

# STOCHASTIC QUANTIZATION AND SPIN-POLARIZED FERMI GASES

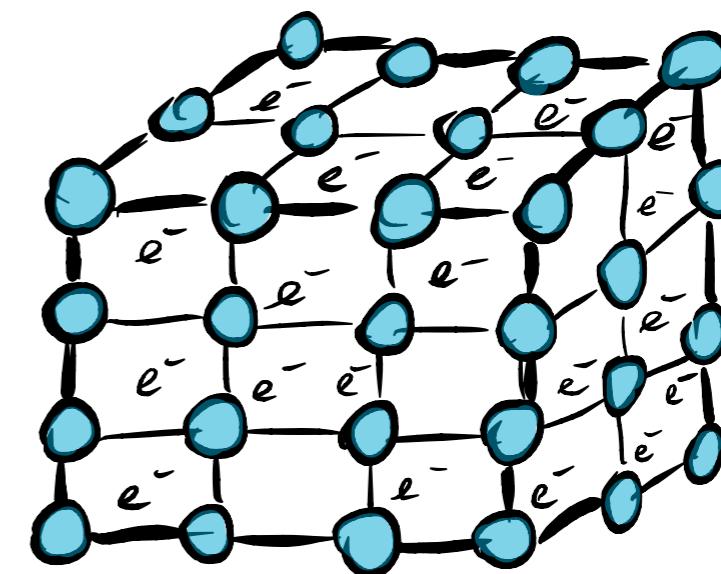
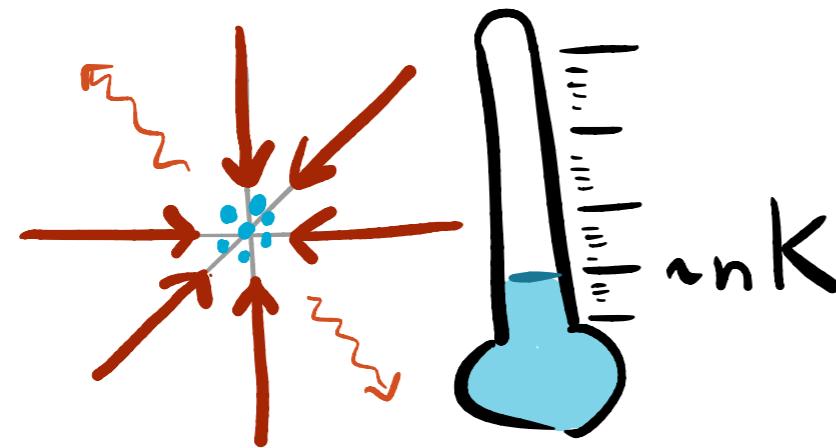
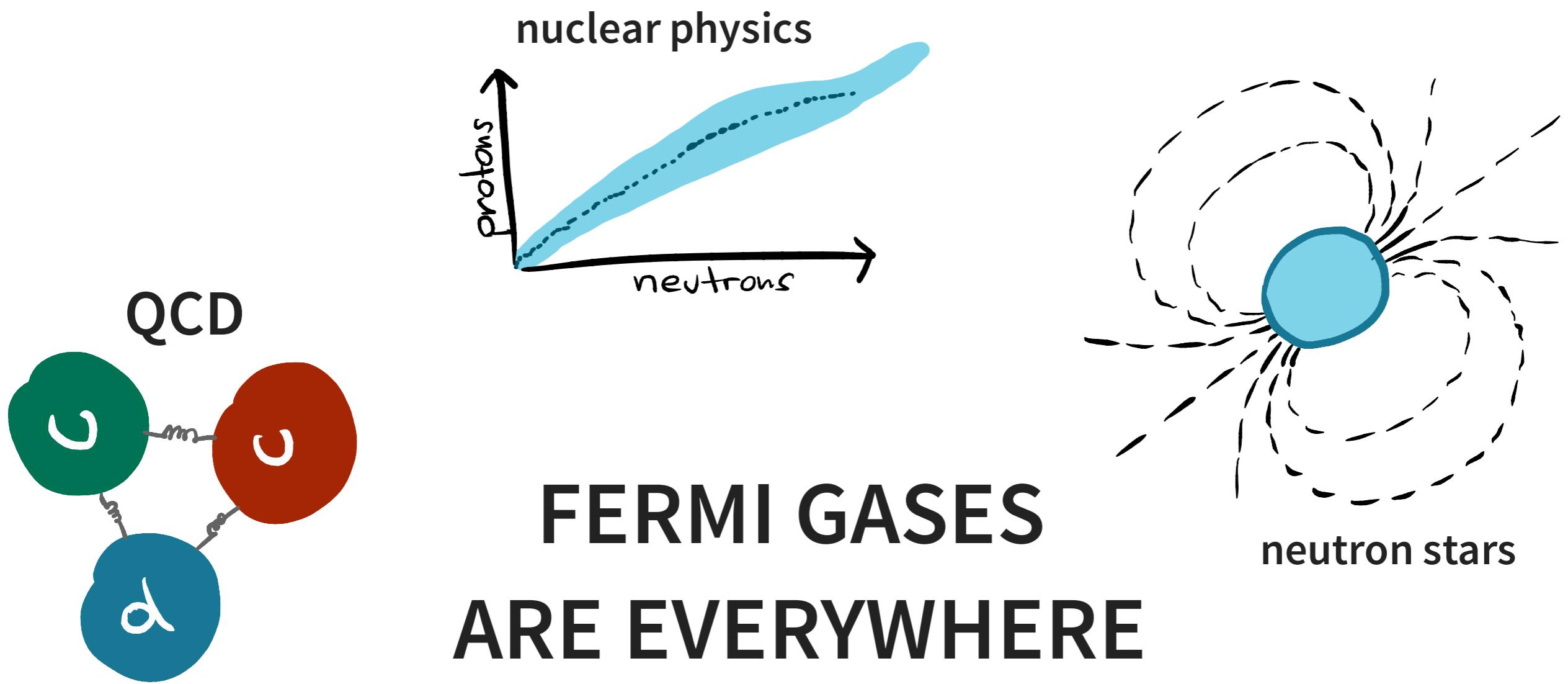
Lukas Rammelmüller, TU Darmstadt

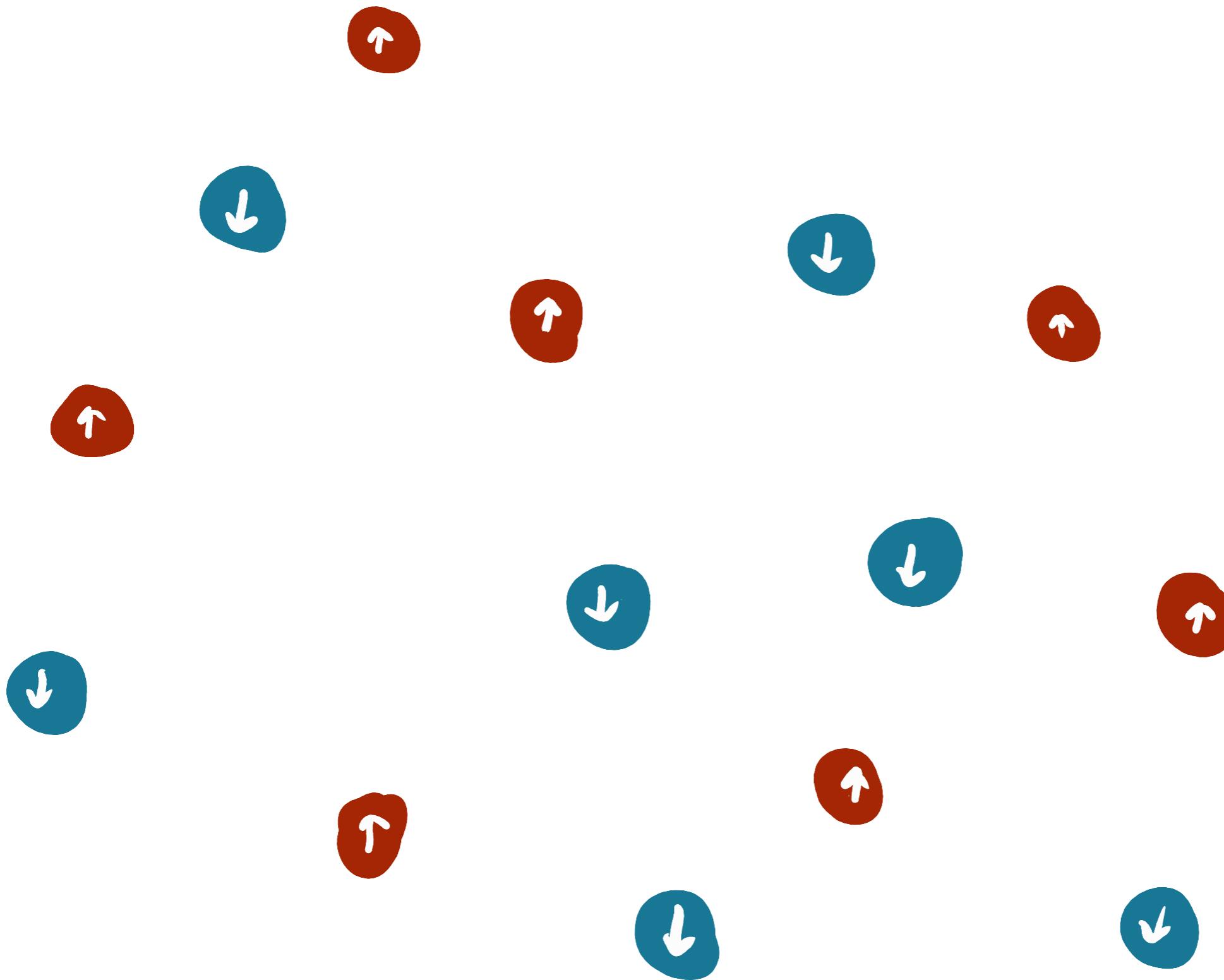
Ludwig-Maximilians-Universität München  
March 11, 2019

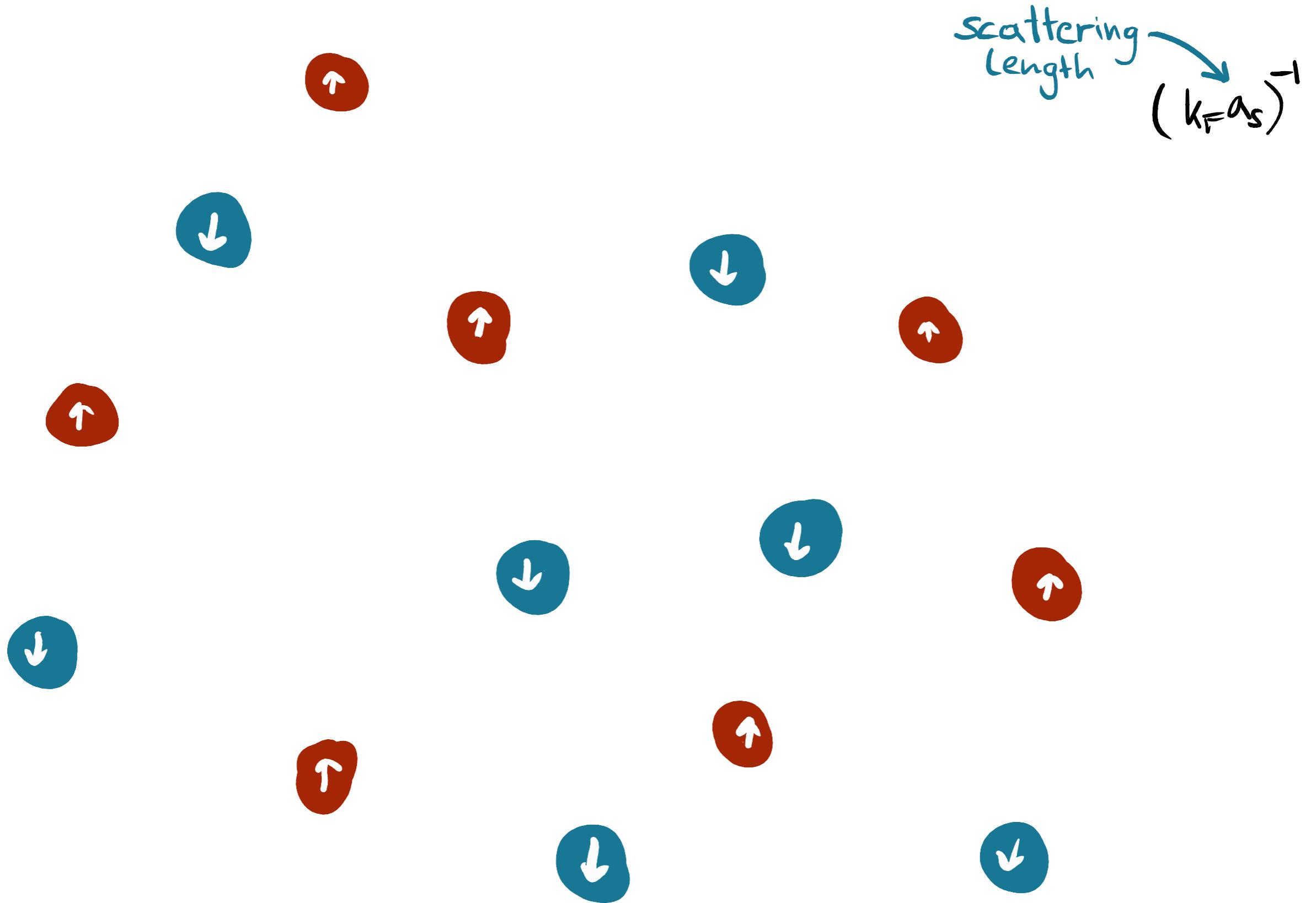
[LR, Drut, Braun *in preparation*]

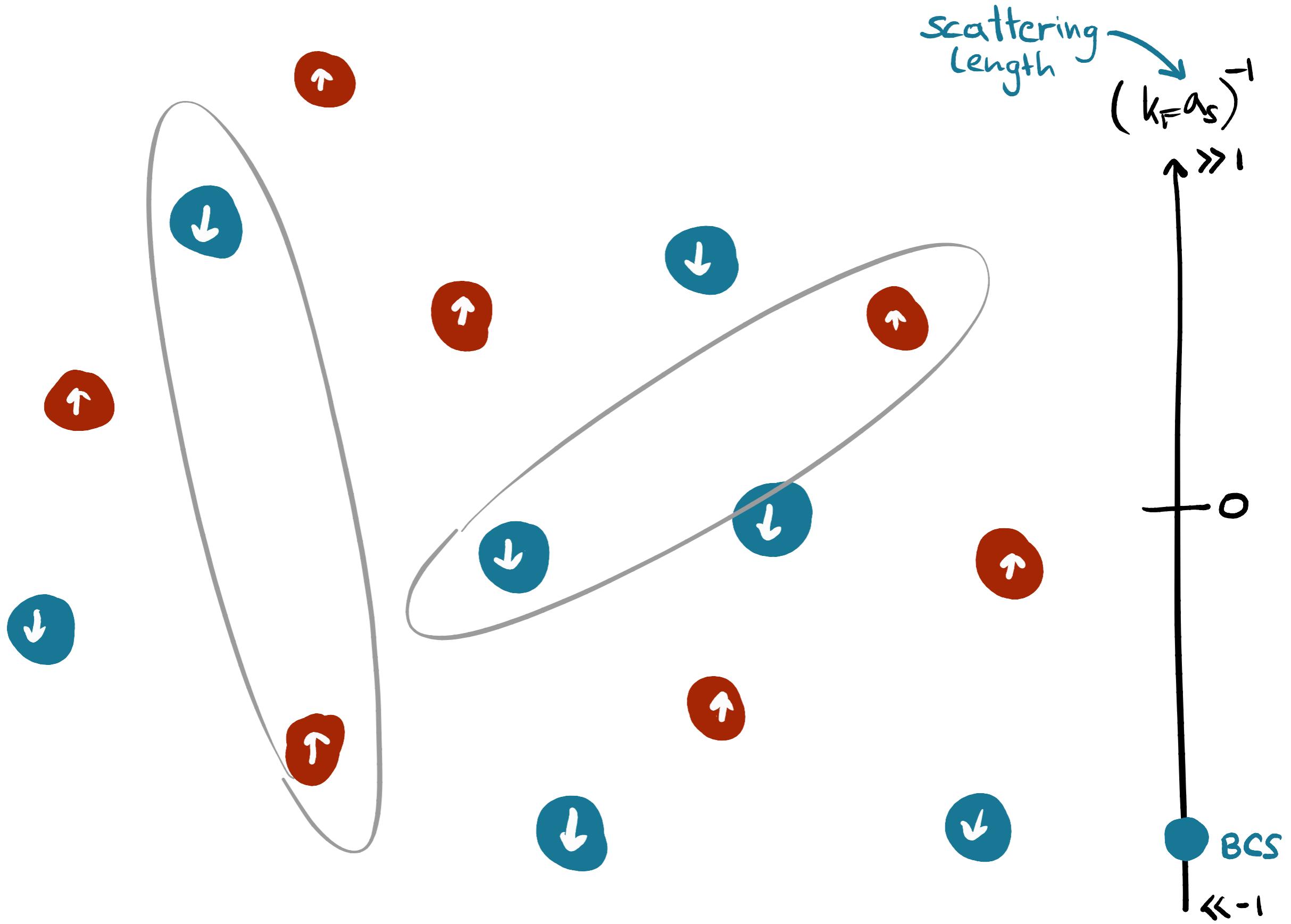
[LR, Loheac, Drut, Braun *Phys. Rev. Lett.* 121, 173001, 2018]

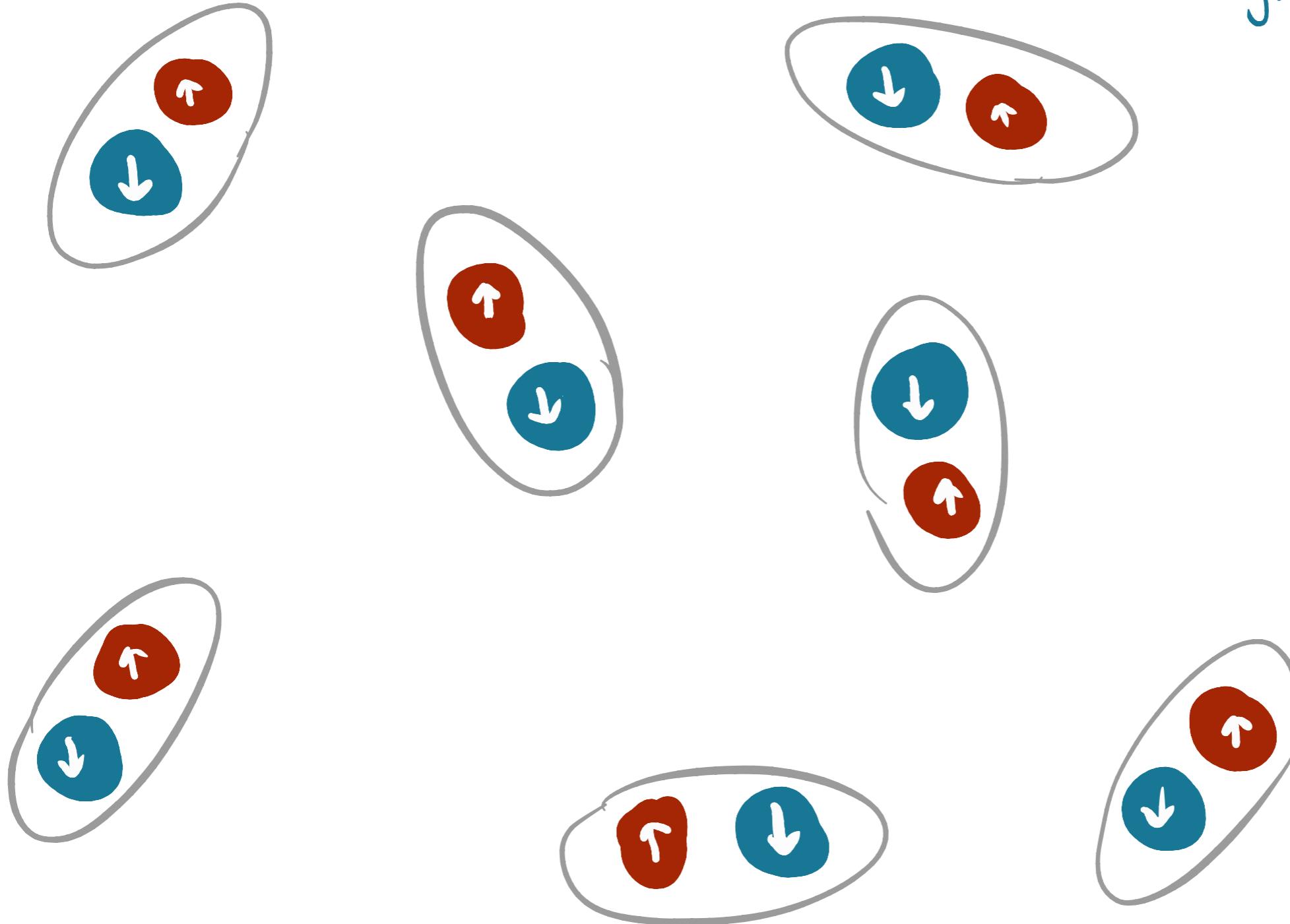
[LR, Porter, Drut, Braun *Phys. Rev. D* 96, 094506, 2017]









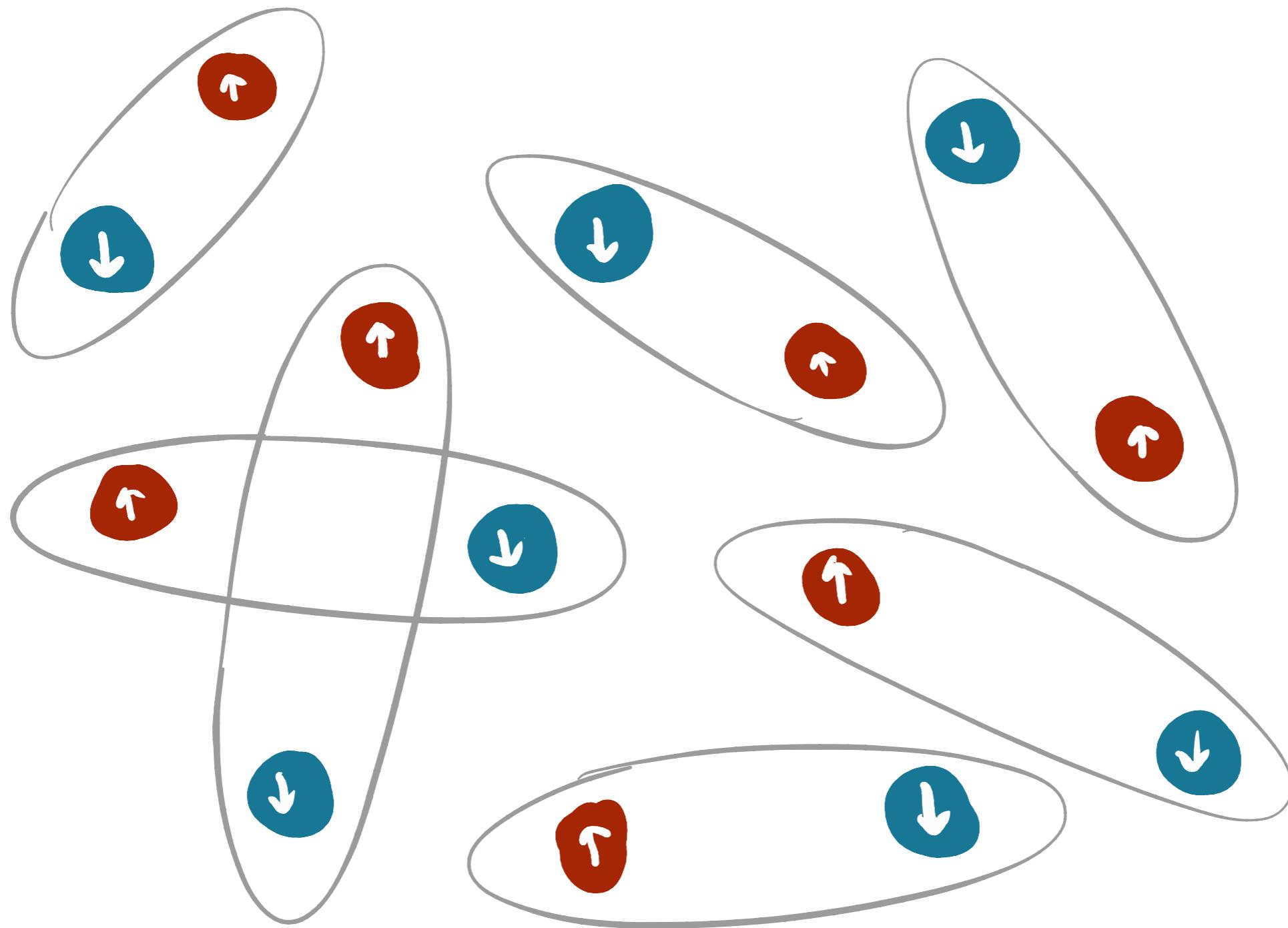


Scattering length  
 $(k_F a_S)^{-1}$   
 $\uparrow \gg 1$   
**BEC**

0

$\ll -1$

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



# the unitary Fermi gas (UFG)

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

density & temperature are the **only** dimensionful scales in the system

**universal** scaling functions:

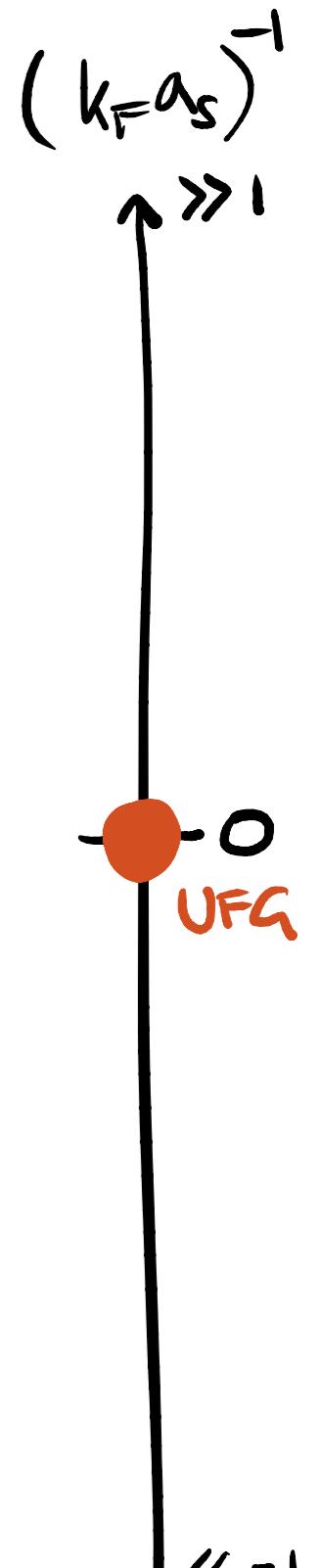
$$E = E_{FG} f_E(\beta\mu)$$

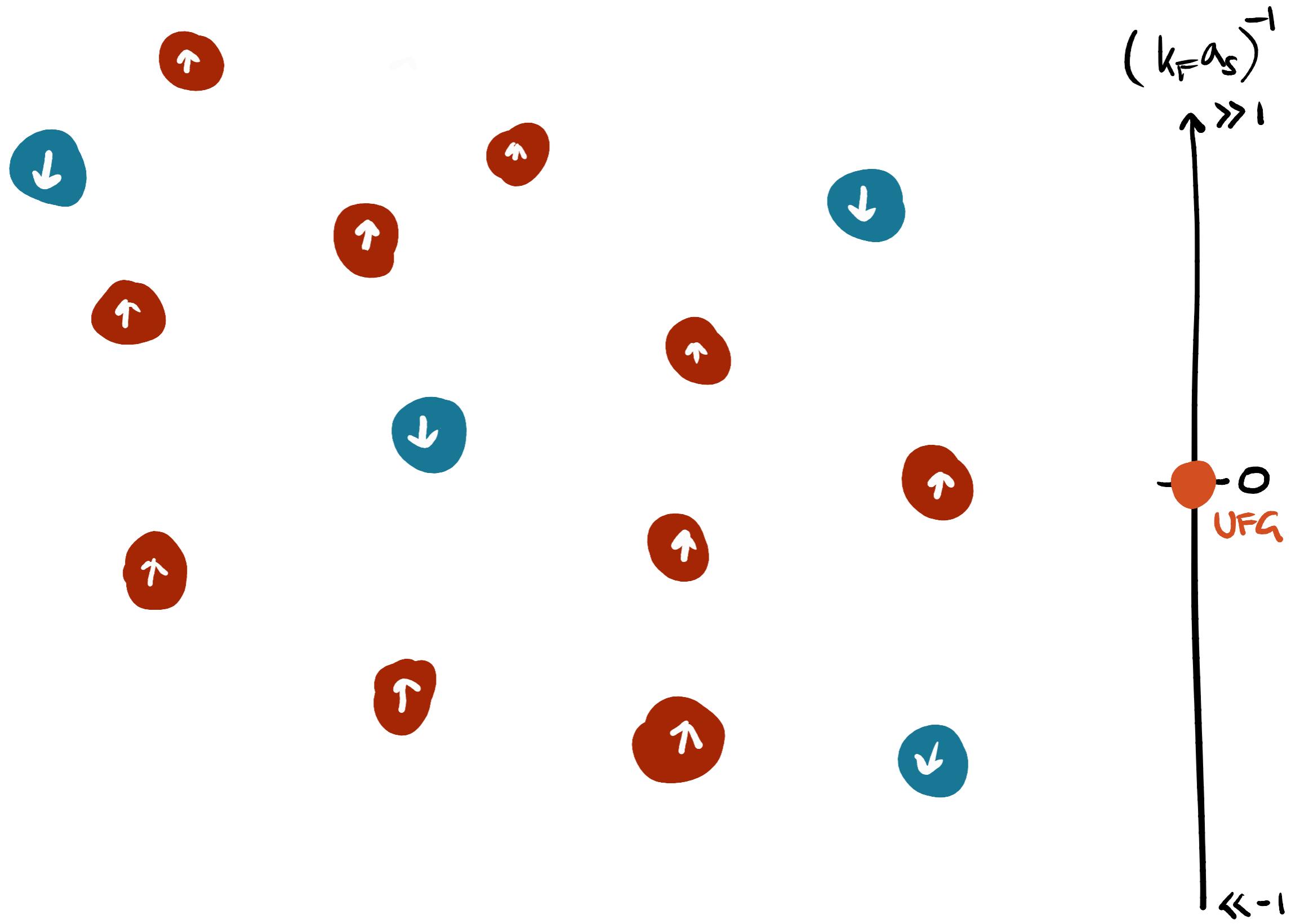
$$P = P_{FG} f_P(\beta\mu)$$

...

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

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(expectation values)

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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]

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fictitious Langevin time  
(not physical)



# stochastic quantization

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

random walk governed by

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

fictitious Langevin time  
(not physical)

noise term

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

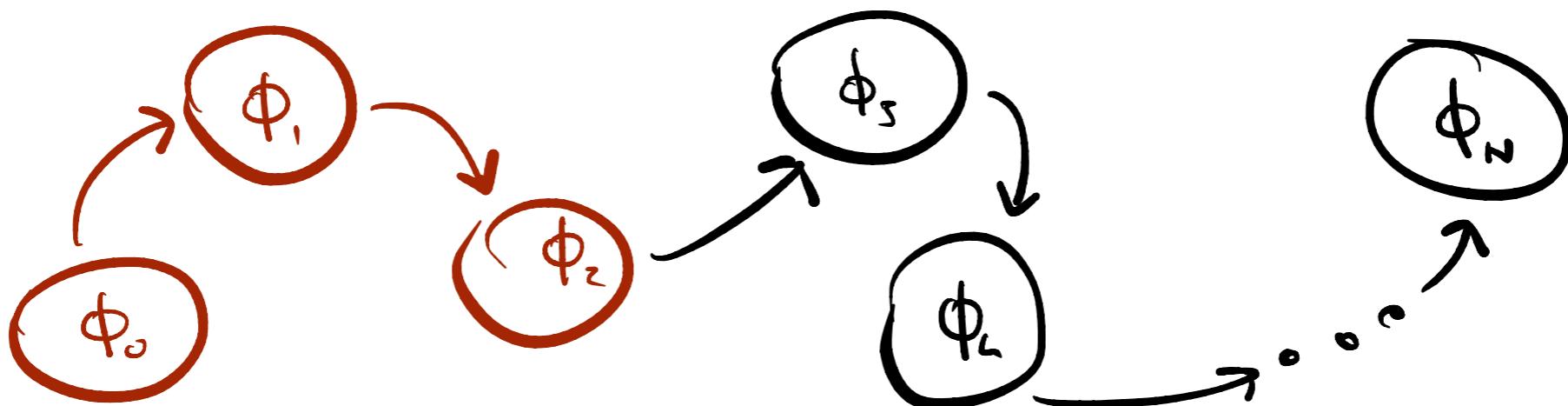
# the Langevin method

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

*discretize*

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

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



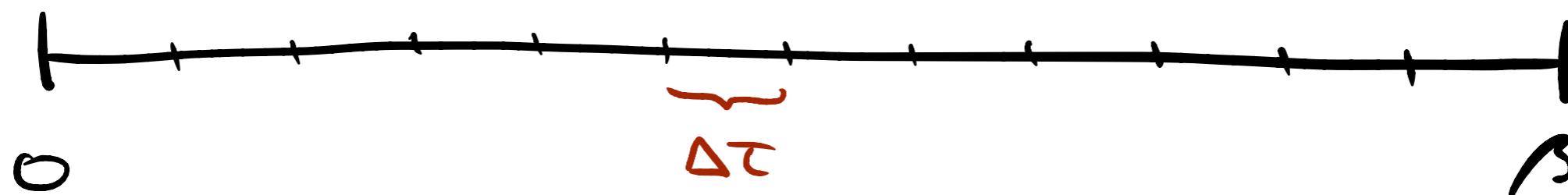
# toy problem: the harmonic oscillator

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 fictitious random process

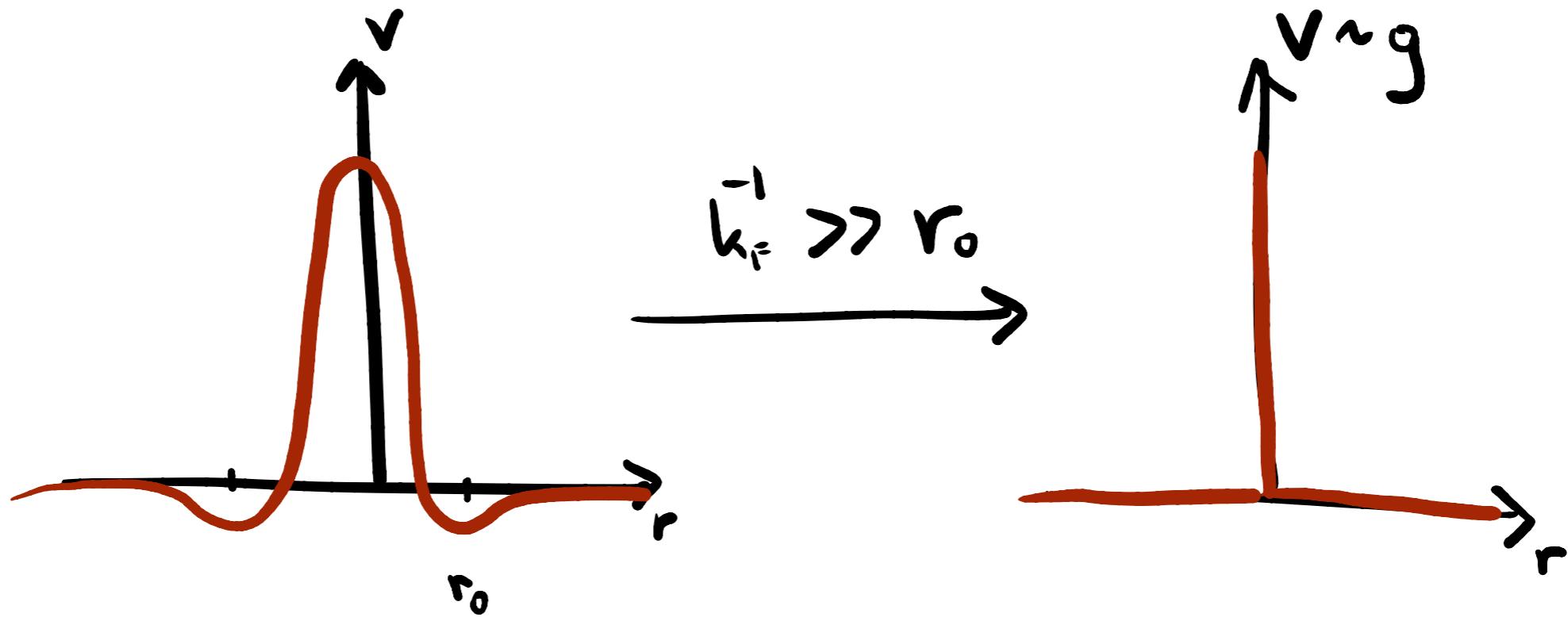
we can use this to construct a numerical method  
based on Markov chains

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?

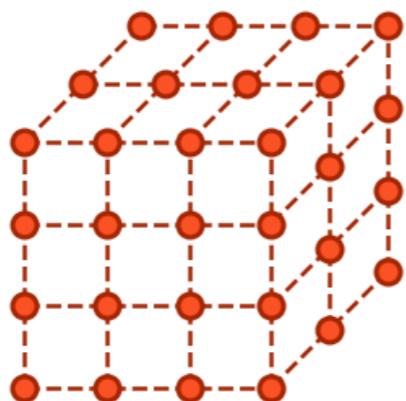
$$\mathcal{Z} = \text{Tr}[\text{e}^{-\beta \hat{H}}] = \text{Tr}[\text{e}^{-\beta(\hat{T} + \hat{V})}]$$

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

# what do we need to compute?

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



+ Trotter decomposition

+ Hubbard-Stratonovich transformation

rewrite the problem as a path-integral:

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

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

# the path integral

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

discrete Langevin equation:

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

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

# the path integral & complex actions

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

discrete Langevin equation:

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

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

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

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

# the path integral & complex actions

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

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

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

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

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

complex action → complex Langevin equation

# complex probabilities & 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?

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Erhard Seiler<sup>†</sup>

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

Ion-Olimpiu Stamatescu<sup>‡</sup>

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



Nuclear Physics A642 (1998) 239c–250c

## Complex Langevin: A Numerical Method?

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<sup>a</sup>Institut für Theoretische Physik,  
Universität Graz, A-8010 Graz, AUSTRIA

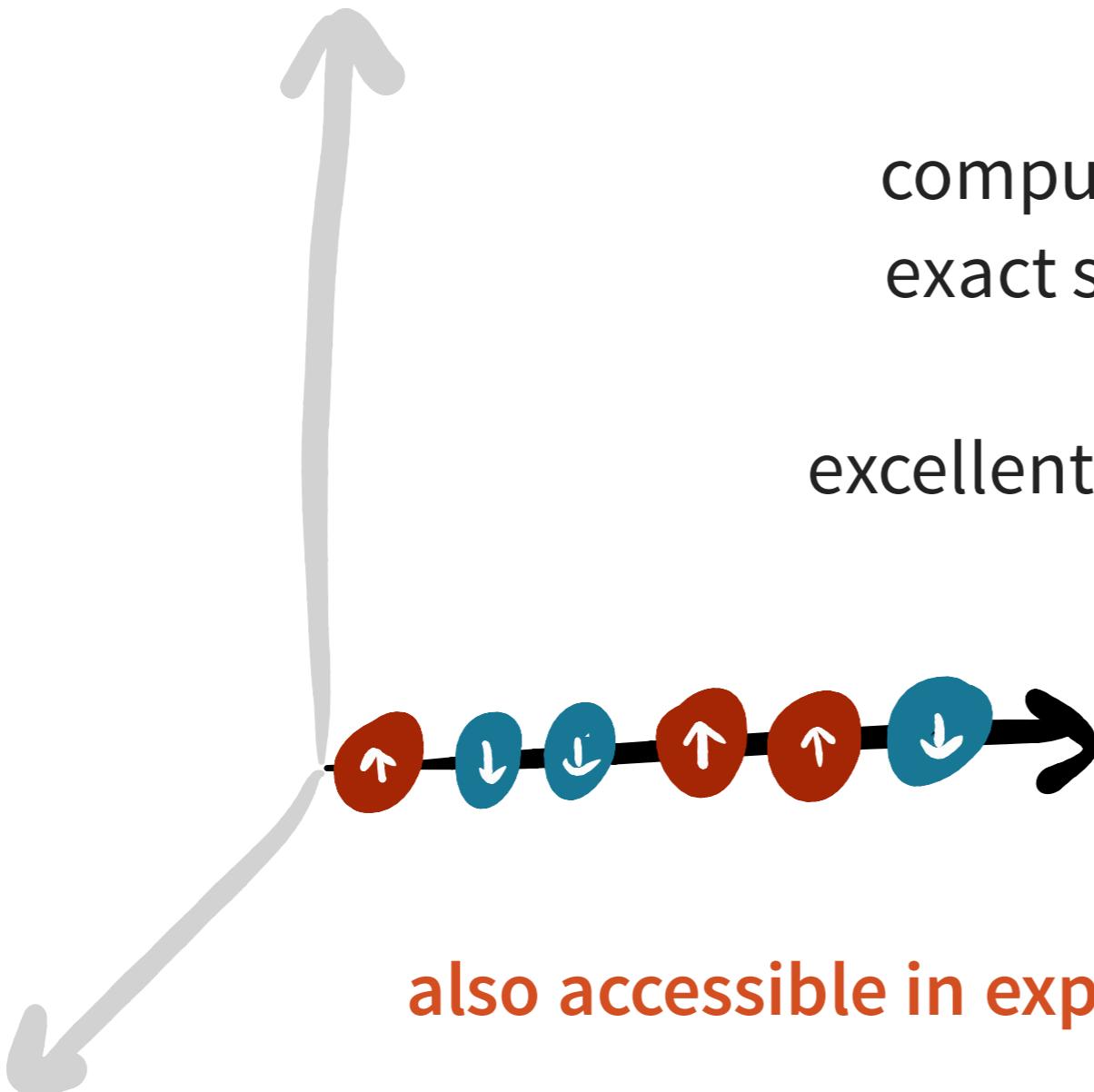
## Does the complex Langevin method give unbiased results?

L.L. Salcedo<sup>¶</sup>

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

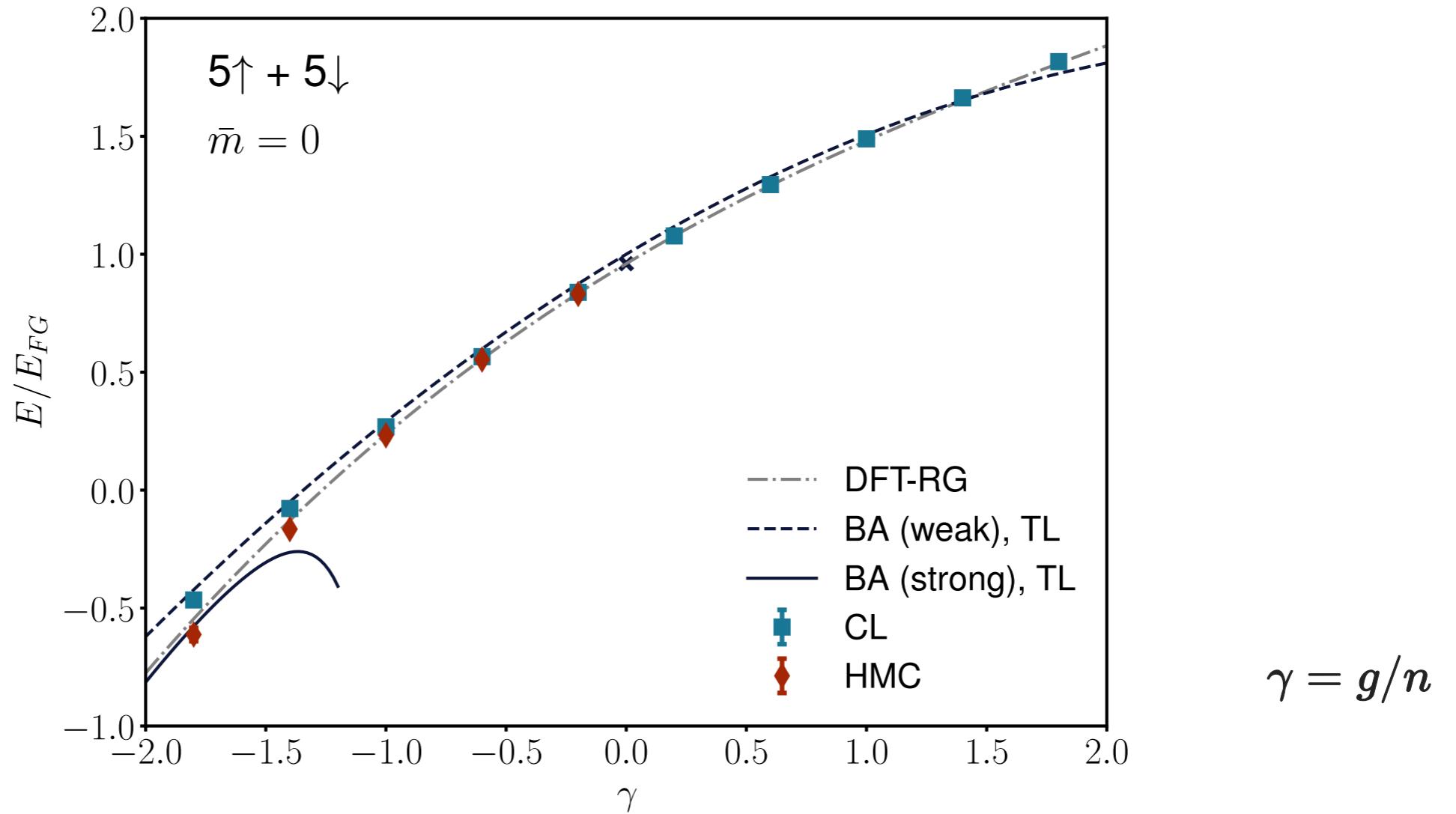
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excellent benchmark systems

also accessible in experiment

# first step: compare to other methods

[LR,Porter,Drut,Braun '17]



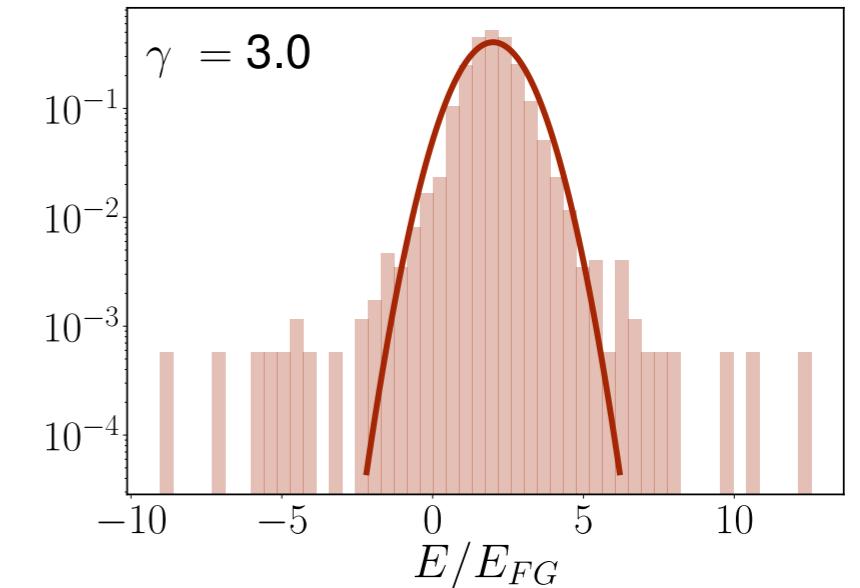
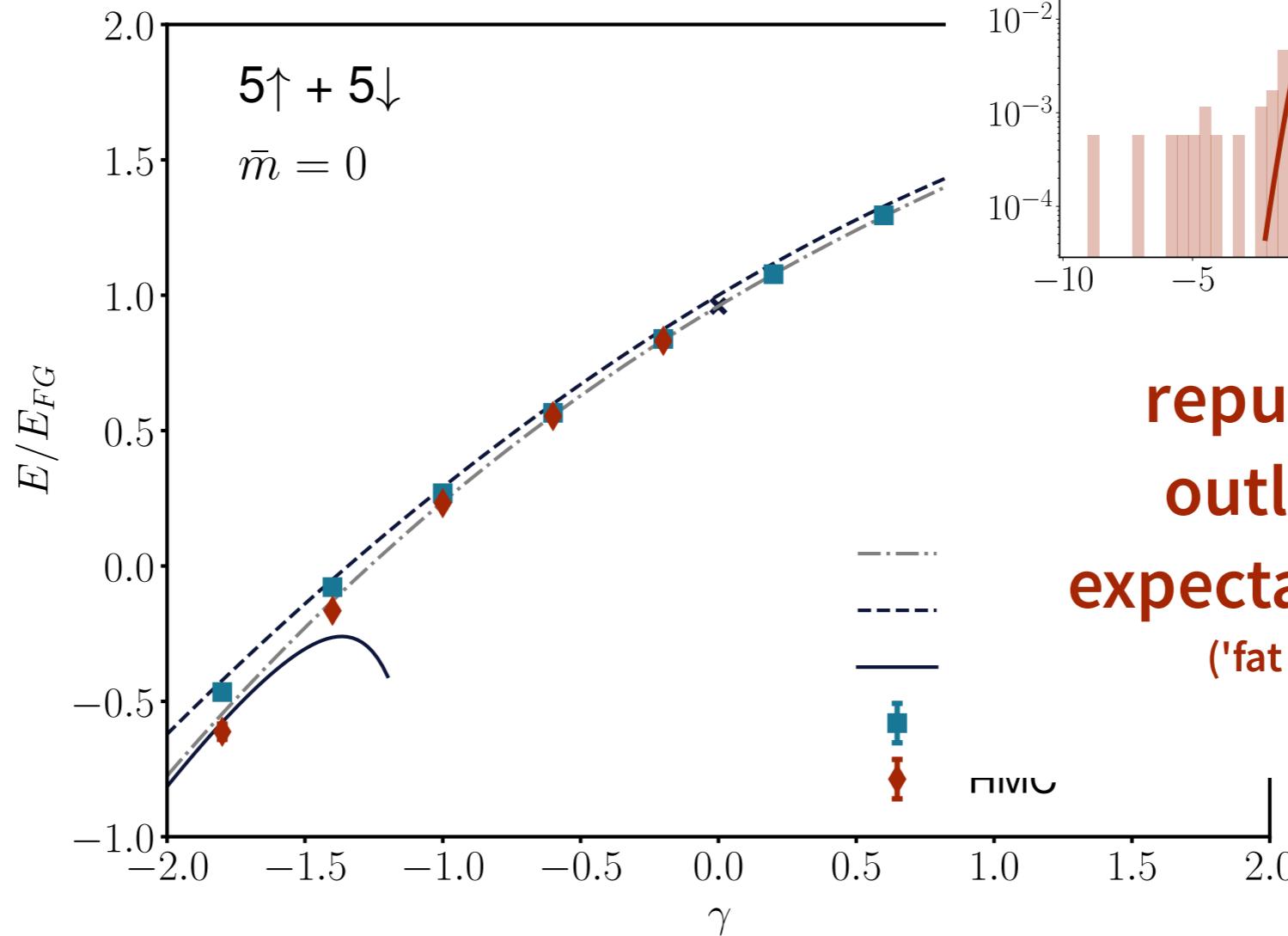
[BA: Iida, Wadati '07; Tracy, Widom '16]

[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]

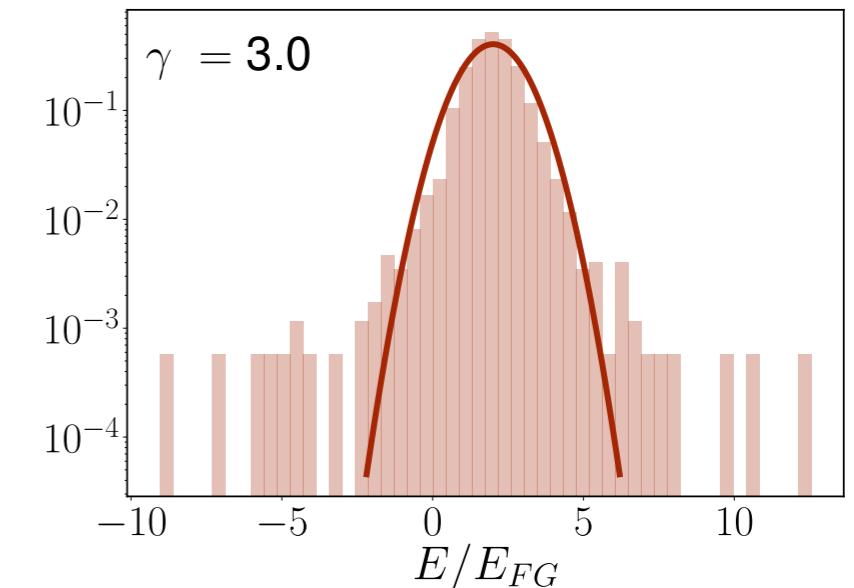
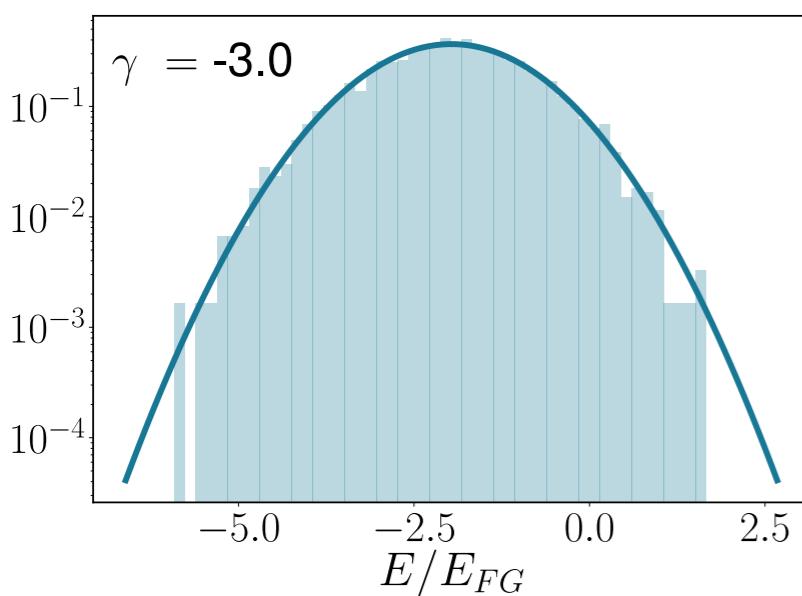
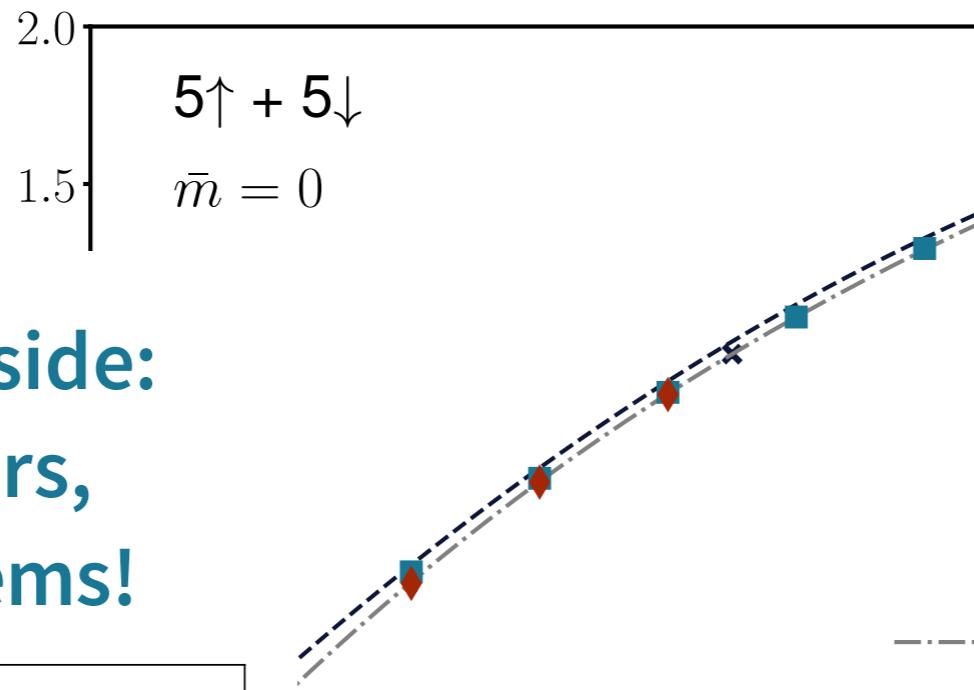
[DFT-RG: Kemler, Pospiech, Braun '17; Kemler '17]

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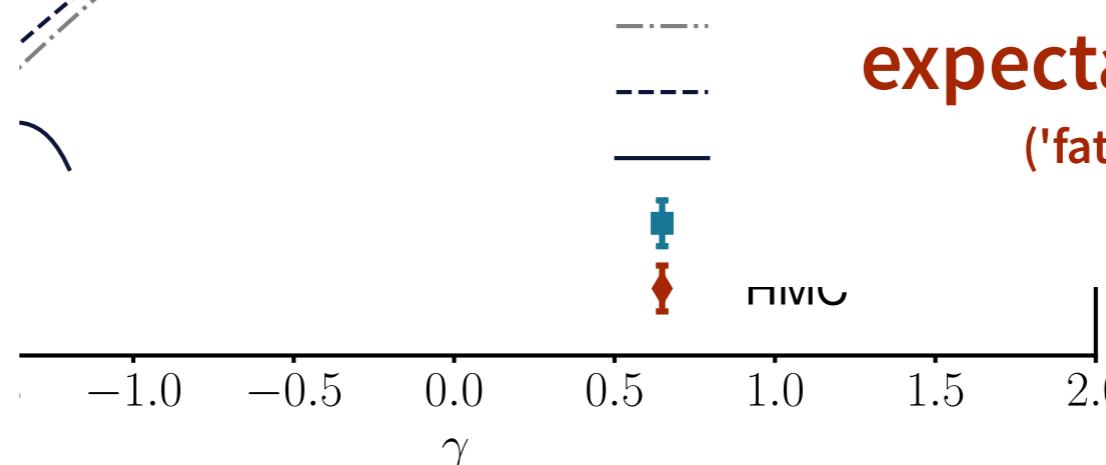
# first step: compare to other methods

[LR,Porter,Drut,Braun '17]

**attractive side:**  
no outliers,  
no problems!



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



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

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

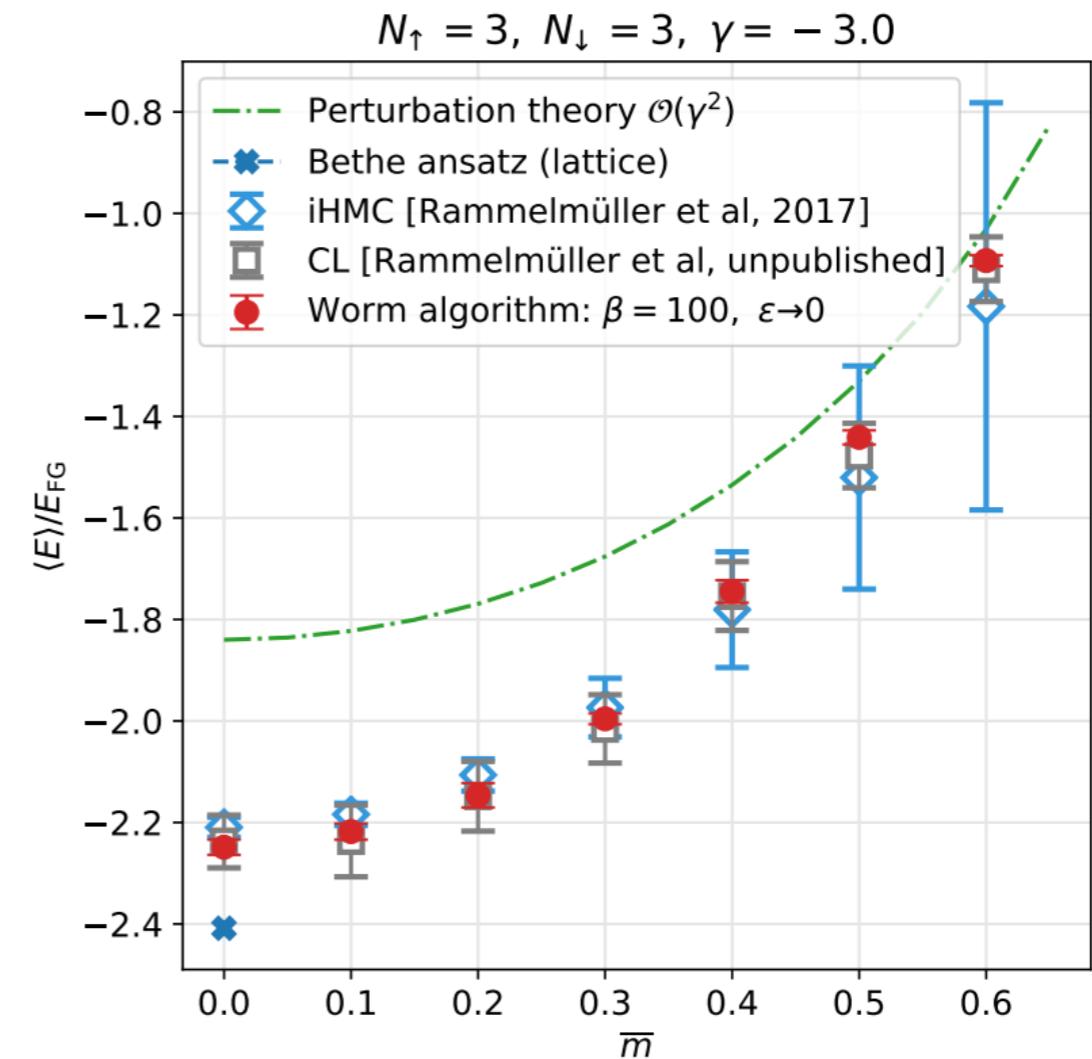
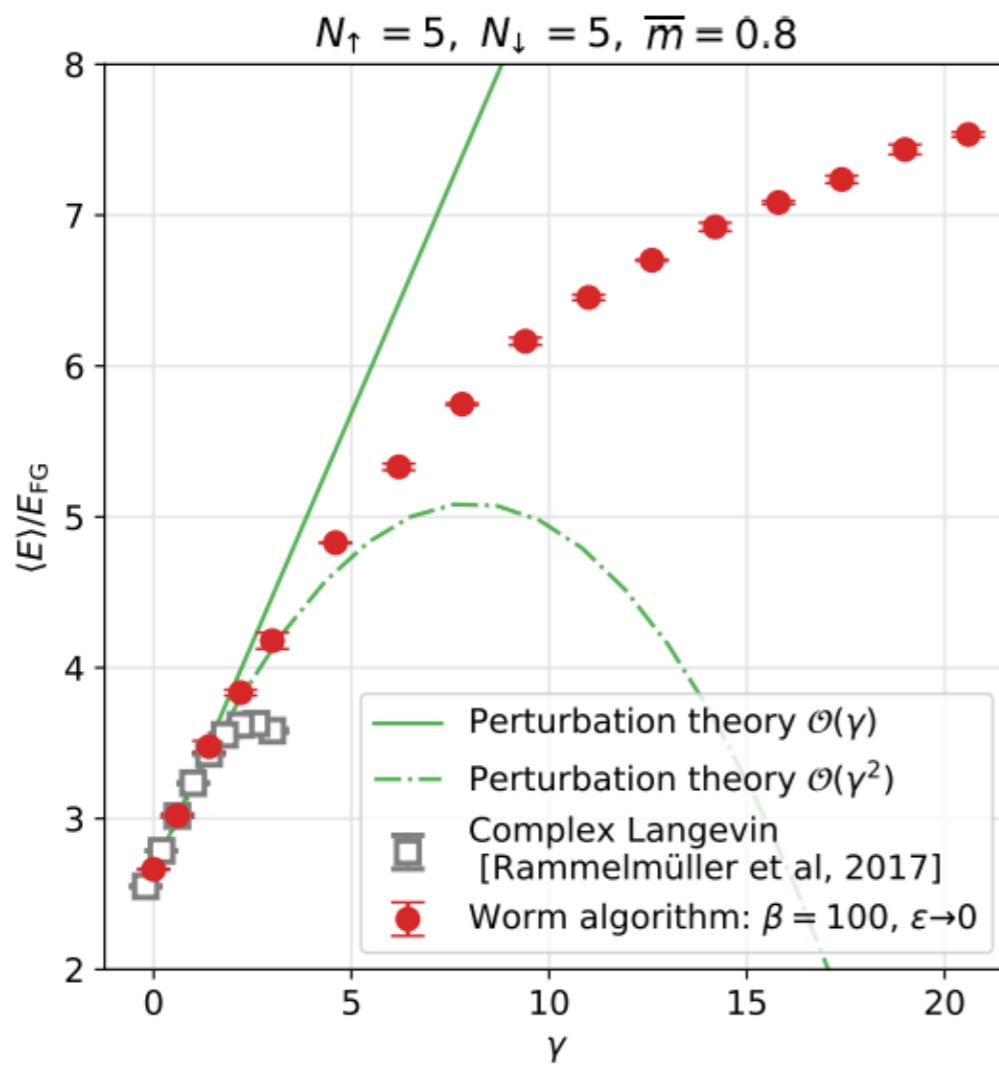
[HMC: LR, Porter, Loheac, Drut '15]

# more comparisons: mass-imbalance

[worldline: Singh,Chandrasekharan '18]

[CL/iHMC: LR,Porter,Drut,Braun '17]

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

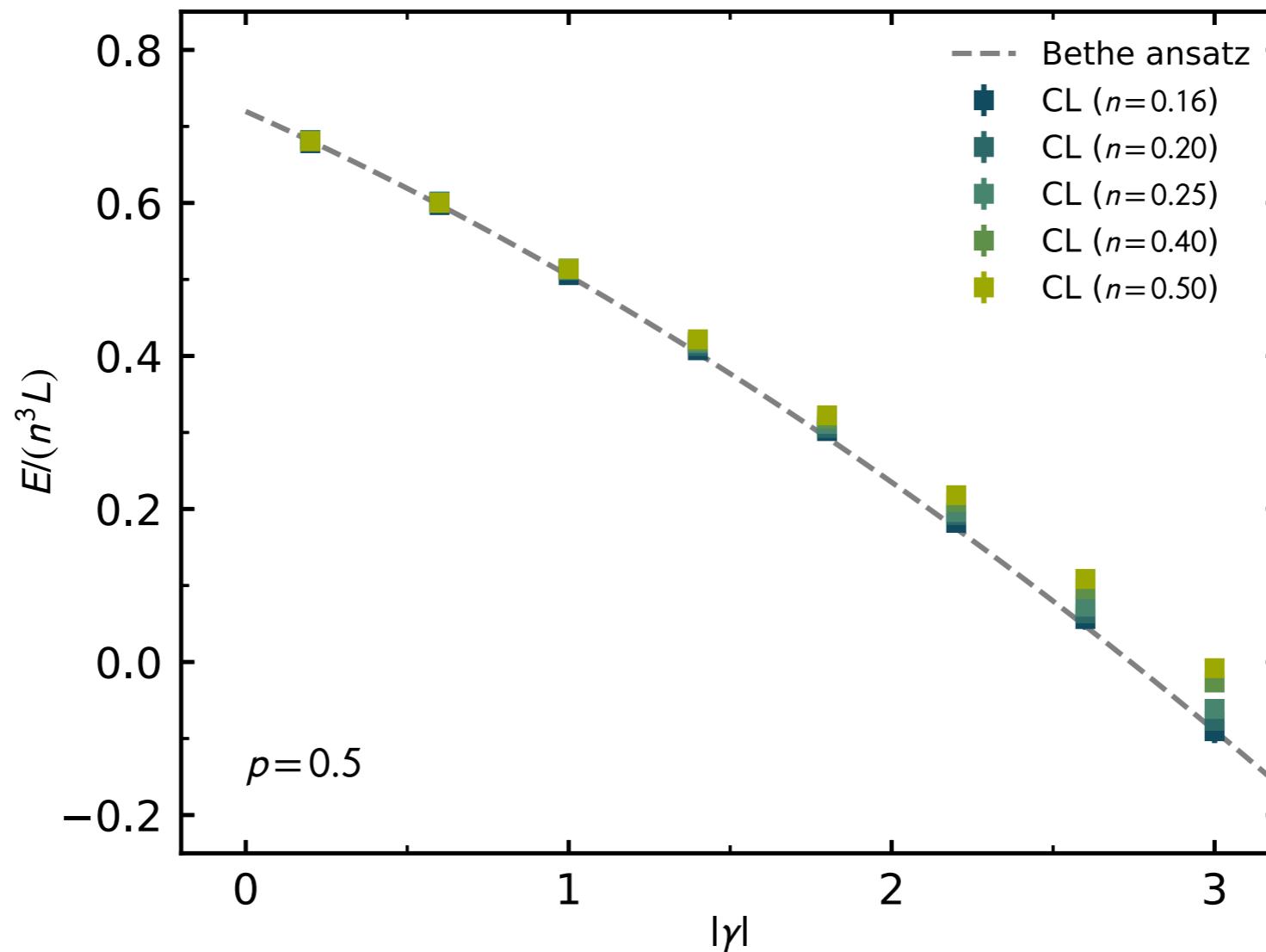


**discrepancy** with worldline methods for **repulsive interaction**

# polarized 1D fermions: equation of state

[LR, Drut, Braun in preparation]

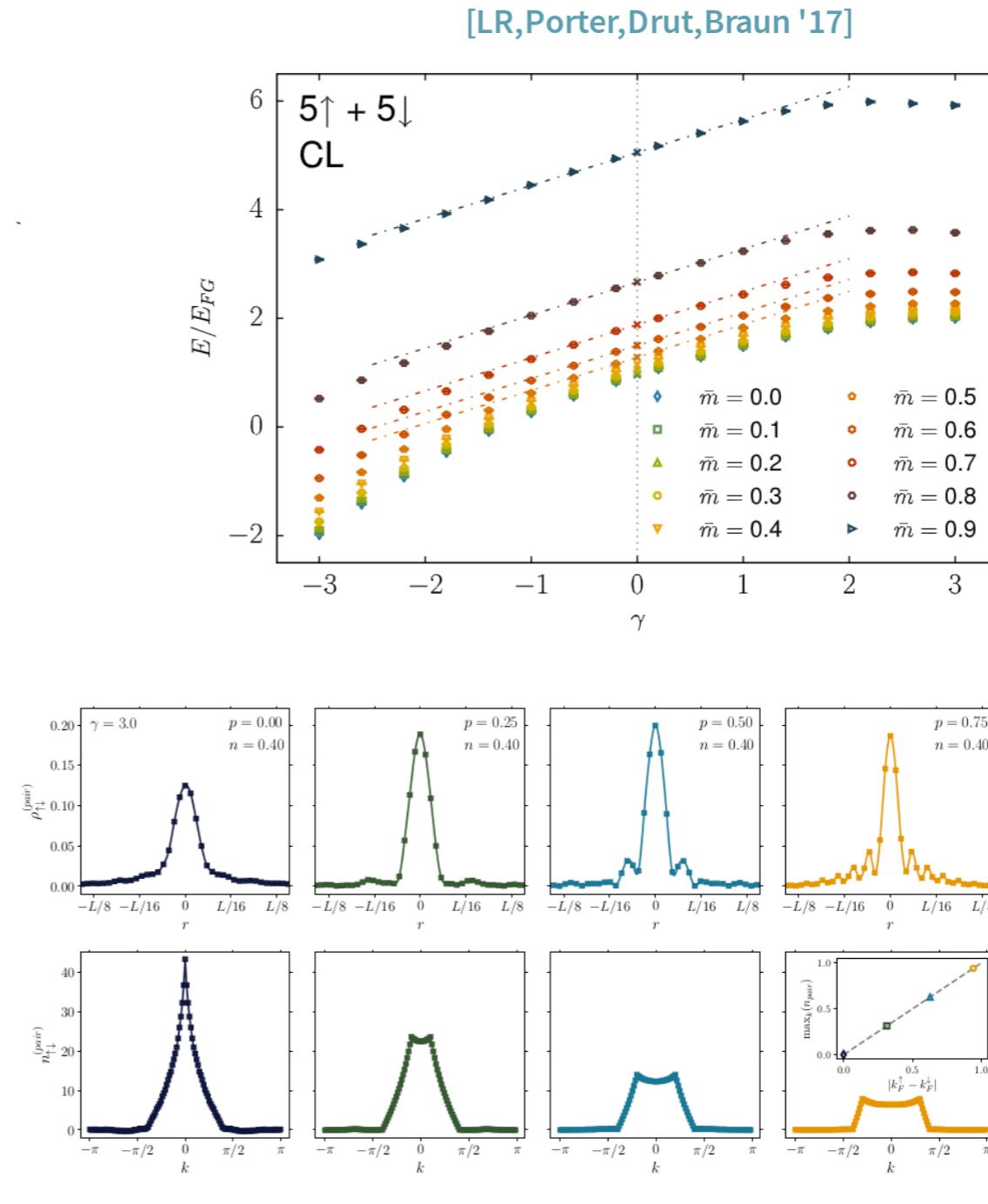
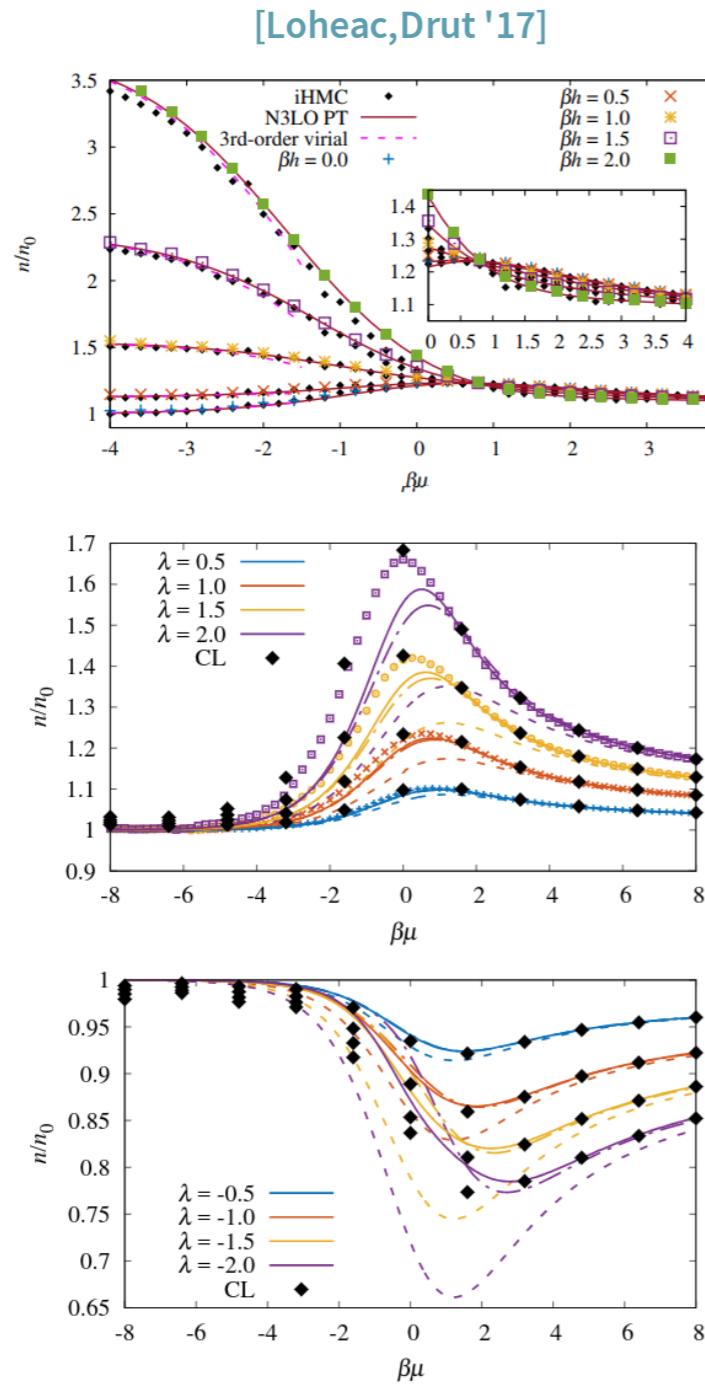
excellent  
agreement at  
low densities  
(zero-range  
limit)



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

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

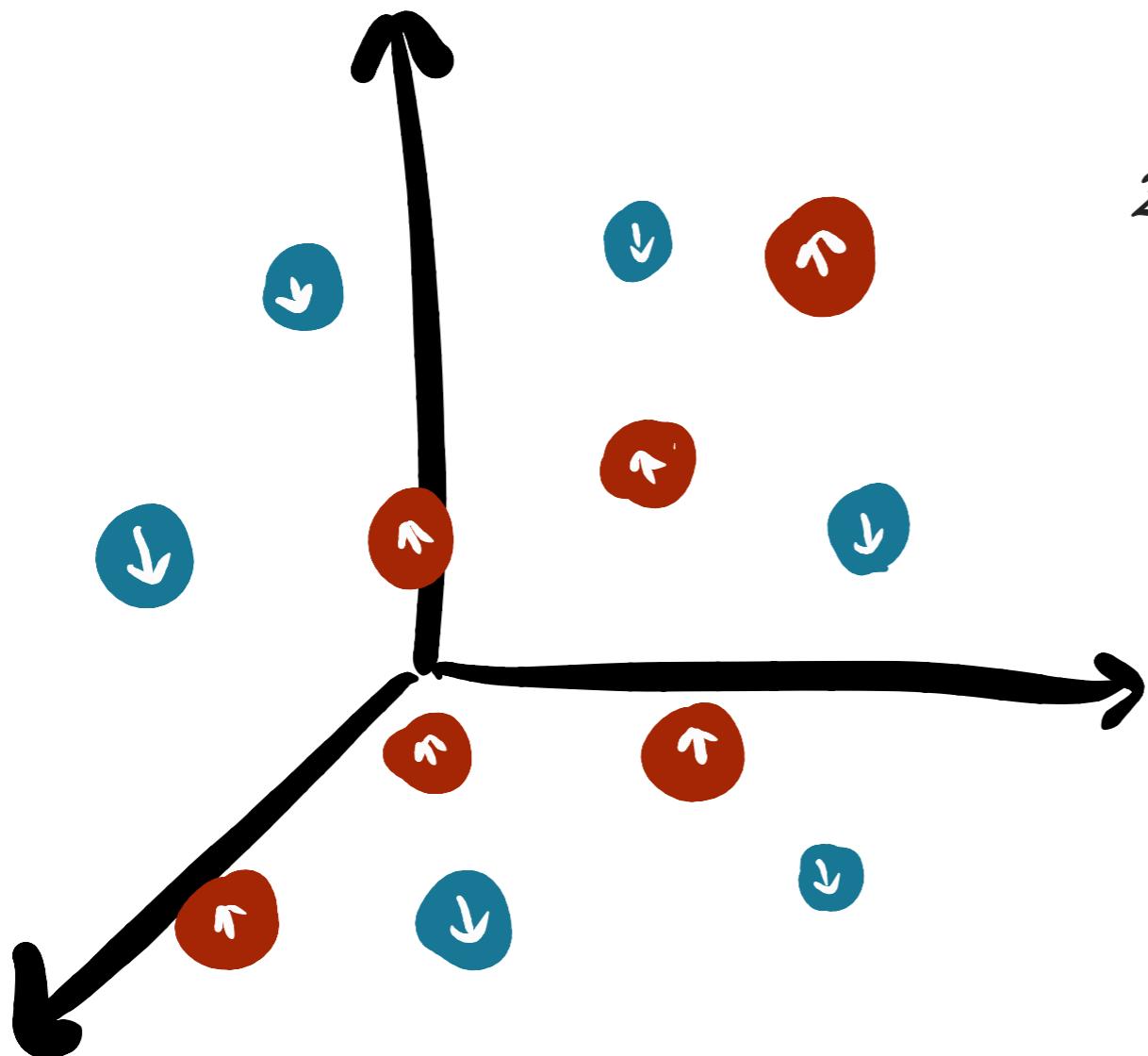
# more CL results for 1D



**[Loheac,Braun,Drut '18]**

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

# the unitary Fermi gas at finite temperature



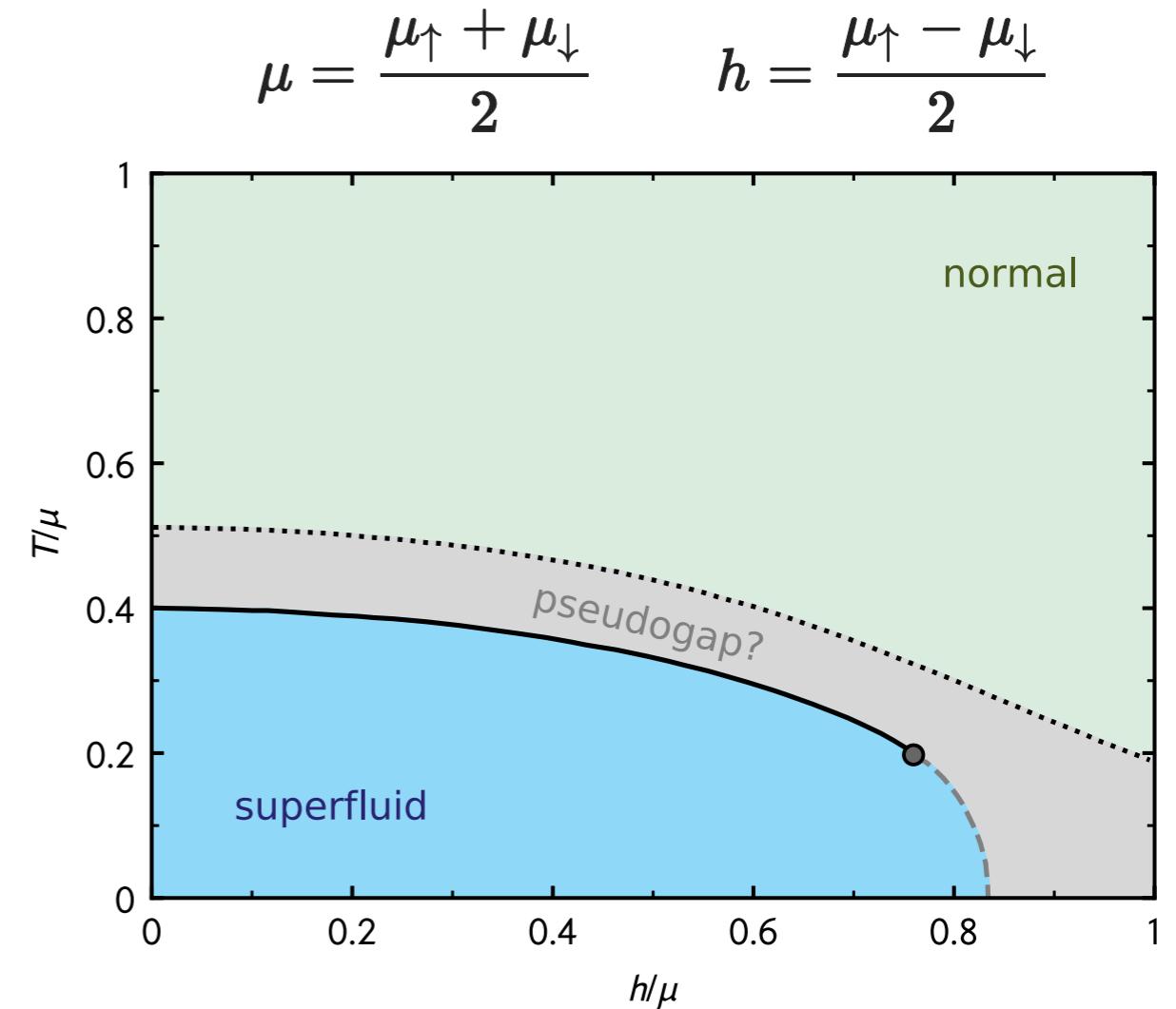
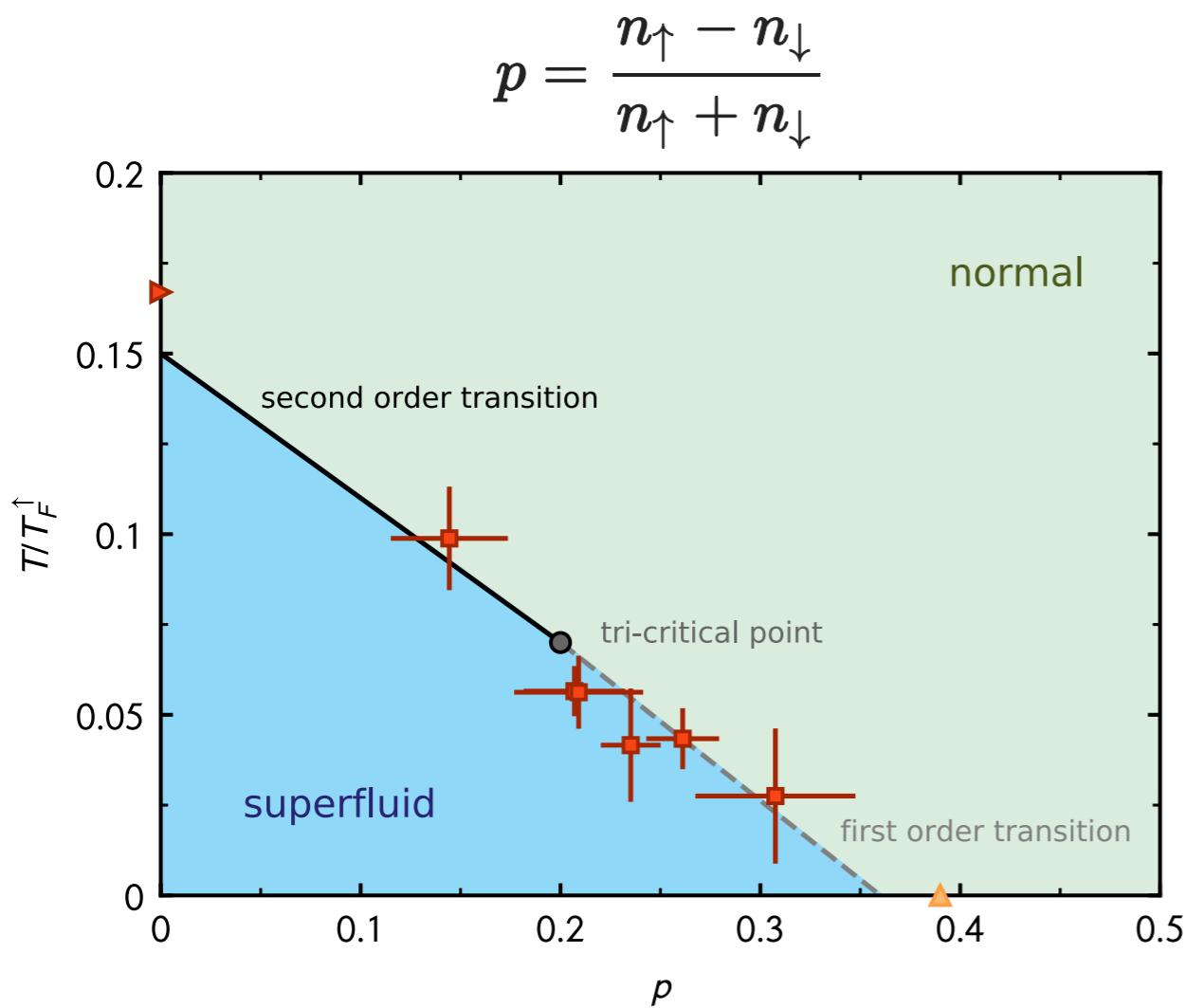
$$\begin{aligned}\mathcal{Z} &= \text{Tr} \left[ e^{-\beta(\hat{H}-\mu_{\uparrow}\hat{N}_{\uparrow}-\mu_{\downarrow}\hat{N}_{\downarrow})} \right] \\ &= \text{Tr} \left[ e^{-\beta(\hat{H}-\mu\hat{N}-h\hat{M})} \right]\end{aligned}$$

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

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

computationally challenging (but feasible)

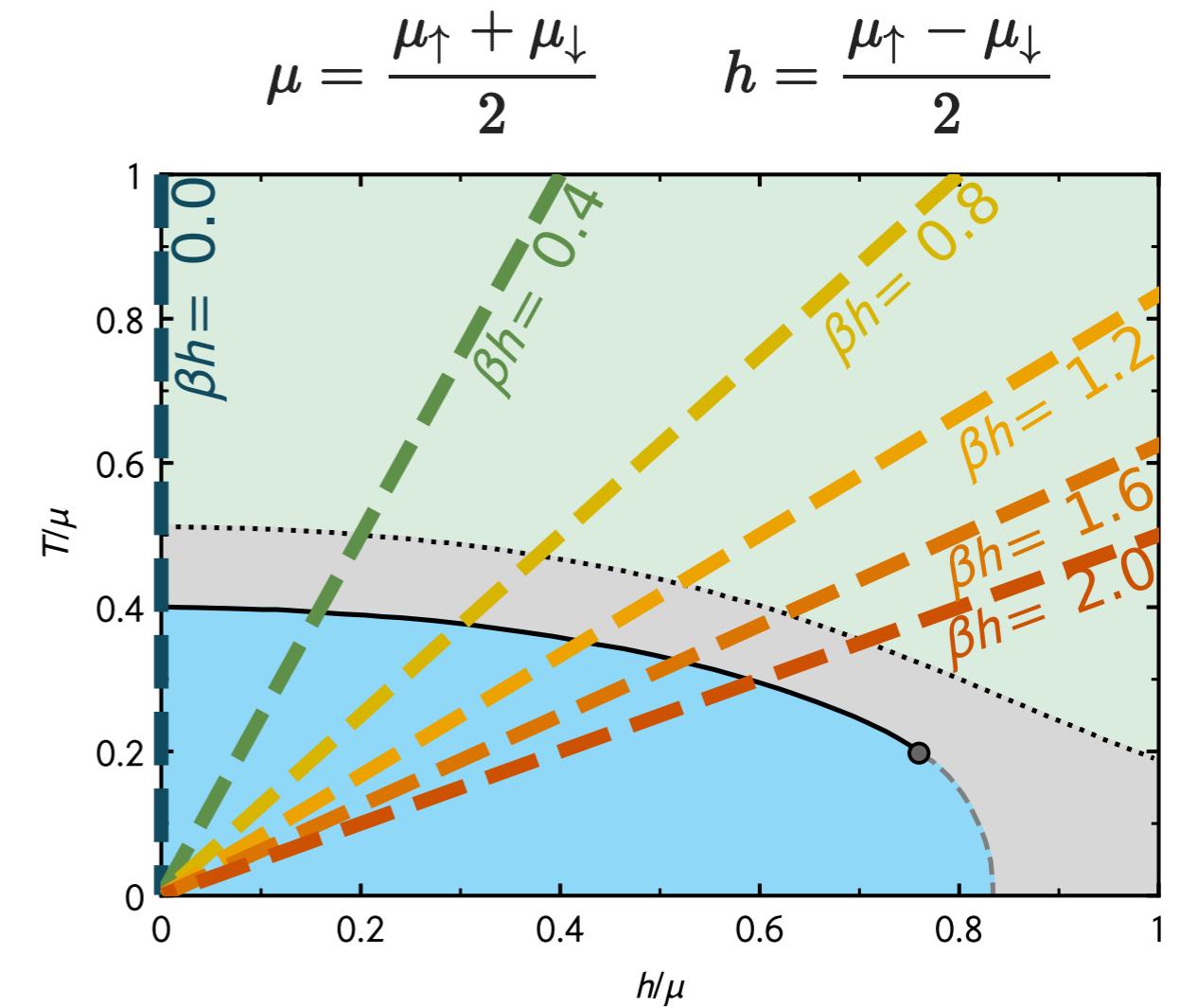
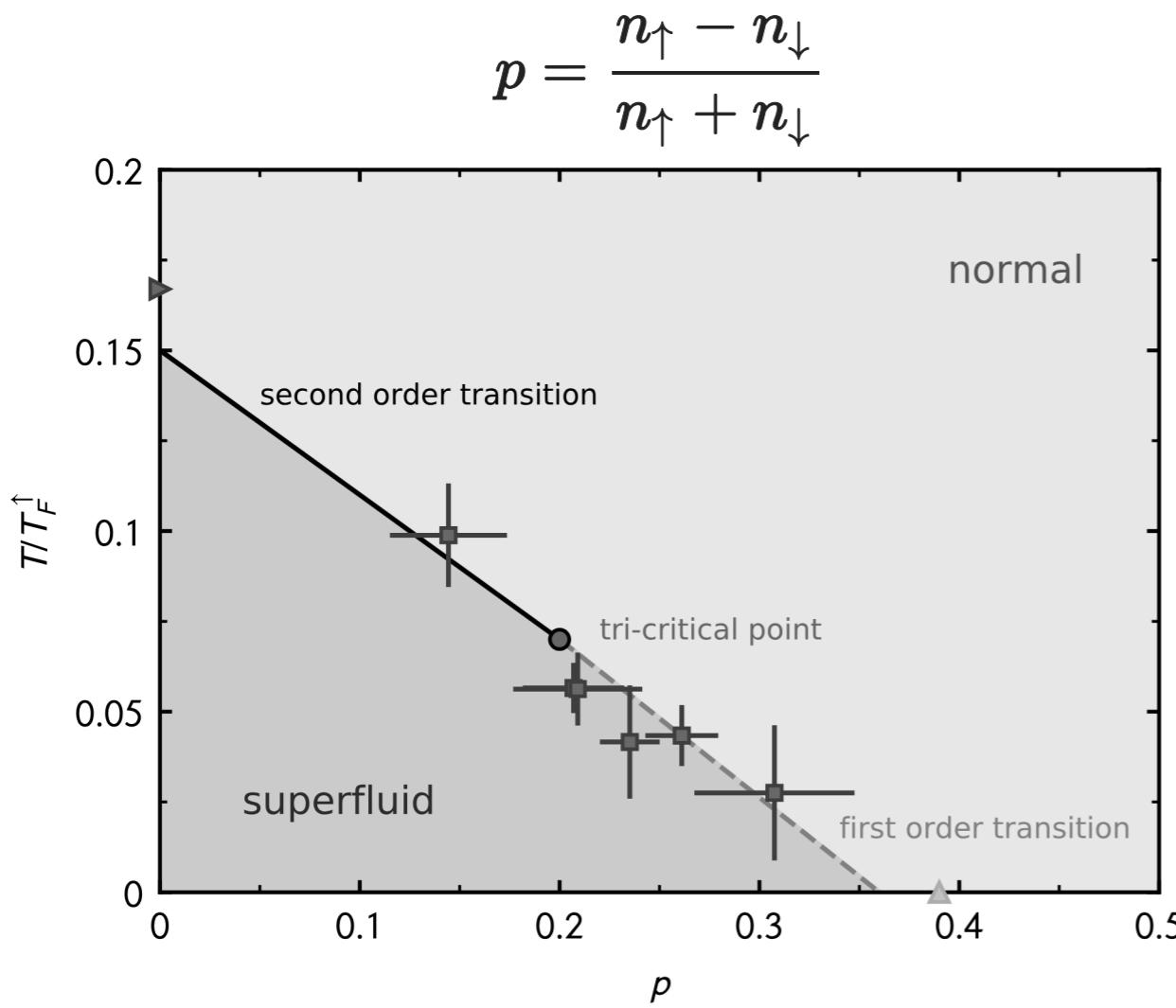
# exploring the phase diagram



[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



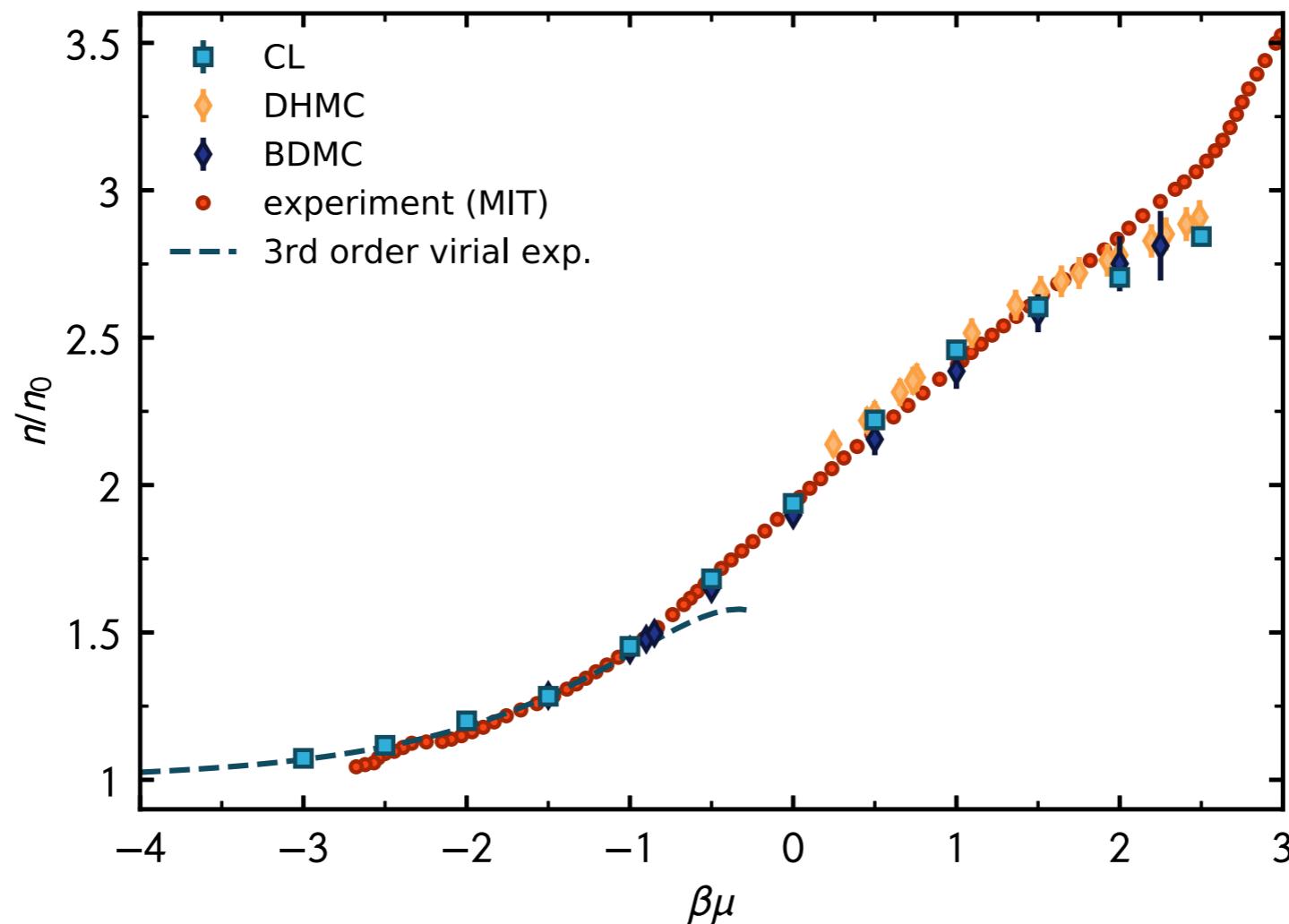
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[fRG: Boettcher et. al '15]

# density equation of state

[LR, Loheac, Drut, Braun '18]

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



classical regime

$k_B T$  dominates

quantum regime

$E_F$  dominates

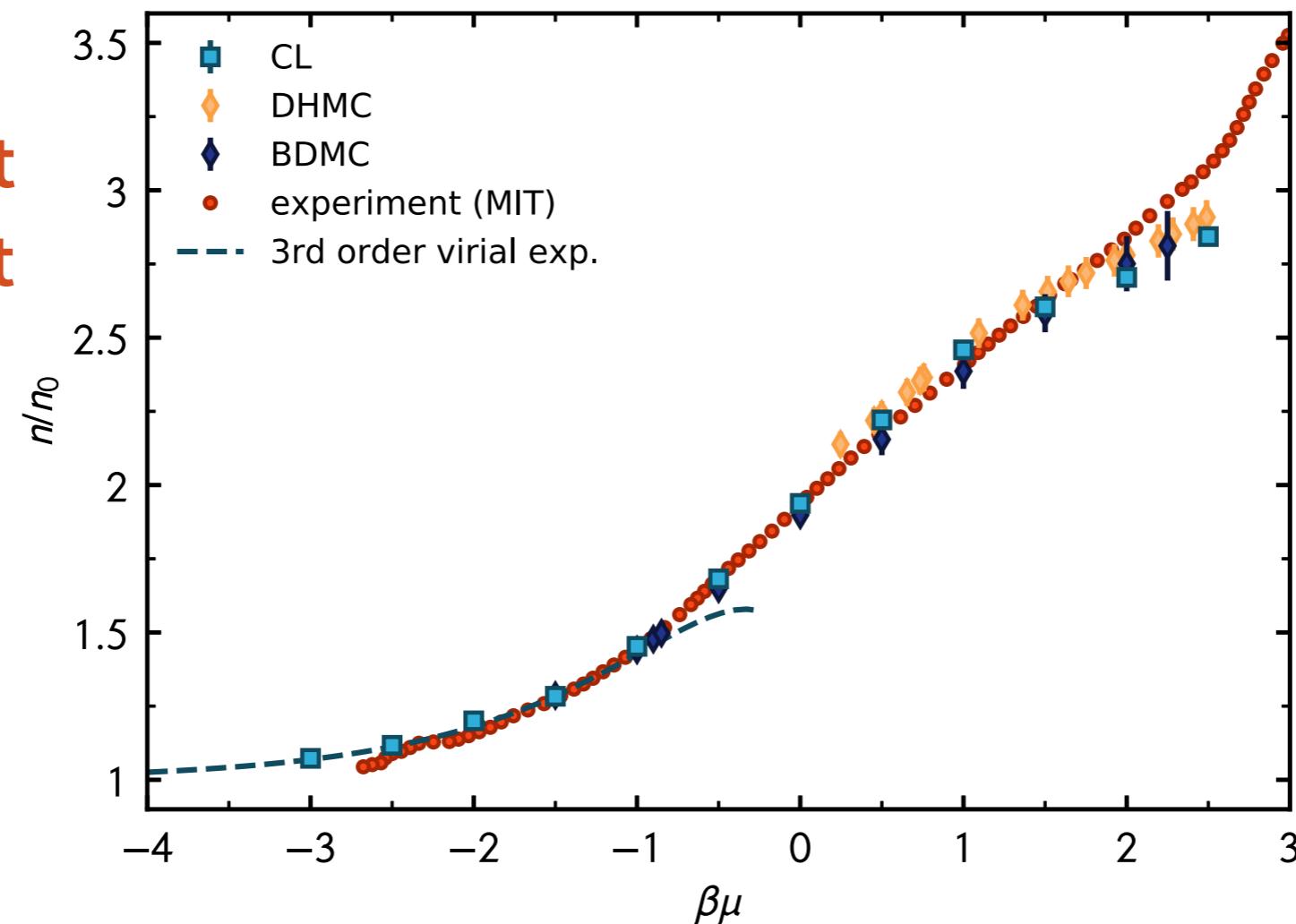
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good agreement  
with experiment  
and other  
methods!

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



classical regime

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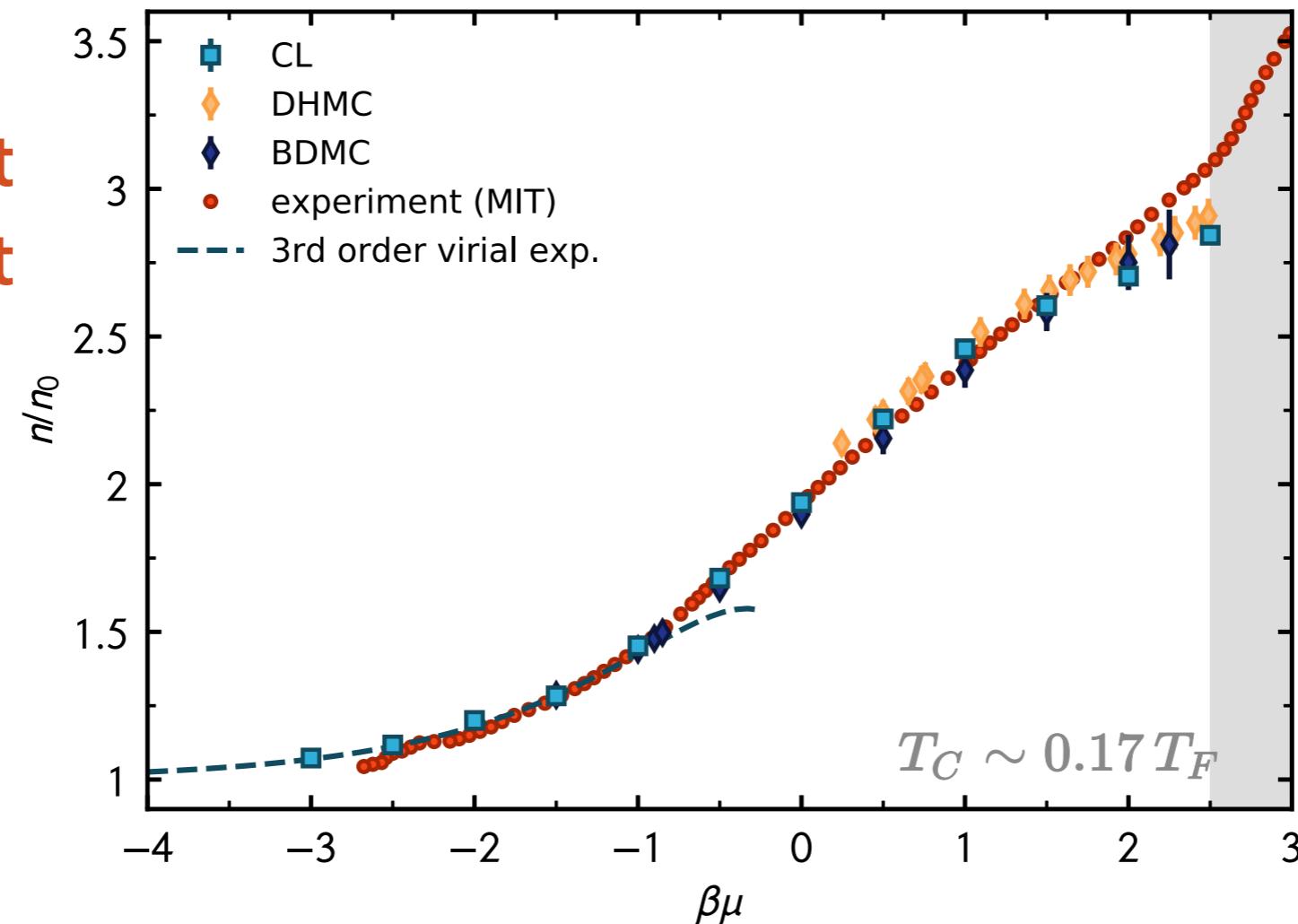
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[DPMC: Drut, Lähde, Wlazłowski, Magierski '12]

good agreement  
with experiment  
and other  
methods!

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



low temperatures:  
 $\lambda_T$  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

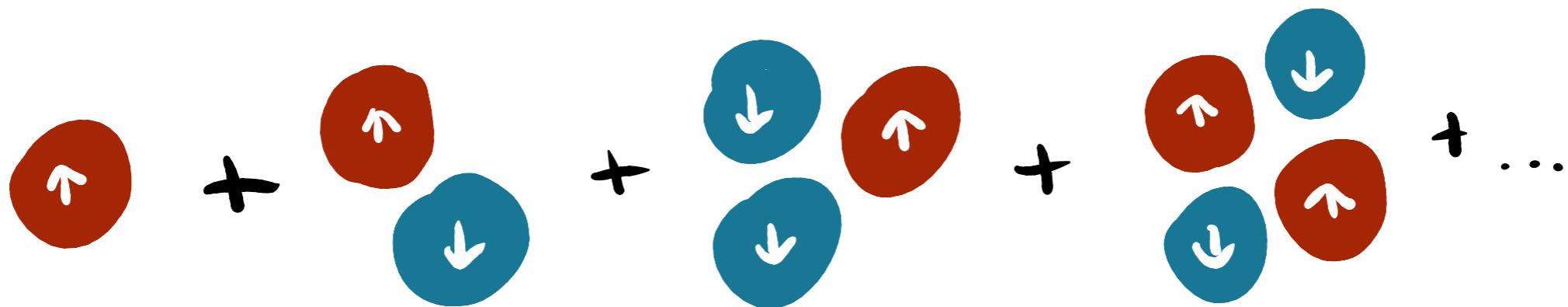
[Liu '13]

dilute gases: few-body correlations dominate

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

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

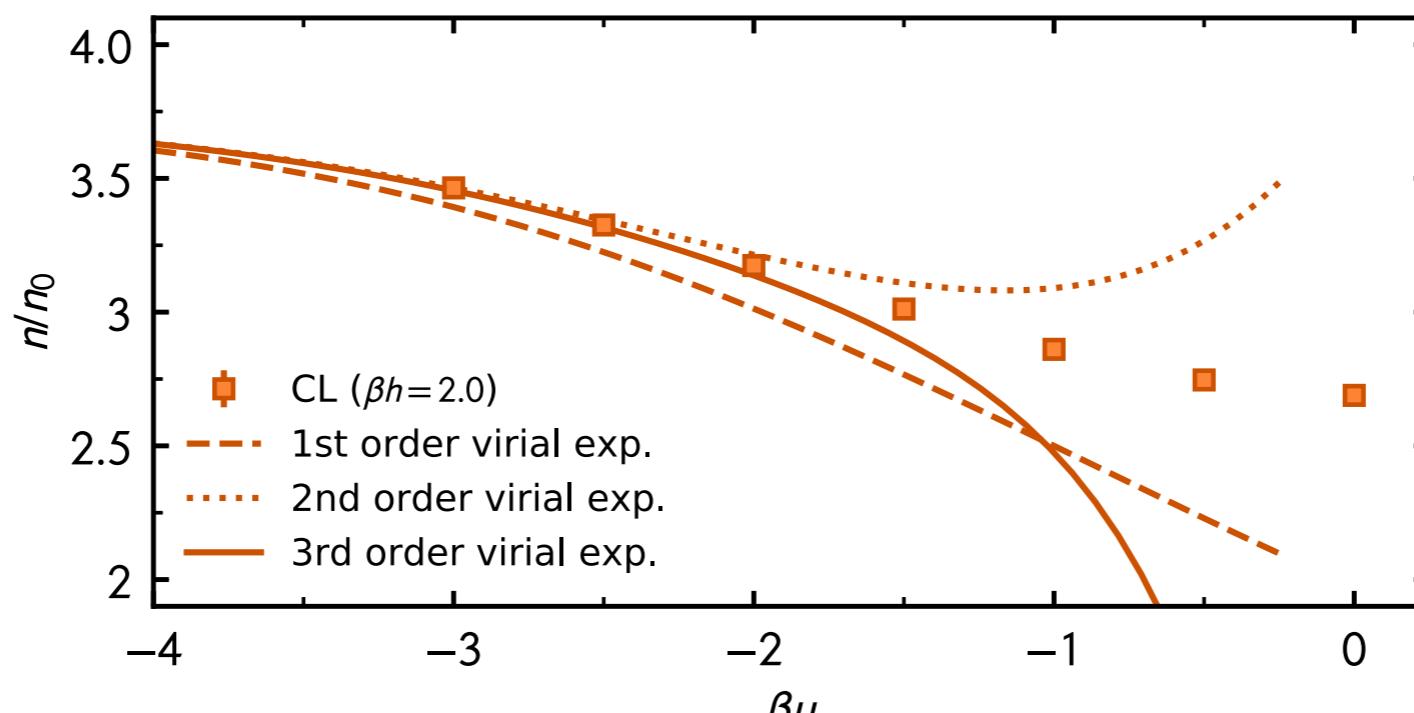
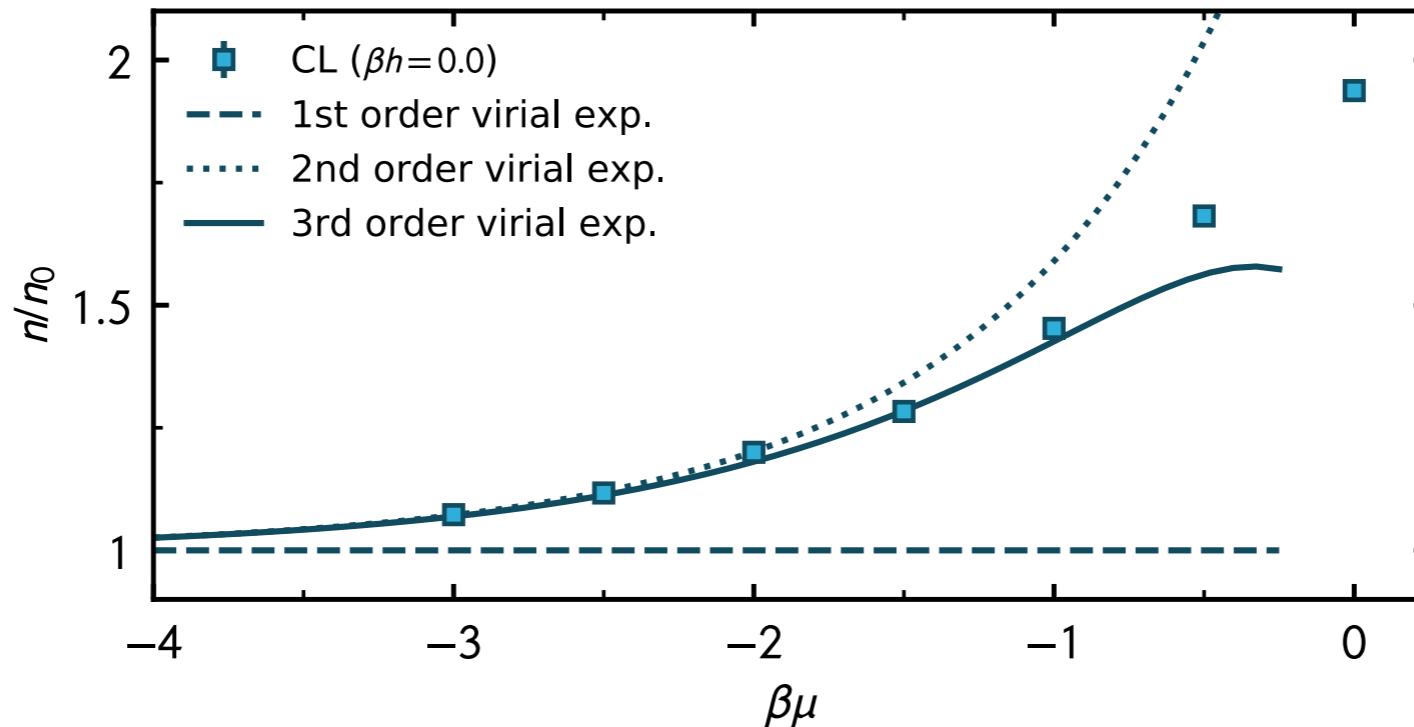
$$\ln \mathcal{Z} = Q_1 \sum_n z^n b_n$$



# density EOS (virial regime)

[LR, Loheac, Drut, Braun '18]

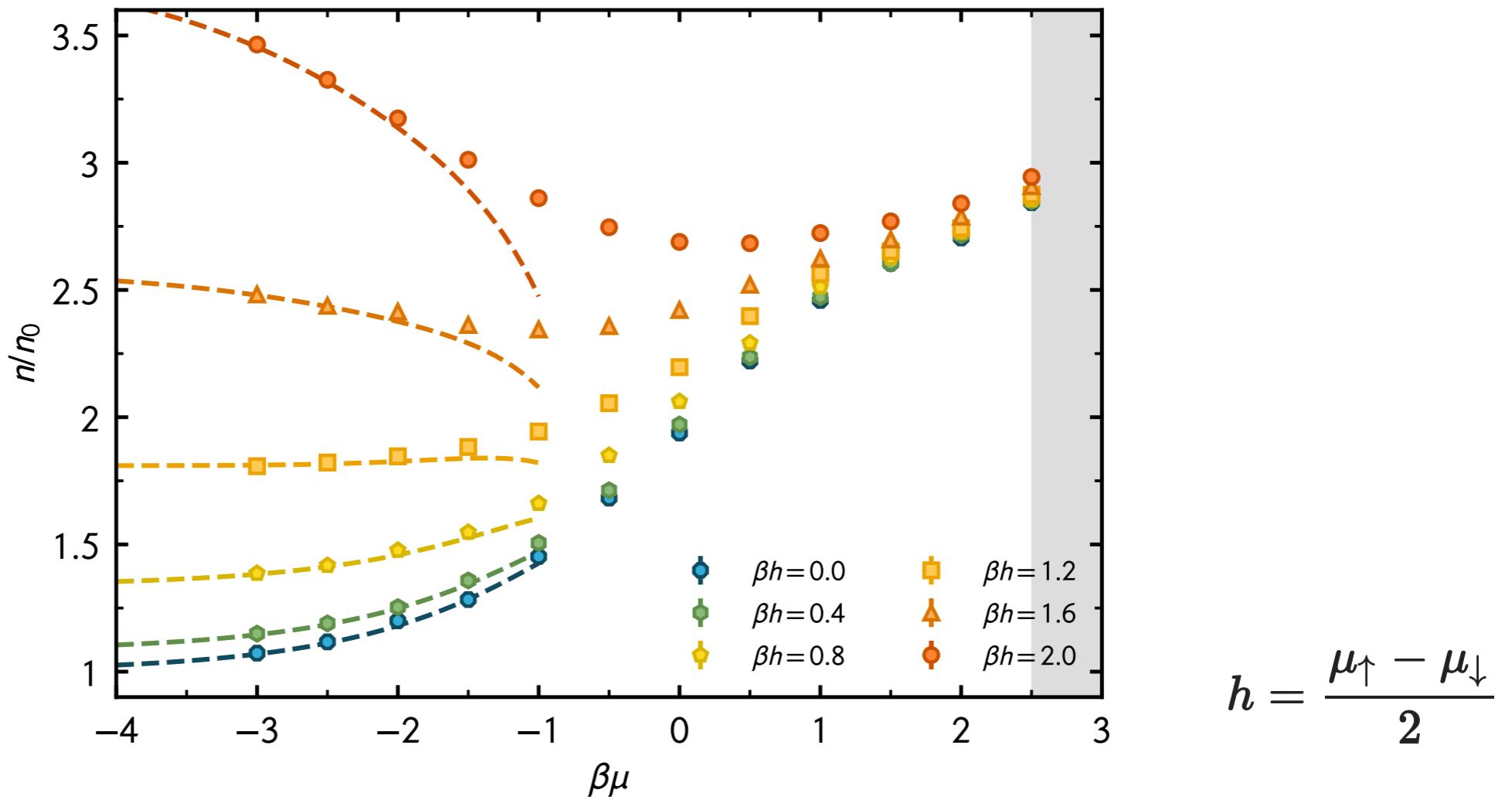
VE approaches  
the CL results  
order-by-order



VE deviates earlier  
for polarized  
systems

# density EOS at finite polarization

[LR, Loheac, Drut, Braun '18]



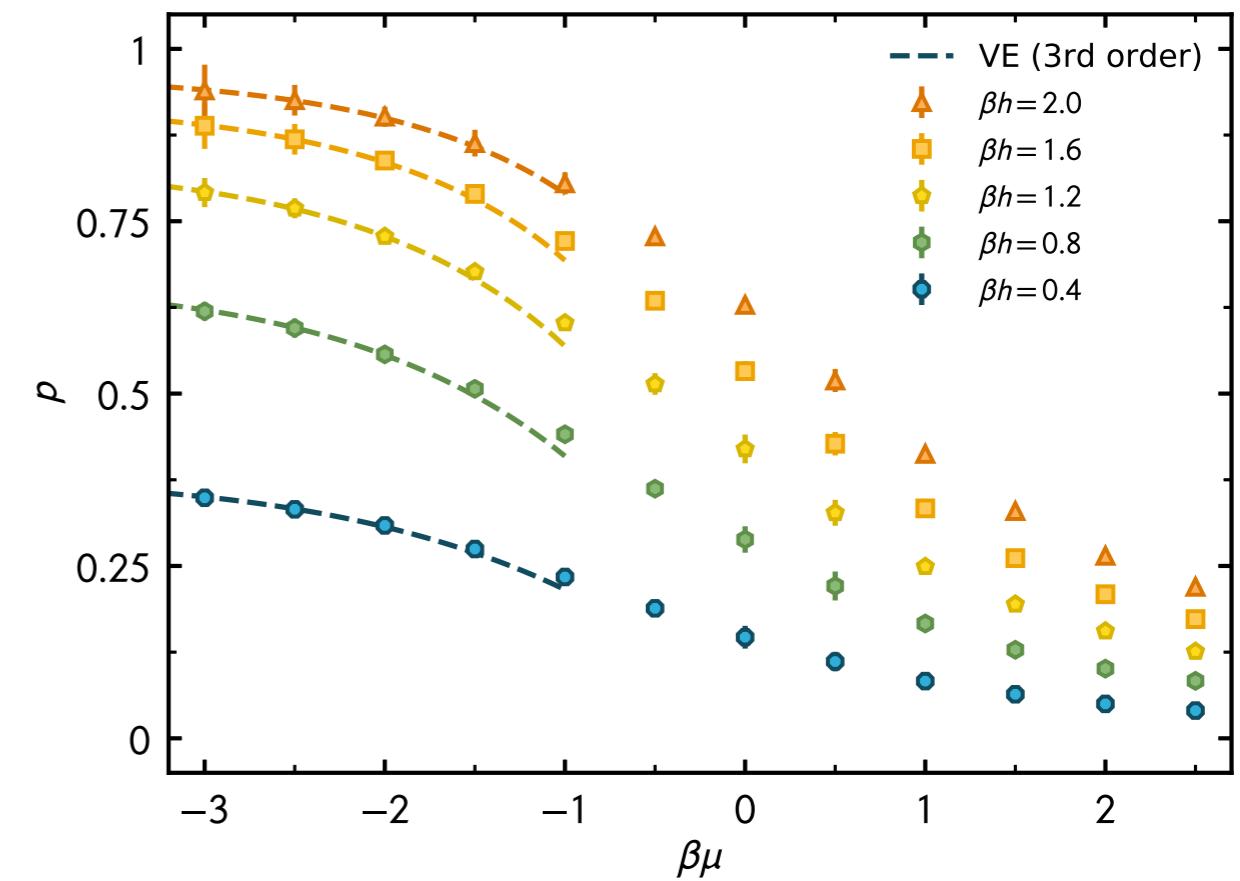
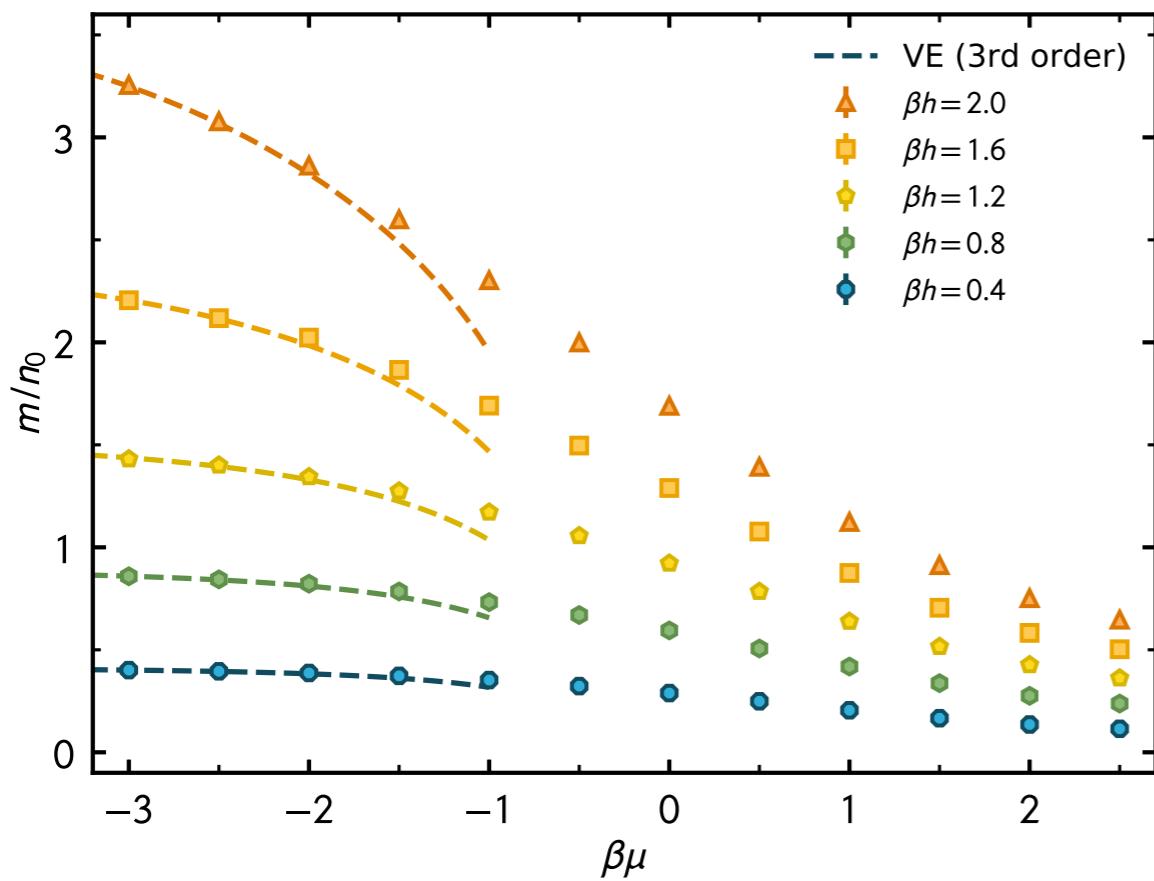
excellent agreement with virial expansion for all polarizations

# magnetization & polarization

[LR, Loheac, Drut, Braun '18]

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

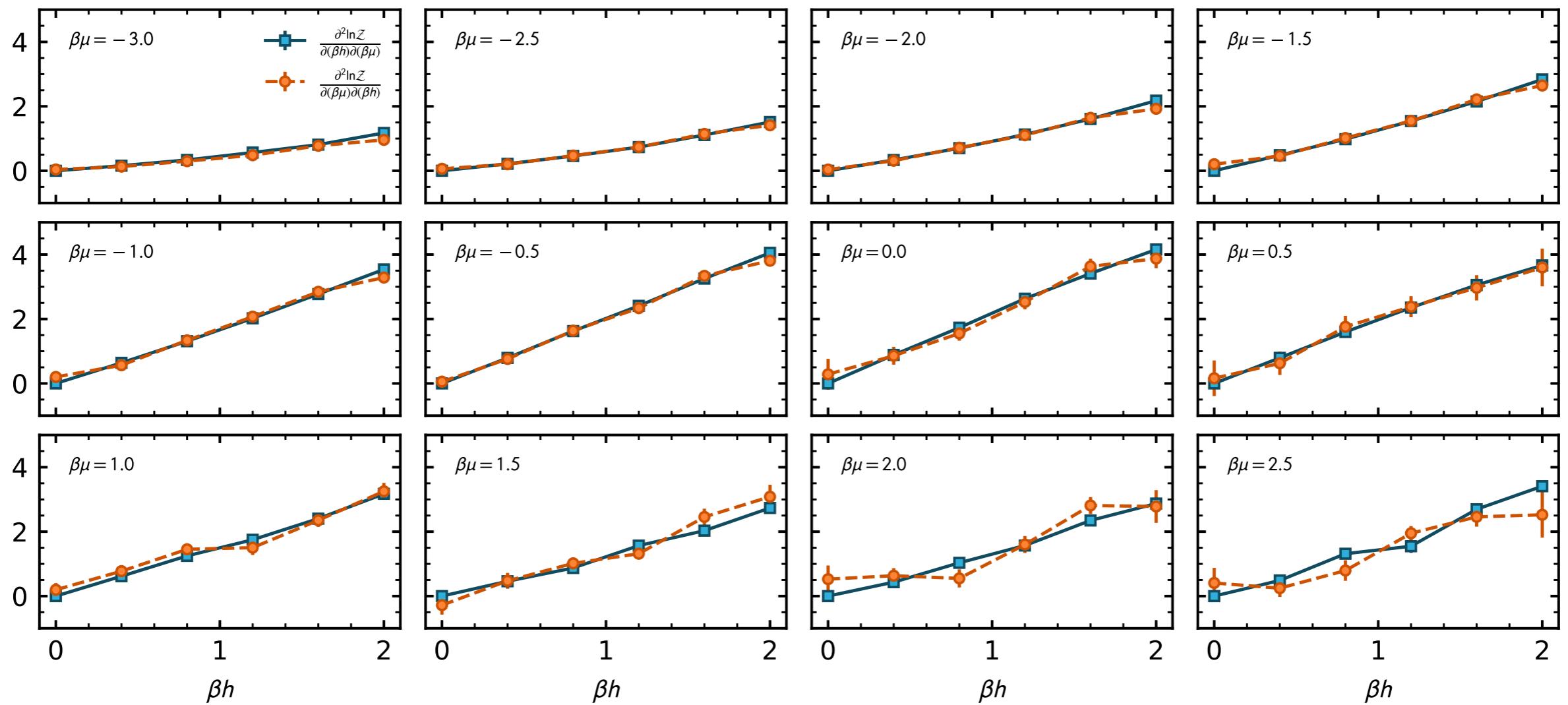
$$p = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}} = \frac{m}{n}$$



# Maxwell relations: consistency check

[LR, Loheac, Drut, Braun '18]

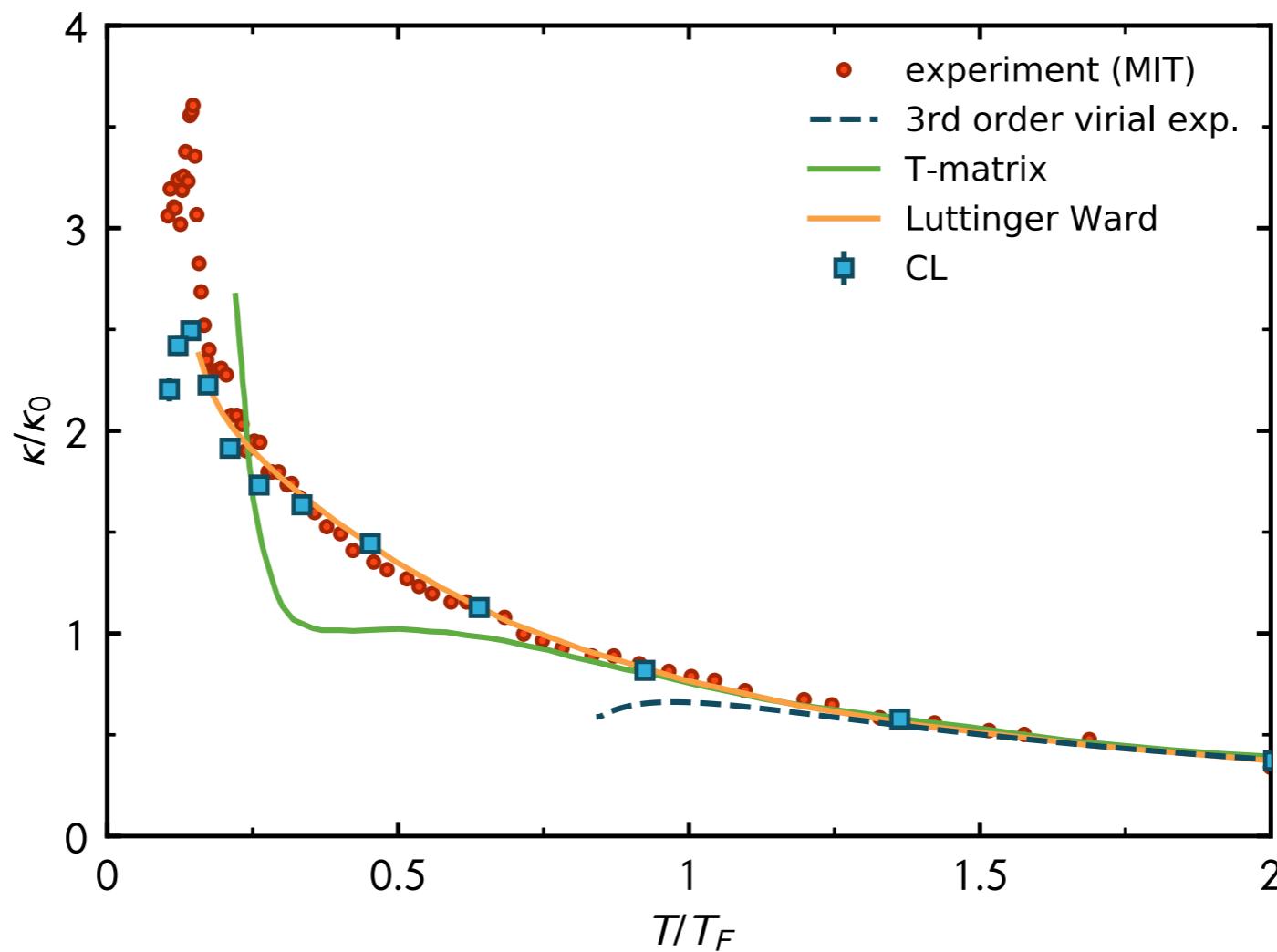
$$\left( \frac{\partial n}{\partial(\beta h)} \right)_{\beta\mu} \stackrel{!}{=} \left( \frac{\partial m}{\partial(\beta\mu)} \right)_{\beta h}$$



# compressibility (unpolarized)

[LR, Loheac, Drut, Braun '18]

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



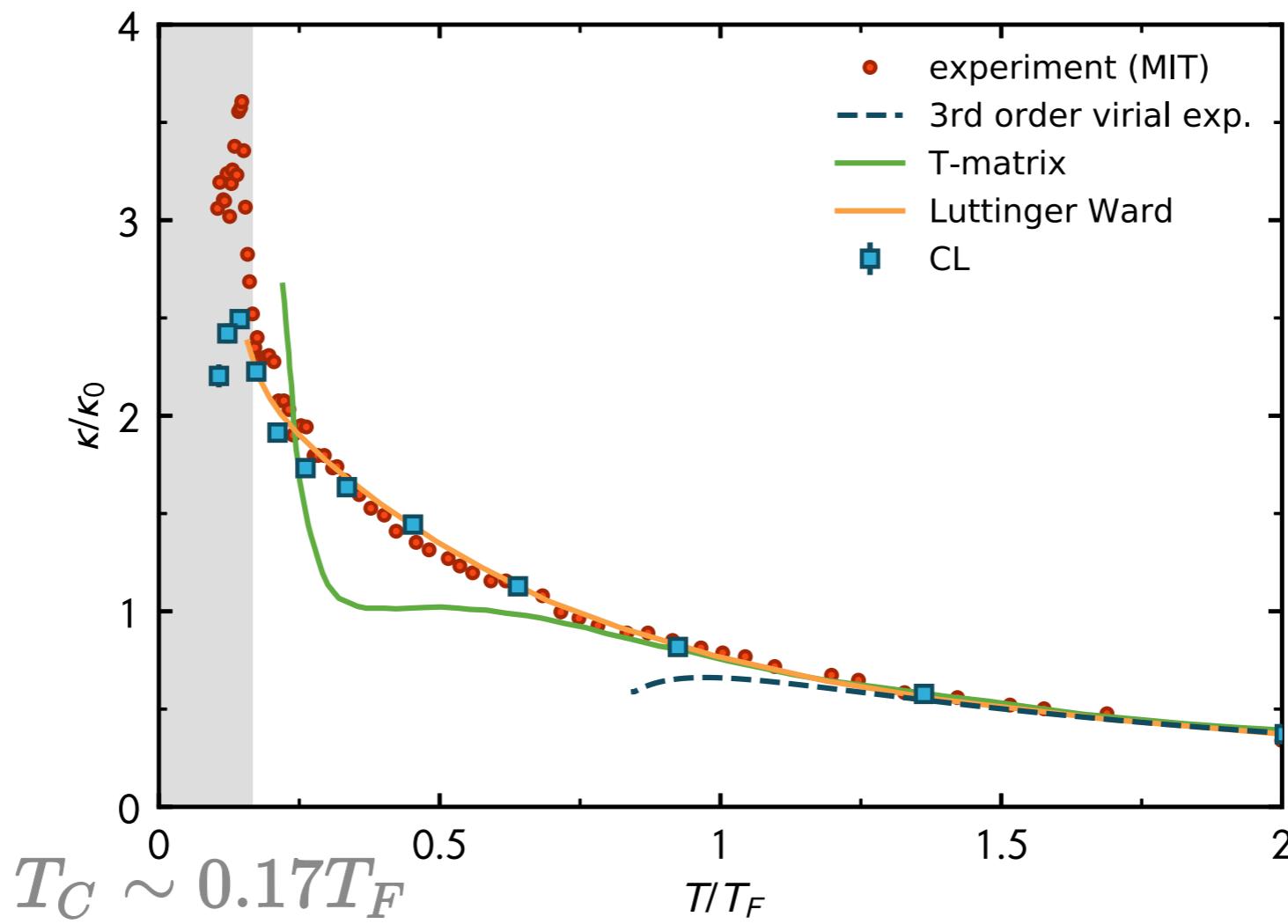
[experiment: Ku,Sommer,Cheuck,Zwierlein '12]  
[Luttinger-Ward: Enns,Haussmann '12]

# 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  $\kappa$   
indicates  
superfluid phase  
transition



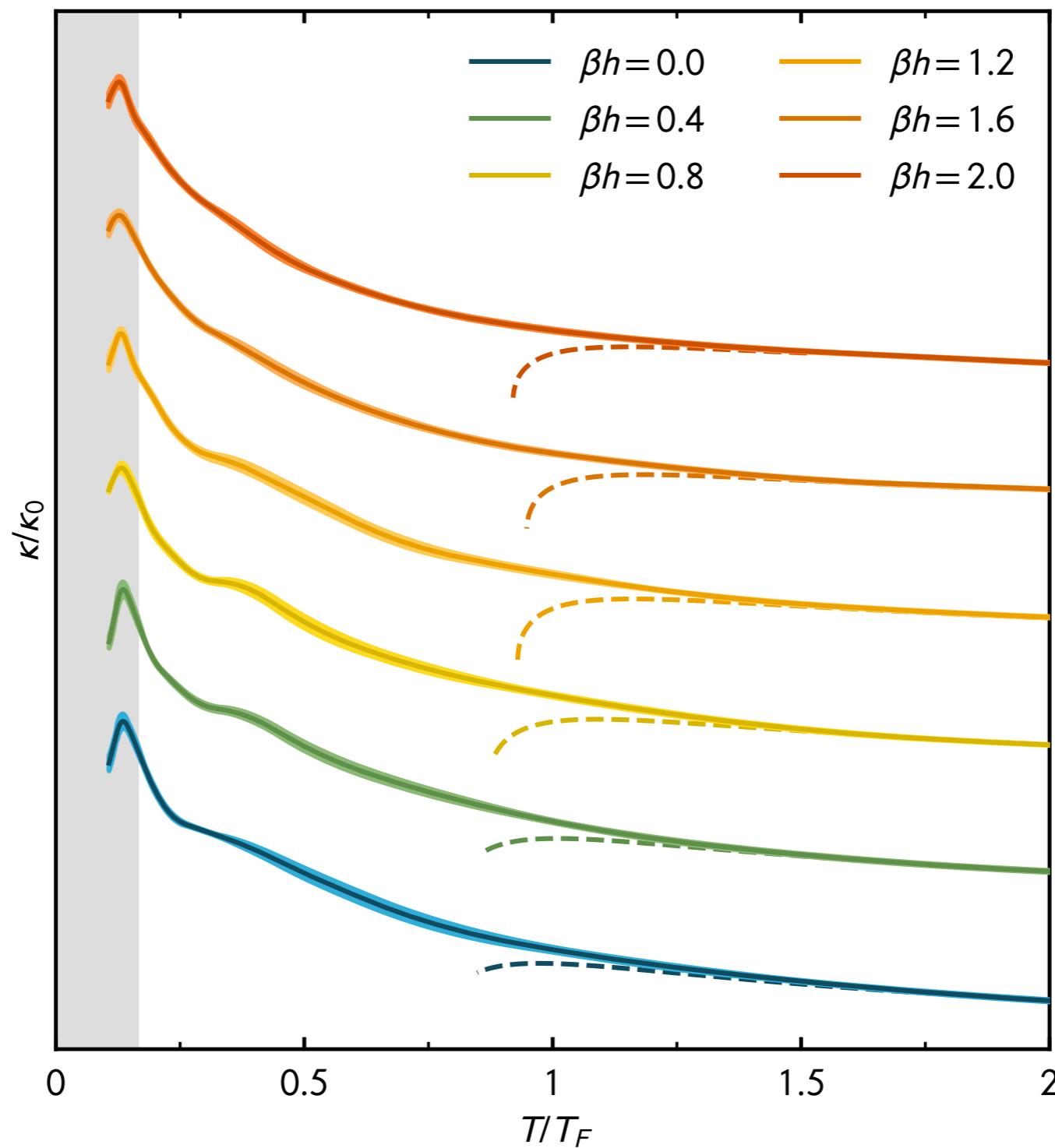
features of curve  
recovered with CL

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]

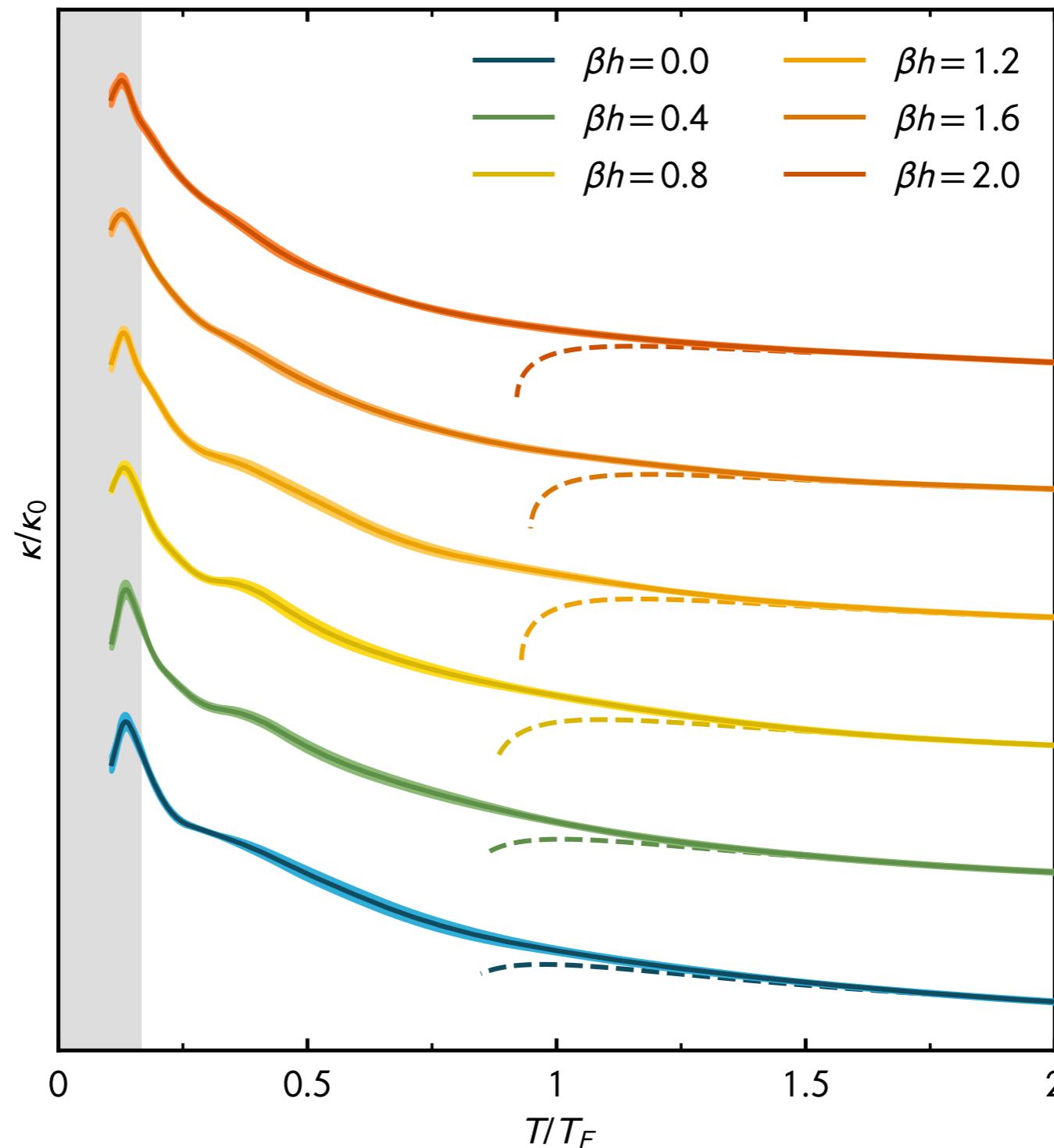


# compressibility for polarized systems

[LR, Loheac, Drut, Braun '18]

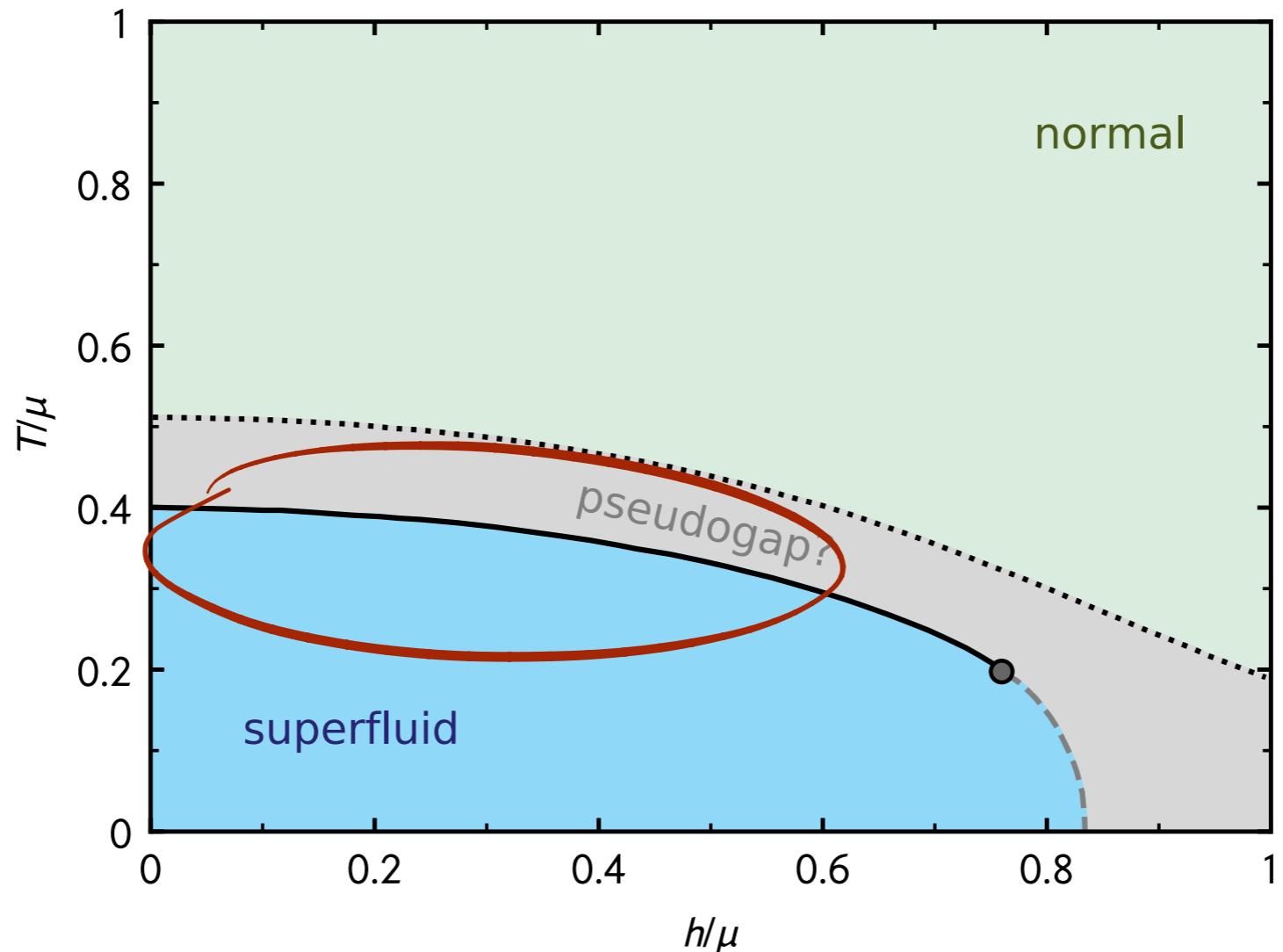
weak dependence  
of the critical  
temperature on  
polarization  
indicated

challenging to  
extract precise  $T_C$



# UFG phase diagram

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

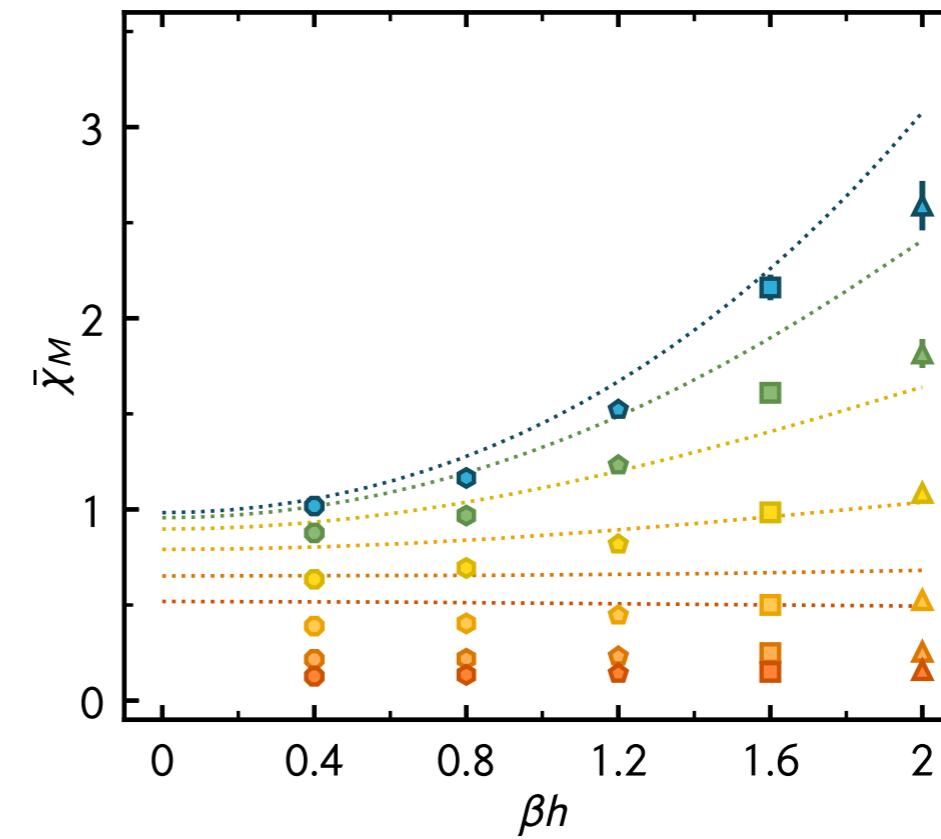
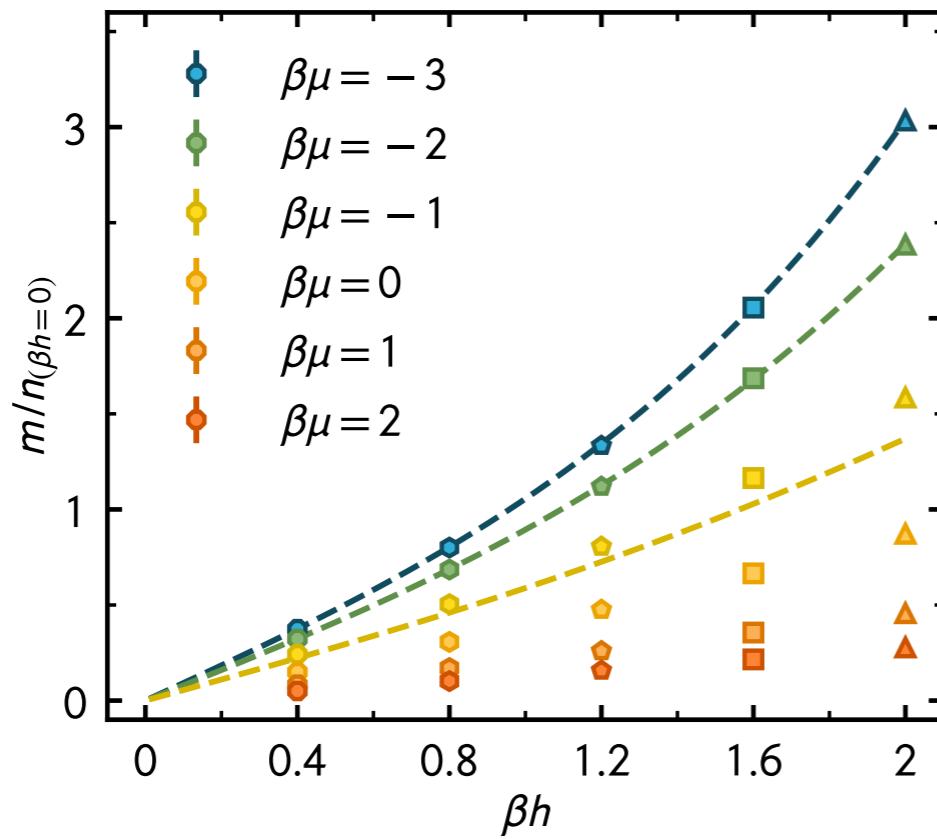


[fRG: Boettcher et. al '15]

# spin susceptibility

[LR, Loheac, Drut, Braun '18]

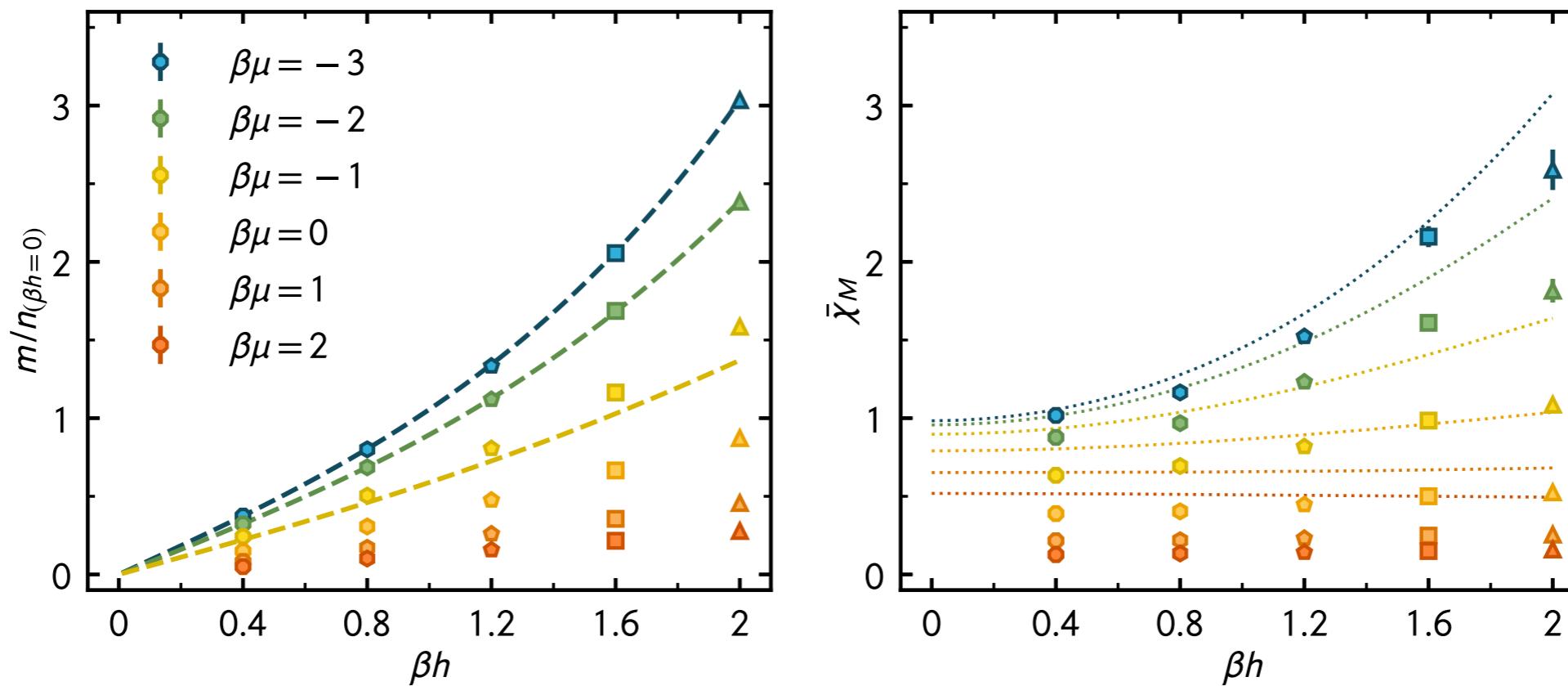
$$\chi = \left( \frac{\partial m}{\partial h} \right)_{T,V,\mu}$$



# spin susceptibility

[LR, Loheac, Drut, Braun '18]

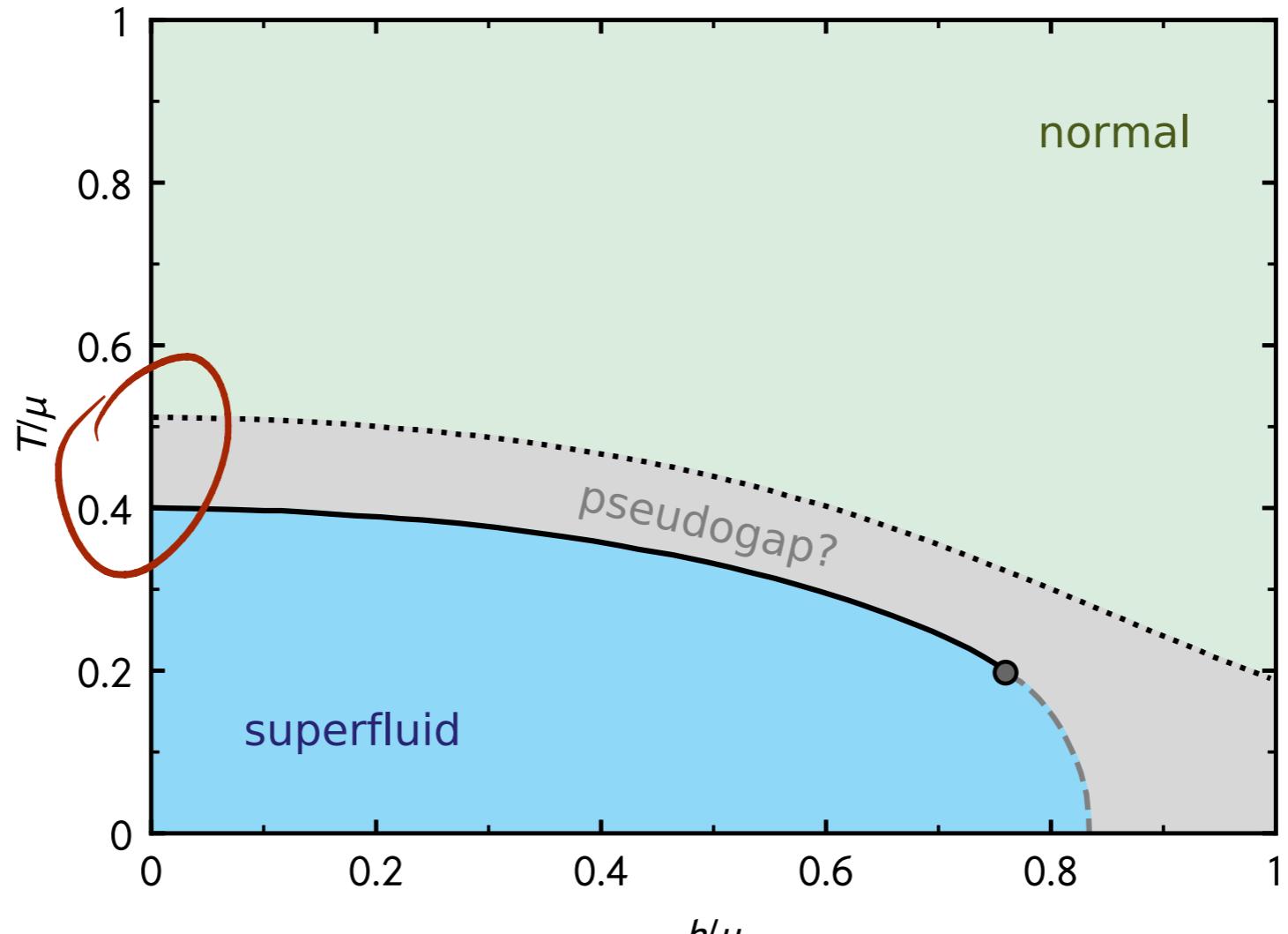
$$\chi = \left( \frac{\partial m}{\partial h} \right)_{T,V,\mu}$$



Pauli susceptibility field independent at low field and temperature

**UFG: dependence on  $\beta h$  very similar to FG, but rescaled**

# UFG phase diagram (sketch)



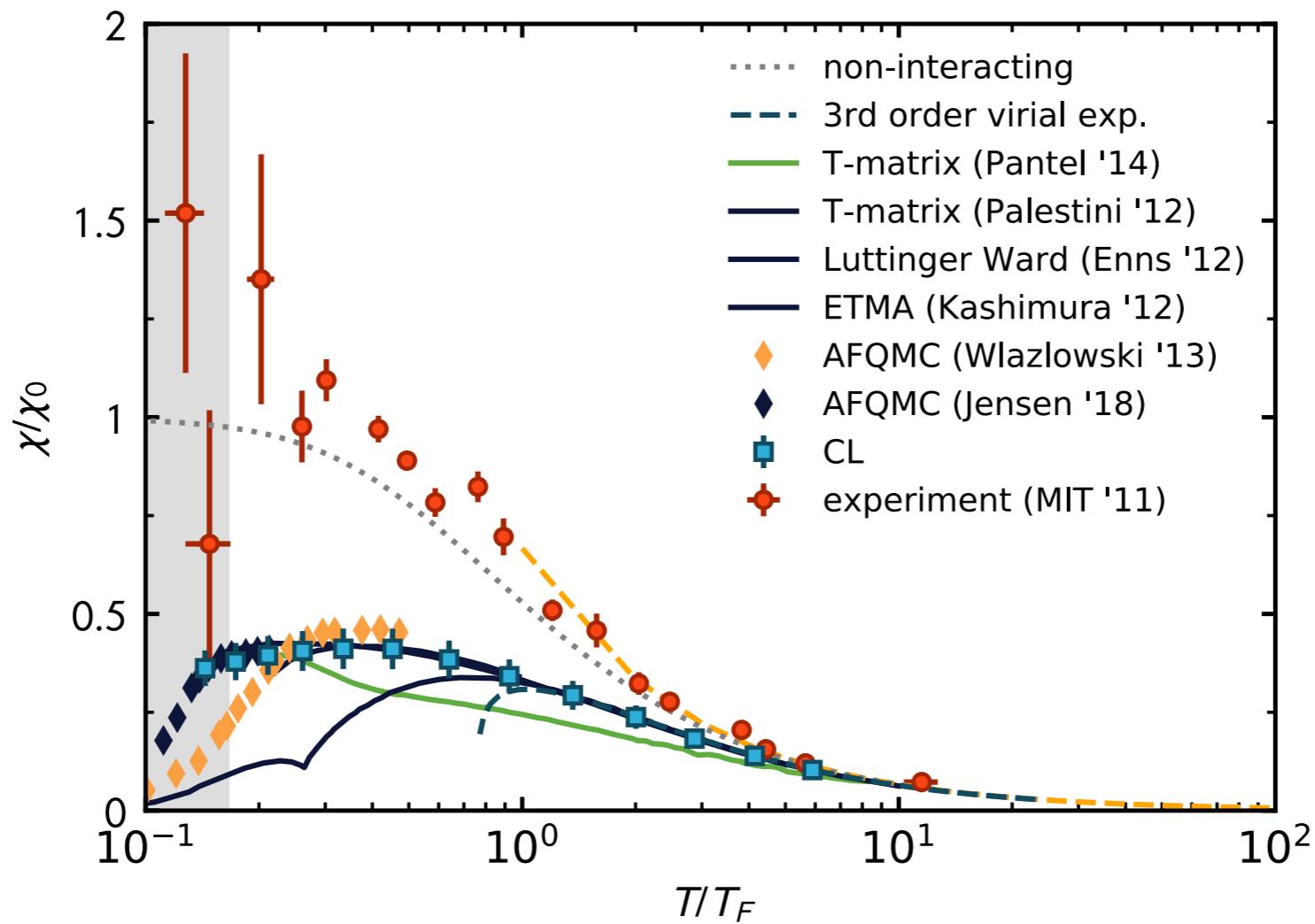
$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$

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

[fRG: Boettcher et. al '15]

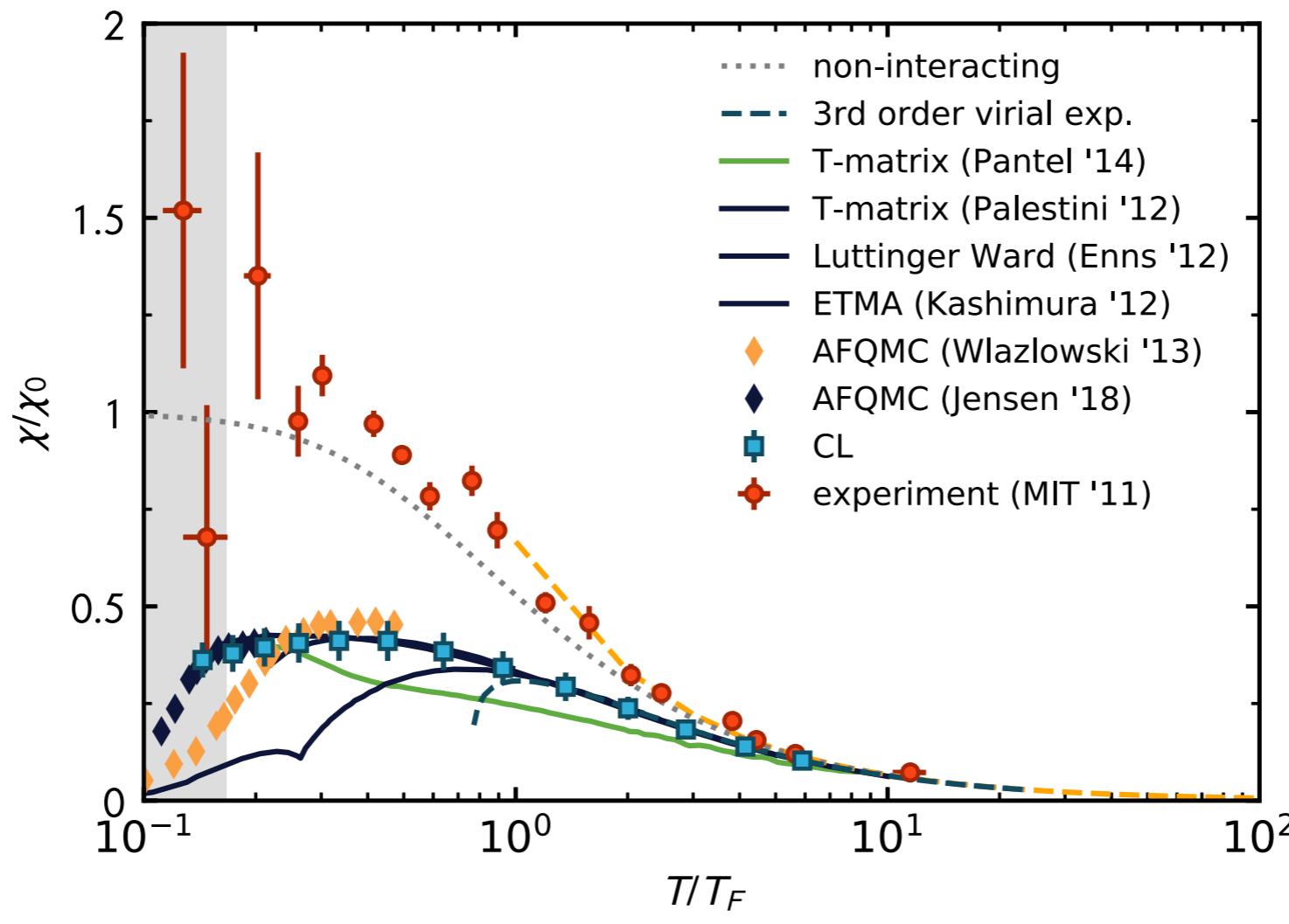
# magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]



# magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]



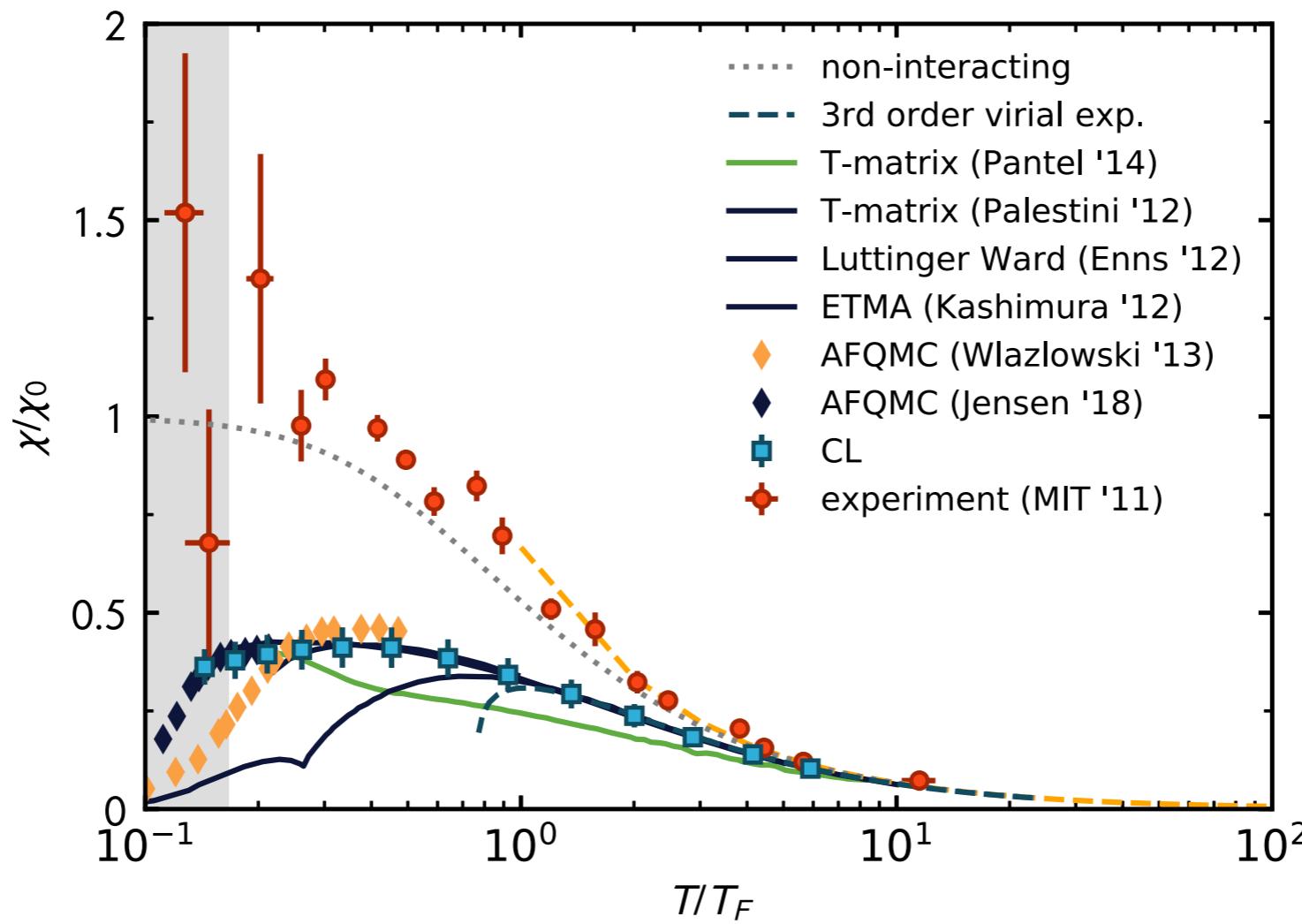
high temperature:  
Curie's law  
 $\chi \propto T^{-1}$

theory & experiment  
agree at high  
temperatures

# magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]

low  
temperature:  
discrepancy  
between  
experiment and  
theory



Pseudogap:  
suppression of  $\chi$  at  $T > T_C$

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

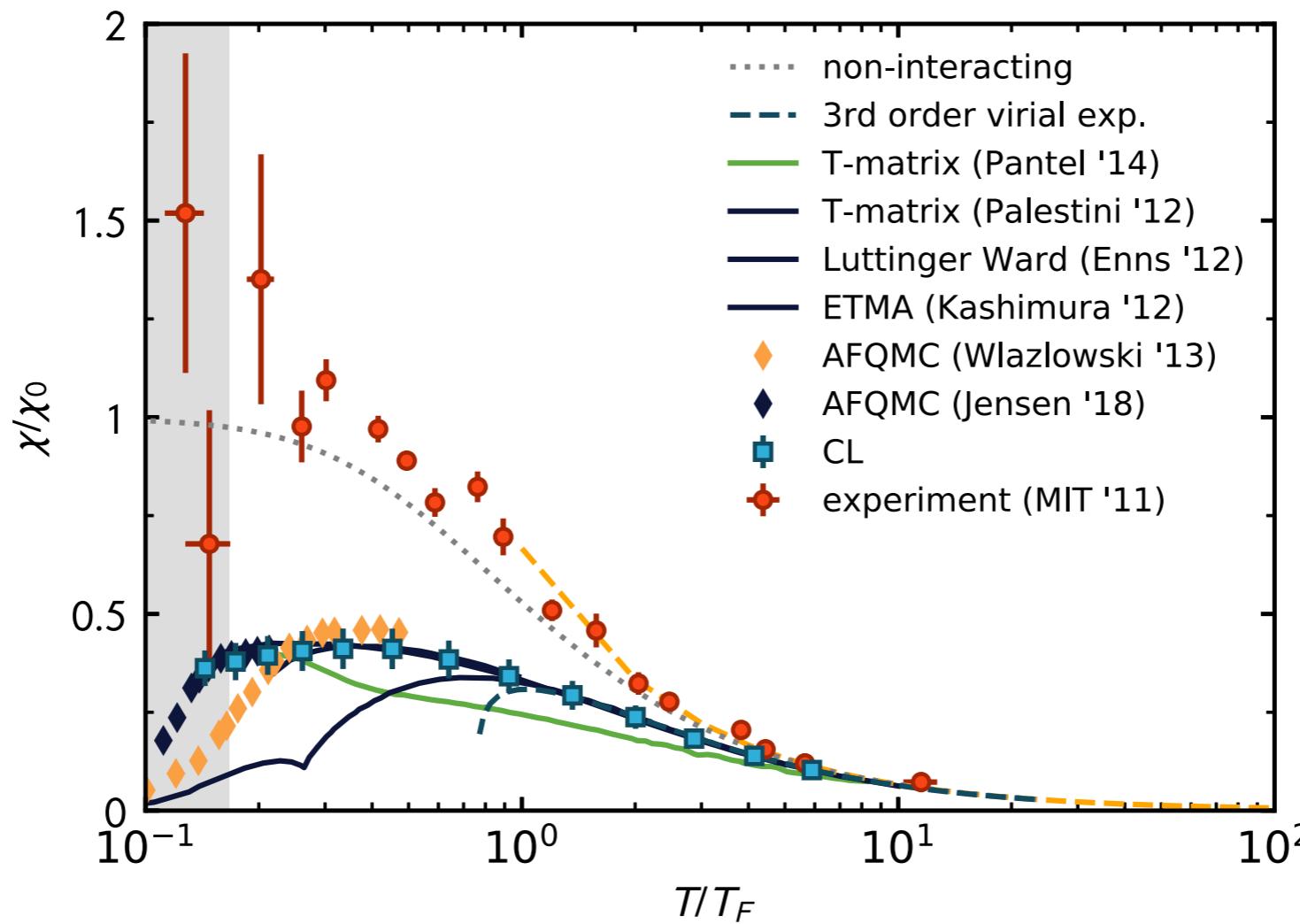
theory & experiment  
agree at high  
temperatures

[recent review: Jensen et al. '18]

# magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]

low  
temperature:  
discrepancy  
between  
experiment and  
theory



Pseudogap:  
suppression of  $\chi$  at  $T > T_C$

[recent review: Jensen et al. '18]

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

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

theory & experiment  
agree at high  
temperatures

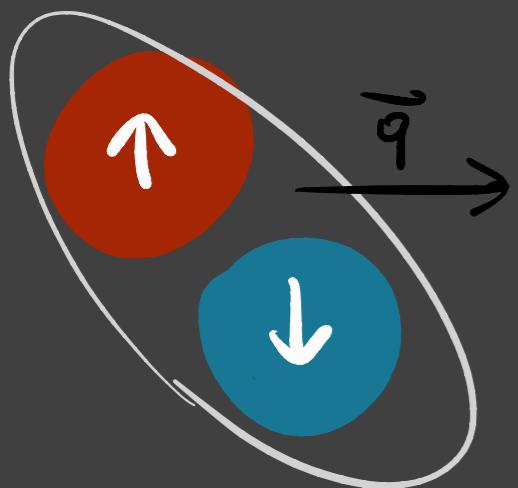
# RECAP

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

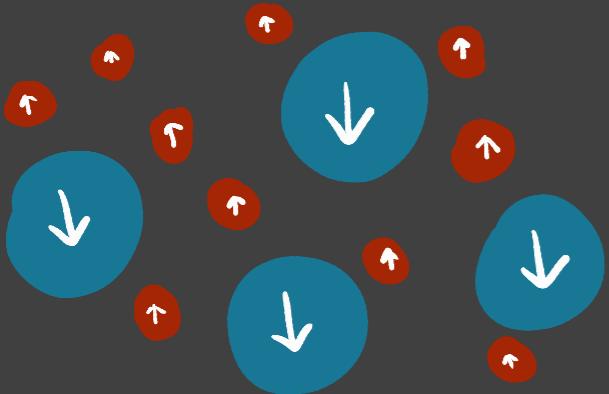
**EOS, magnetic properties & response** accessible  
for the unitary Fermi gas at finite temperature and polarization  
**in ab initio fashion**

# STAY TUNED!

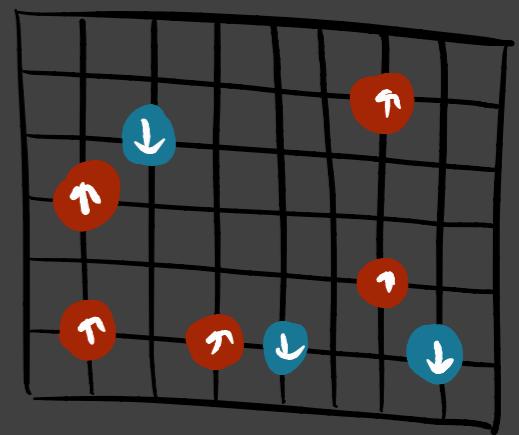


**looking for inhomogeneous phases in the UFG**  
[ongoing work with Florian Ehmann, Joaquin Drut & Jens Braun]

**thermodynamics of 2D fermions at finite polarization**  
[ongoing work with Josh McKenney, Andrew Loheac, Joaquin Drut & Jens Braun]



**effect of mass-imbalance on fermion pair formation**

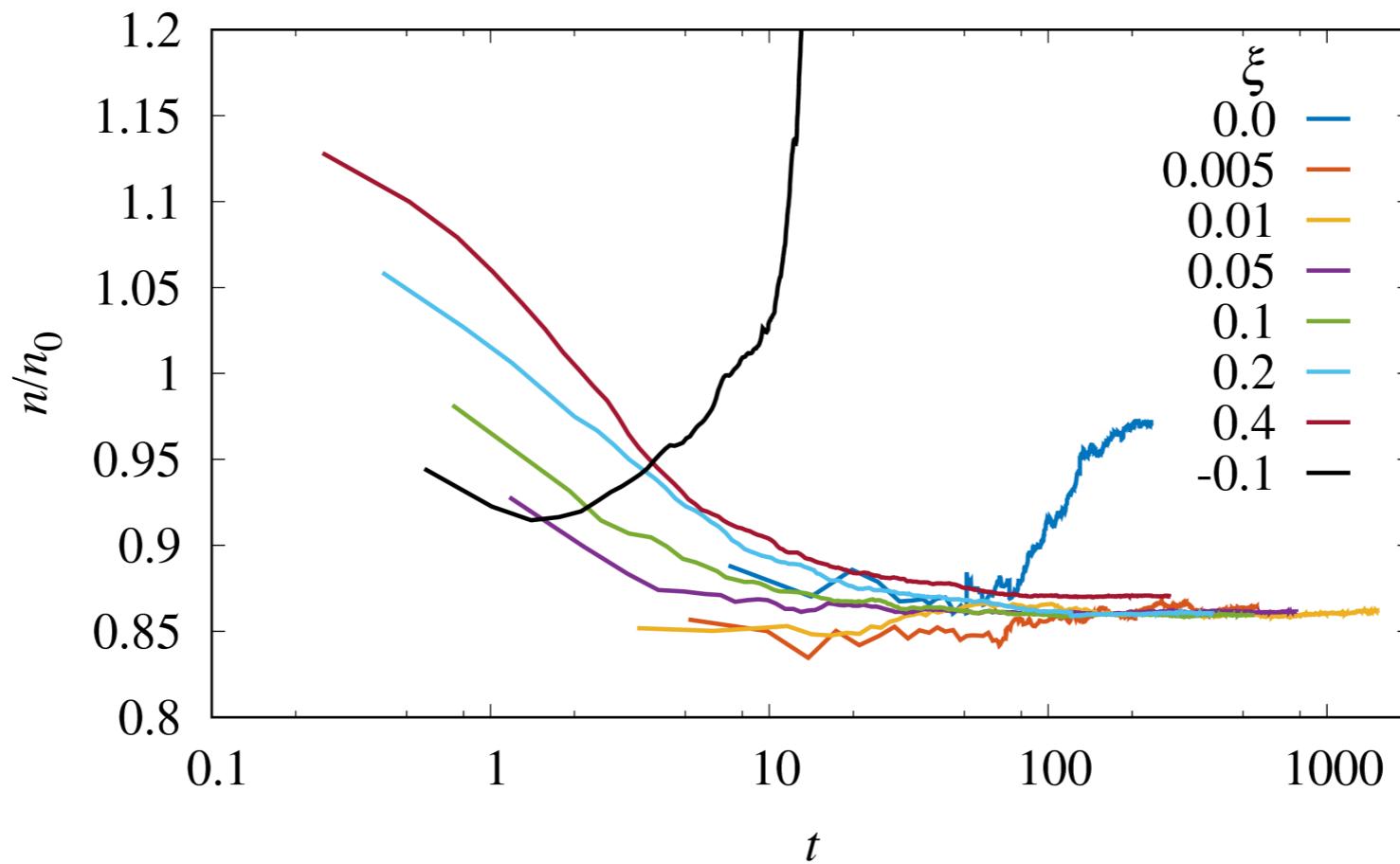


# APPENDIX

# regulator to stabilize numerics

[Loheac,Drut '17]

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

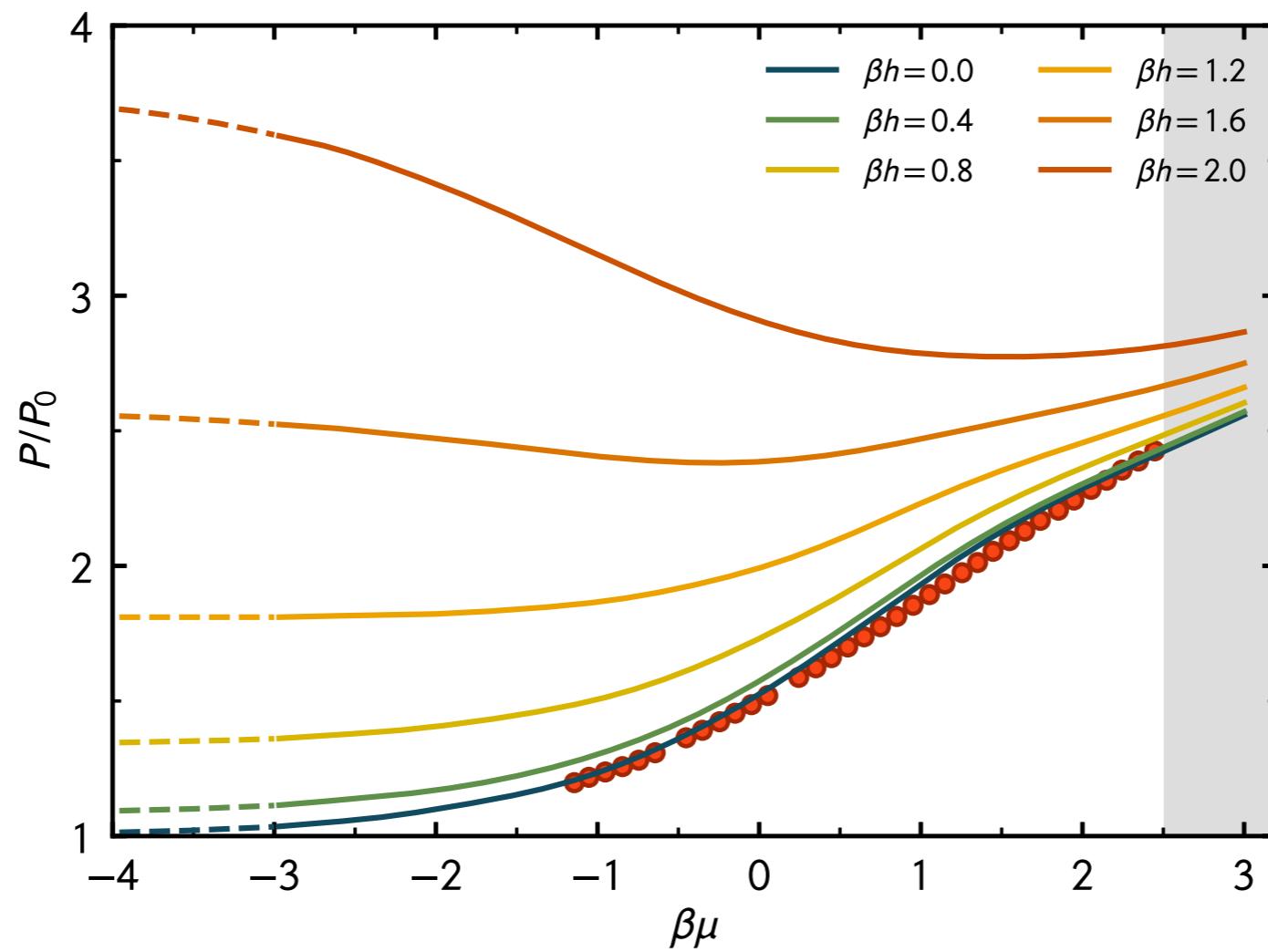


unregulated runs tend to fail:  $\xi$  stabilizes CL trajectories

# pressure equation of state

[LR, Loheac, Drut, Braun '18]

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

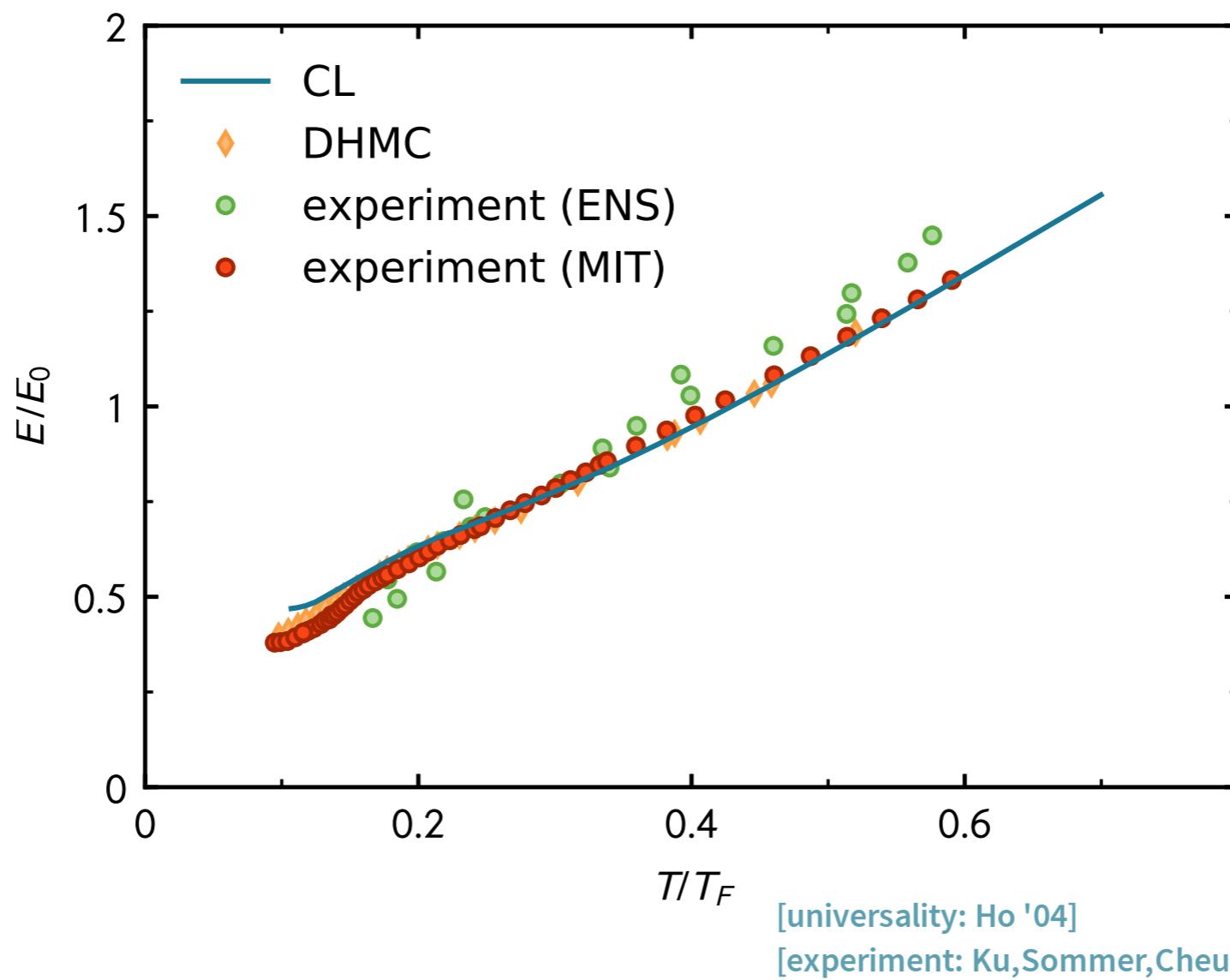


[experiment: Ku,Sommer,Cheuck,Zwierlein '12]

# energy equation of state

[LR, Loheac, Drut, Braun in preparation]

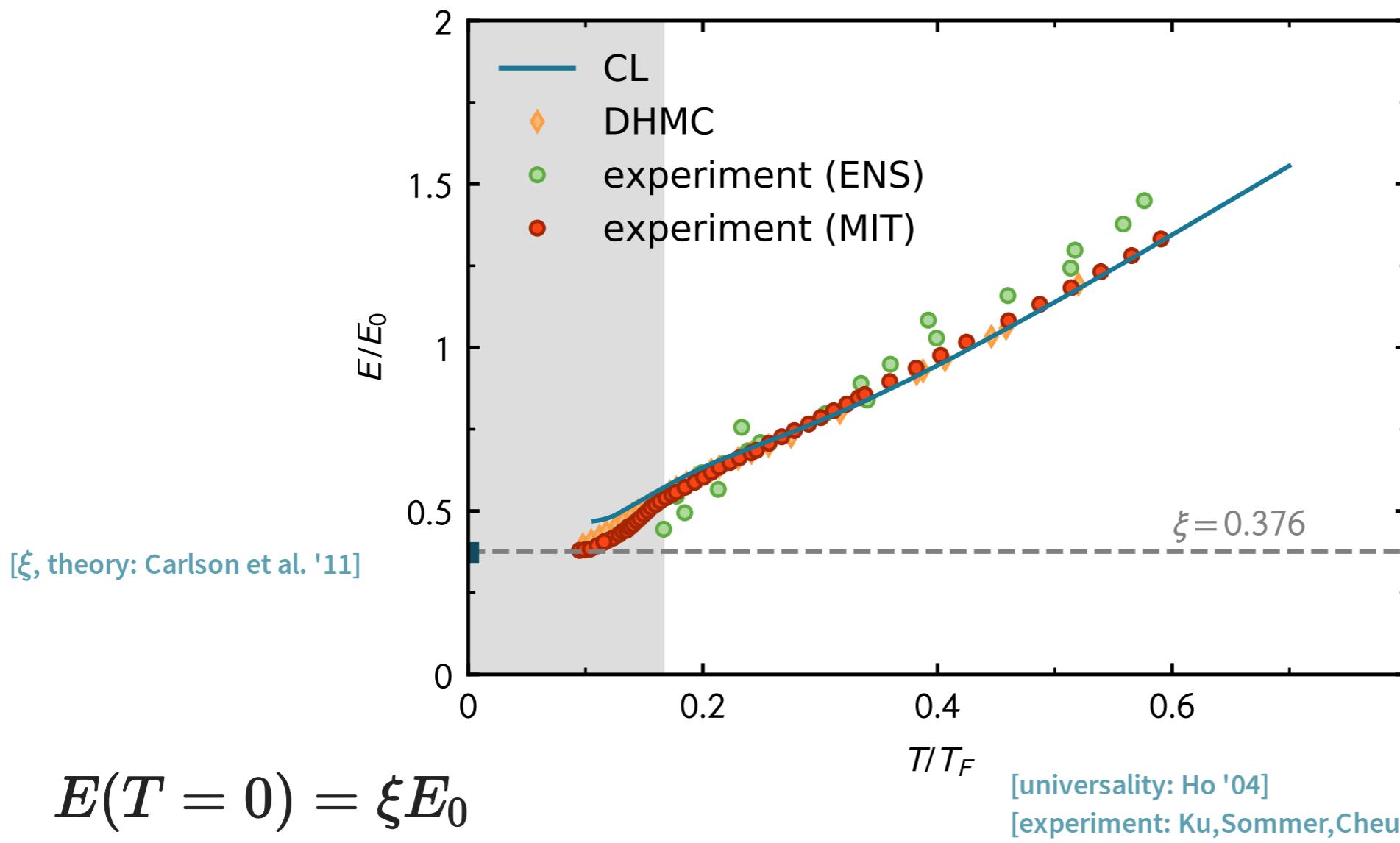
$$E = \frac{3}{2} PV$$



# energy equation of state

[LR, Loheac, Drut, Braun in preparation]

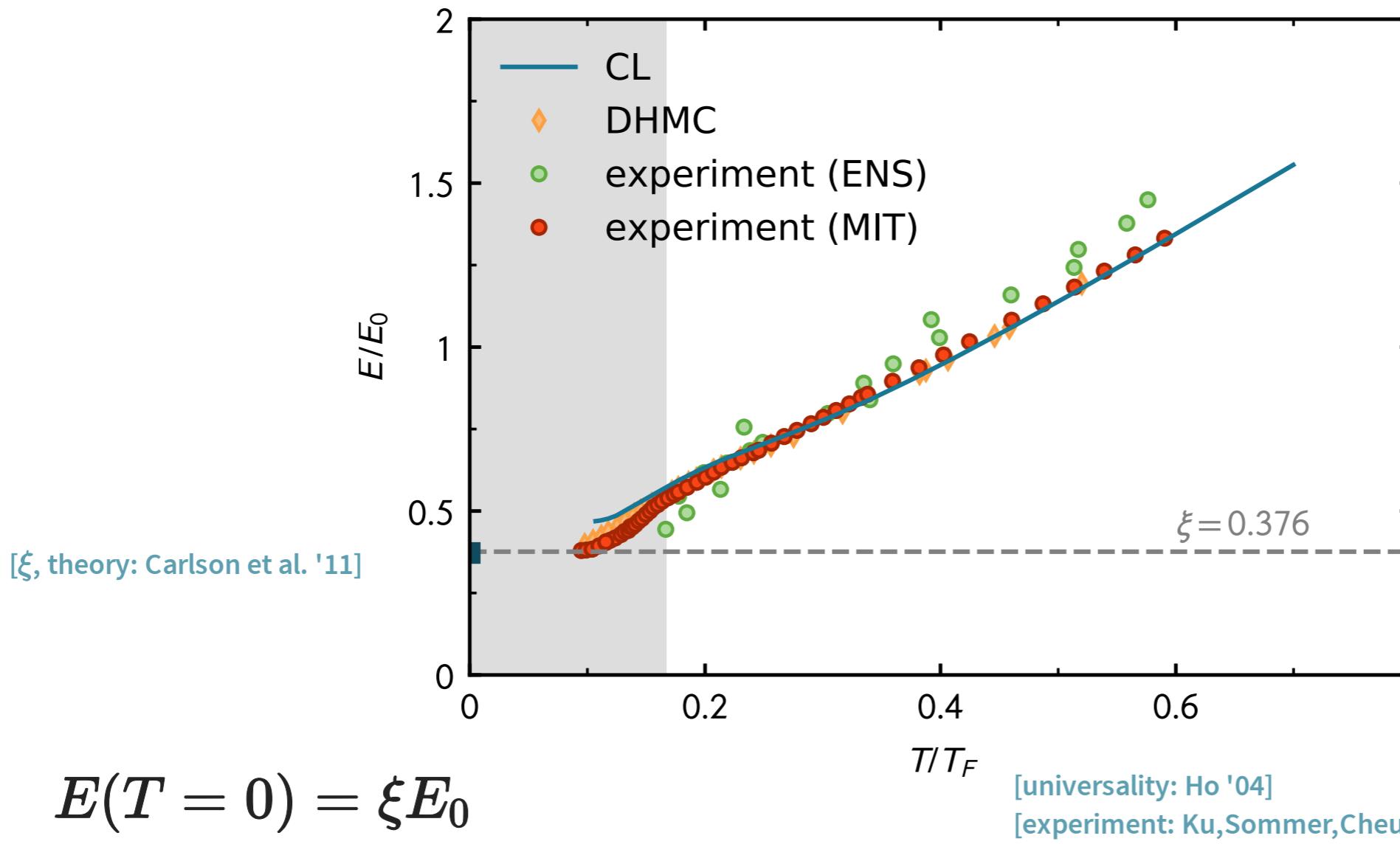
$$E = \frac{3}{2} PV$$



# energy equation of state

[LR, Loheac, Drut, Braun in preparation]

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



at low temperature:  
larger lattices,  
improved operators

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

[universality: Ho '04]

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