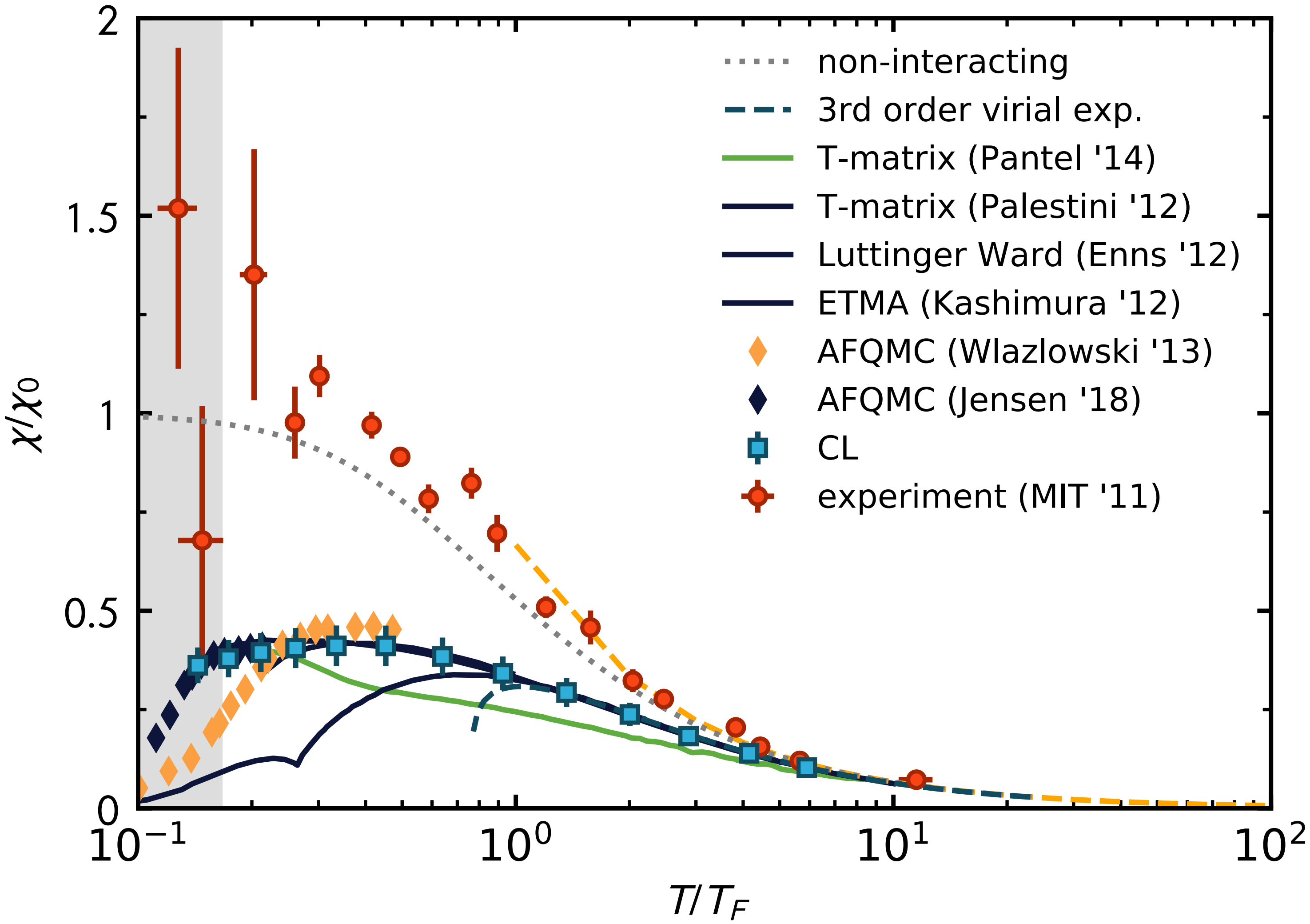


high temperature: Curie's law $\chi \propto T^{-1}$

theory & experiment agree at high temperatures

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

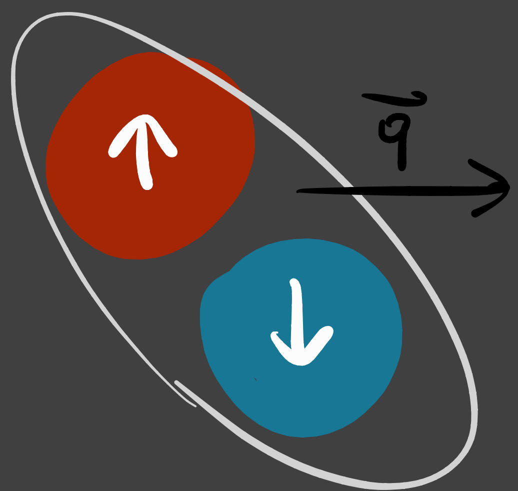
RECAP

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

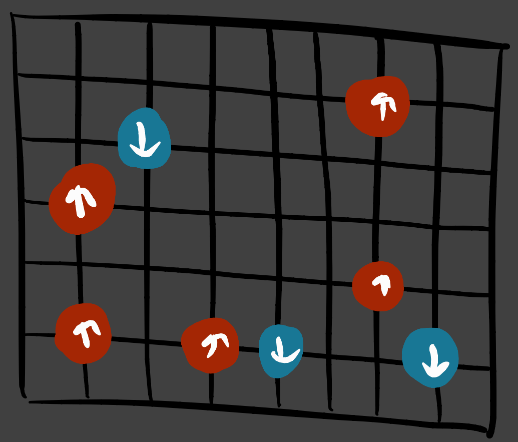
complex Langevin **matches state-of-the art results from other methods** wherever available

EOS, magnetic properties & response accessible for the unitary Fermi gas at finite temperature and polarization **in ab initio fashion**

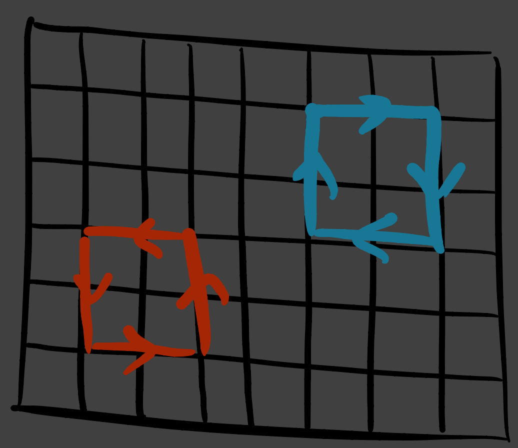
STAY TUNED!



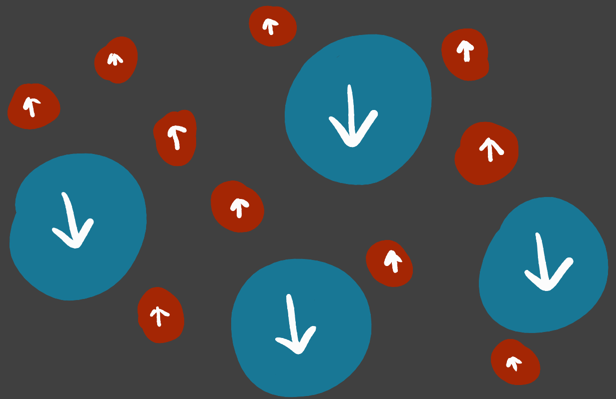
looking for inhomogeneous phases in the UFG



thermodynamics of 2D fermions at finite polarization
[with Josh McKenney, Andrew Loheac & Joaquin Drut, UNC Chapel Hill]



vortex formation in 2D rotating bosons
[Casey Berger & Joaquin Drut, UNC Chapel Hill]



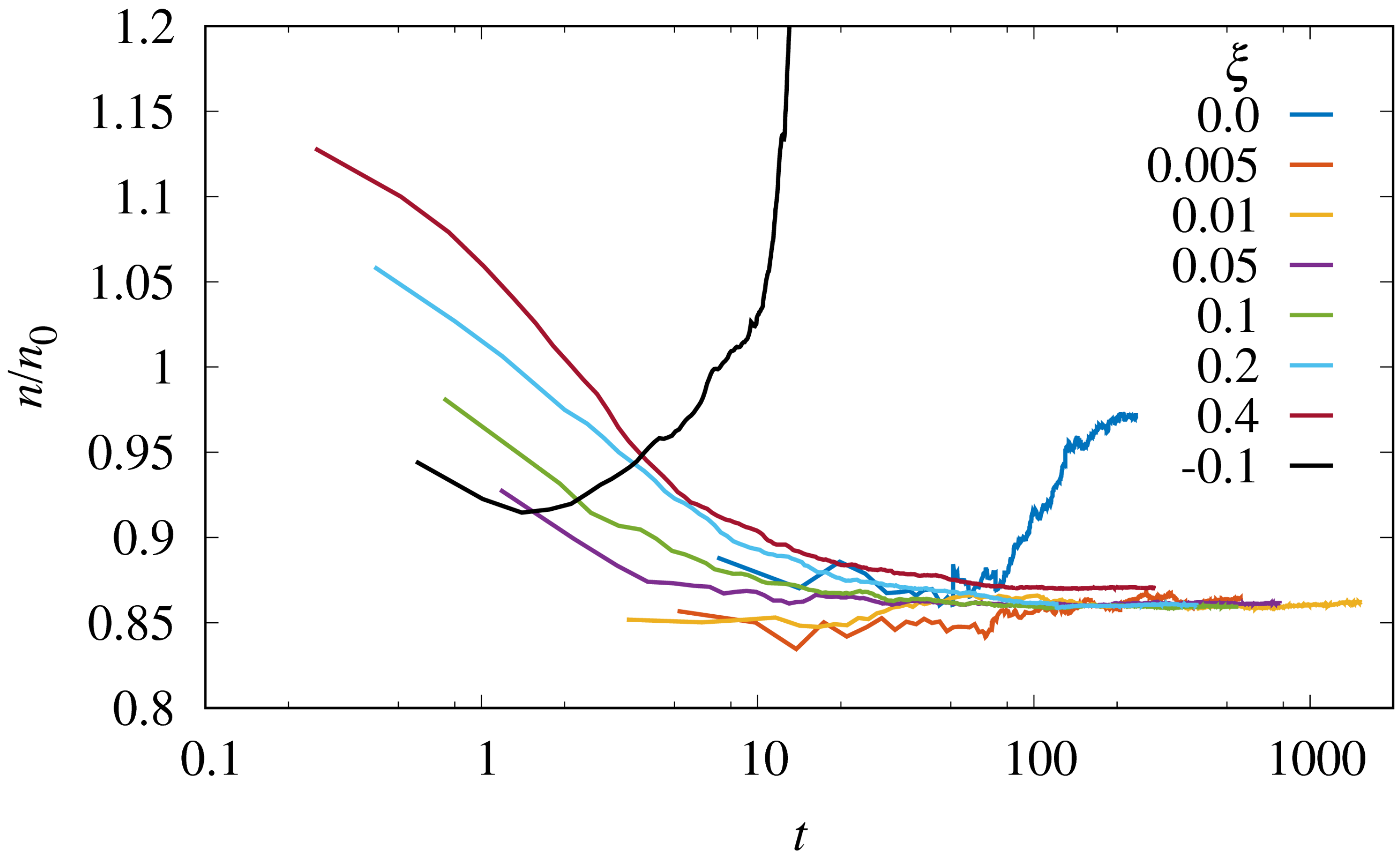
effect of mass-imbalance on fermion pair formation

APPENDIX

regulator to stabilize numerics

[Loheac,Drut '17]

$$\phi^{(n+1)} = \phi^{(n)} - \left.\frac{\delta S[\phi]}{\delta\phi}\right|_{\phi^{(n)}} \Delta t_L - 2\xi\phi^{(n)} + \sqrt{2\Delta t_L}\,\eta$$

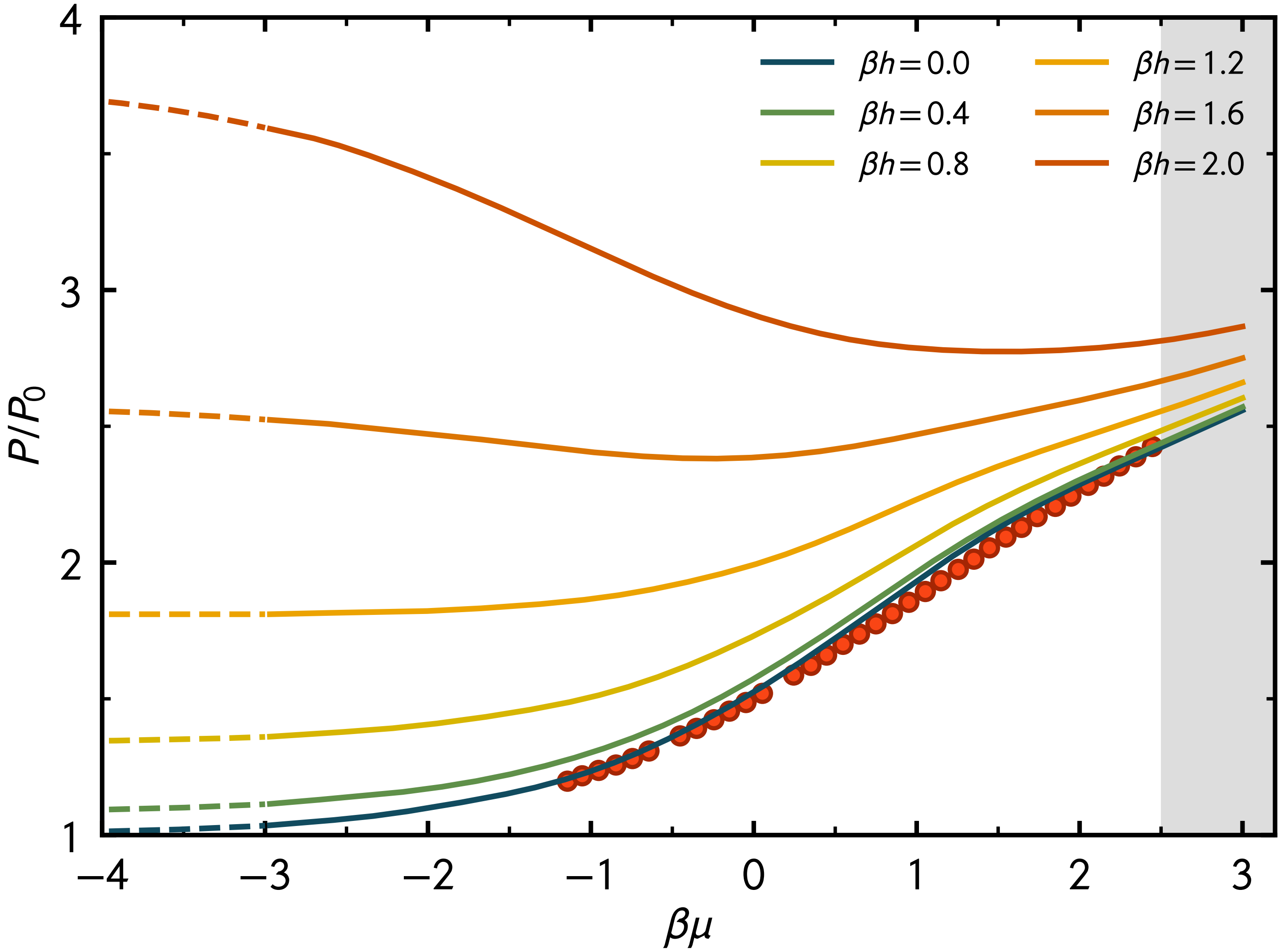


unregulated runs tend to fail: **ξ stabilizes CL trajectories**

pressure equation of state

[LR, Loheac, Drut, Braun '18]

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

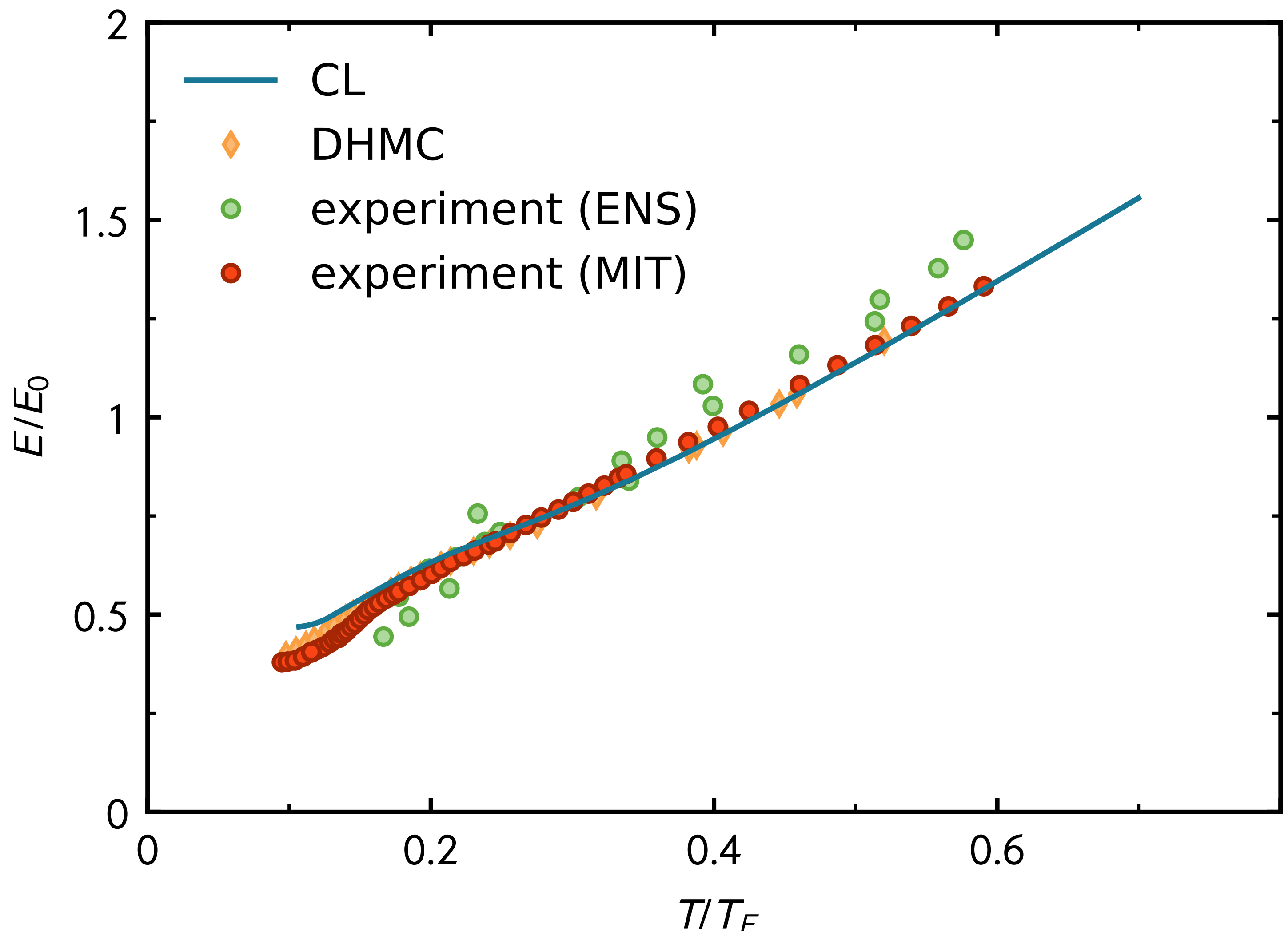


[experiment: Ku,Sommer,Cheuck,Zwierlein '12]

energy equation of state

[LR, Loheac, Drut, Braun in preparation]

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



[universality: Ho '04]
[experiment: Ku,Sommer,Cheuck,Zwierlein '12; Nascimbène et al. '10]

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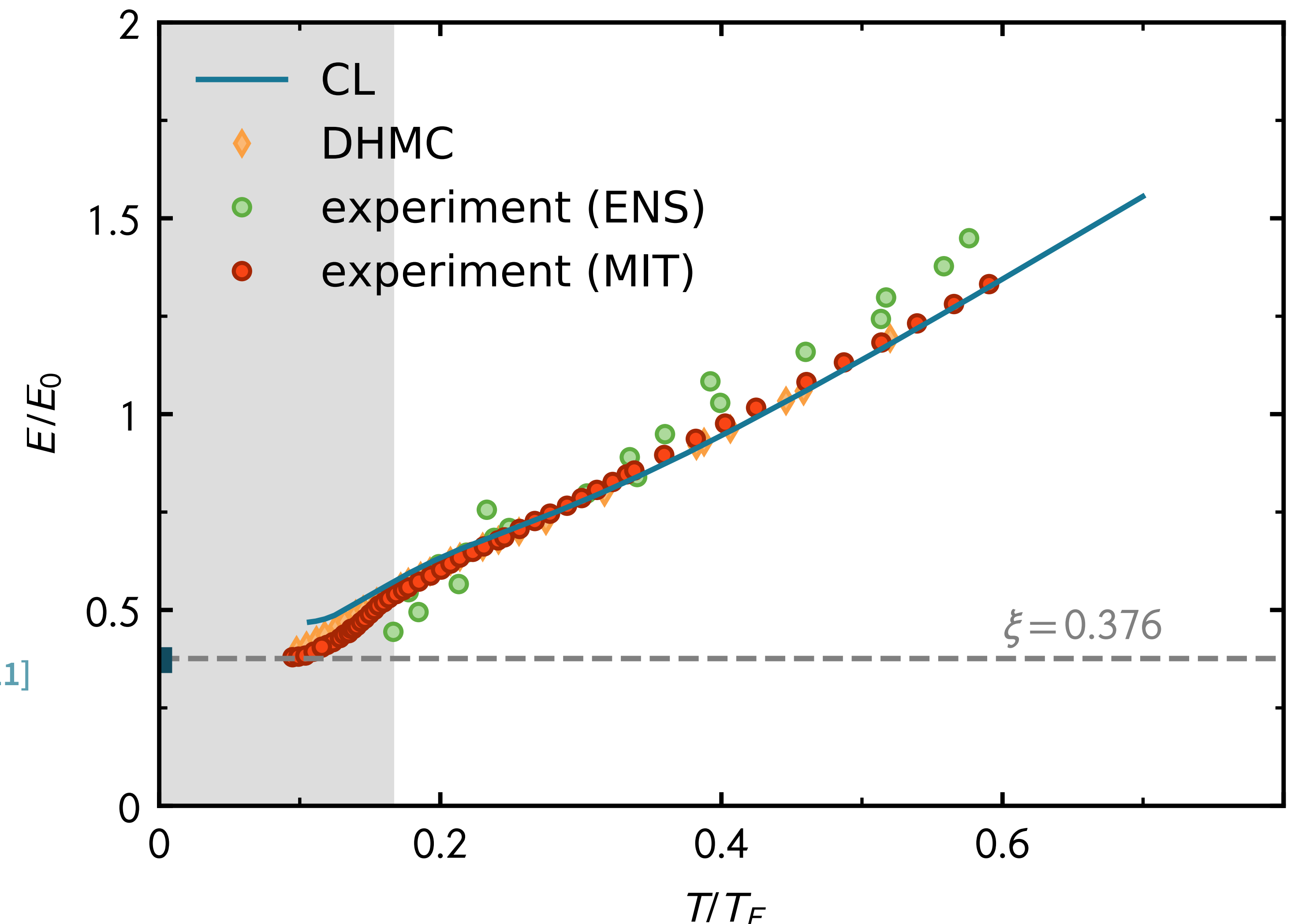

[ξ, theory: Carlson et al. '11]

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

[universality: Ho '04]

[experiment: Ku,Sommer,Cheuck,Zwierlein '12; Nascimbène et al. '10]

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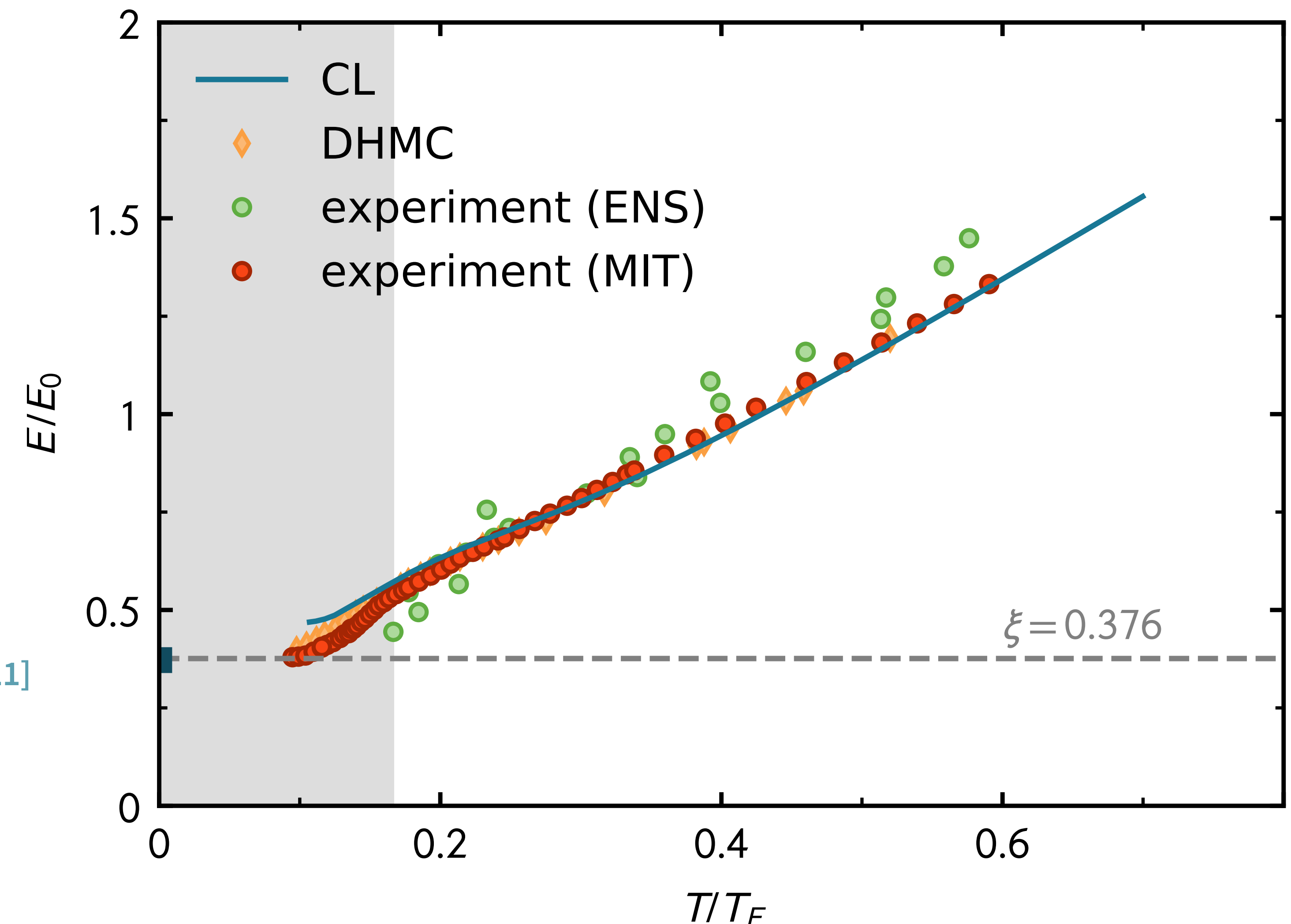

at low temperature: larger lattices, improved operators

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

[ξ, theory: Carlson et al. '11]

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

[universality: Ho '04]

[experiment: Ku,Sommer,Cheuck,Zwierlein '12; Nascimbène et al. '10]