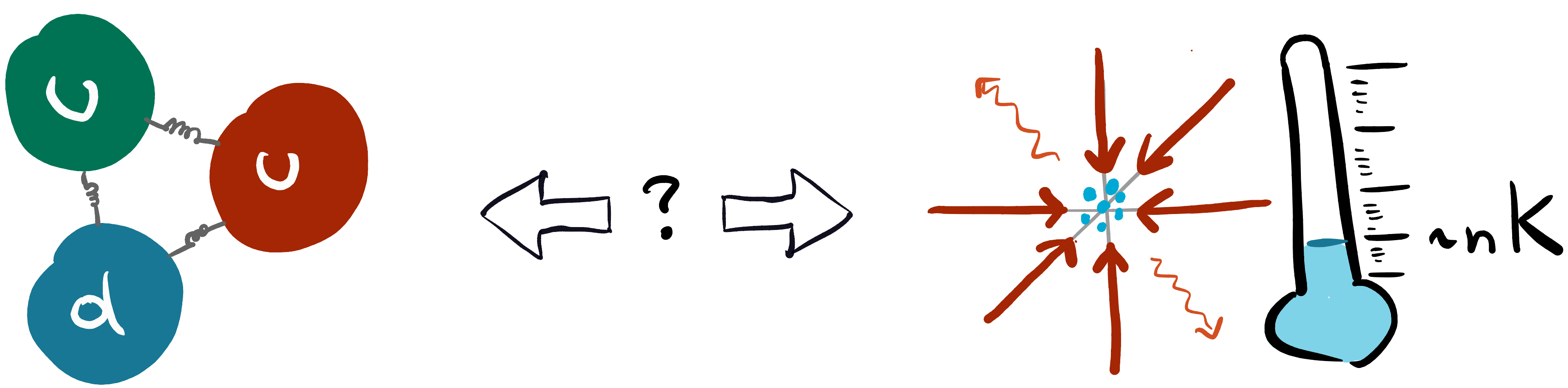
Approaching imbalanced Fermi gases via complex Langevin



Lukas Rammelmüller, TU Darmstadt

ECT workshop "High-energy physics at ultra-cold temperatures" - June 10, 2019*

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Helmholtz Graduate School for Hadron and Ion Research

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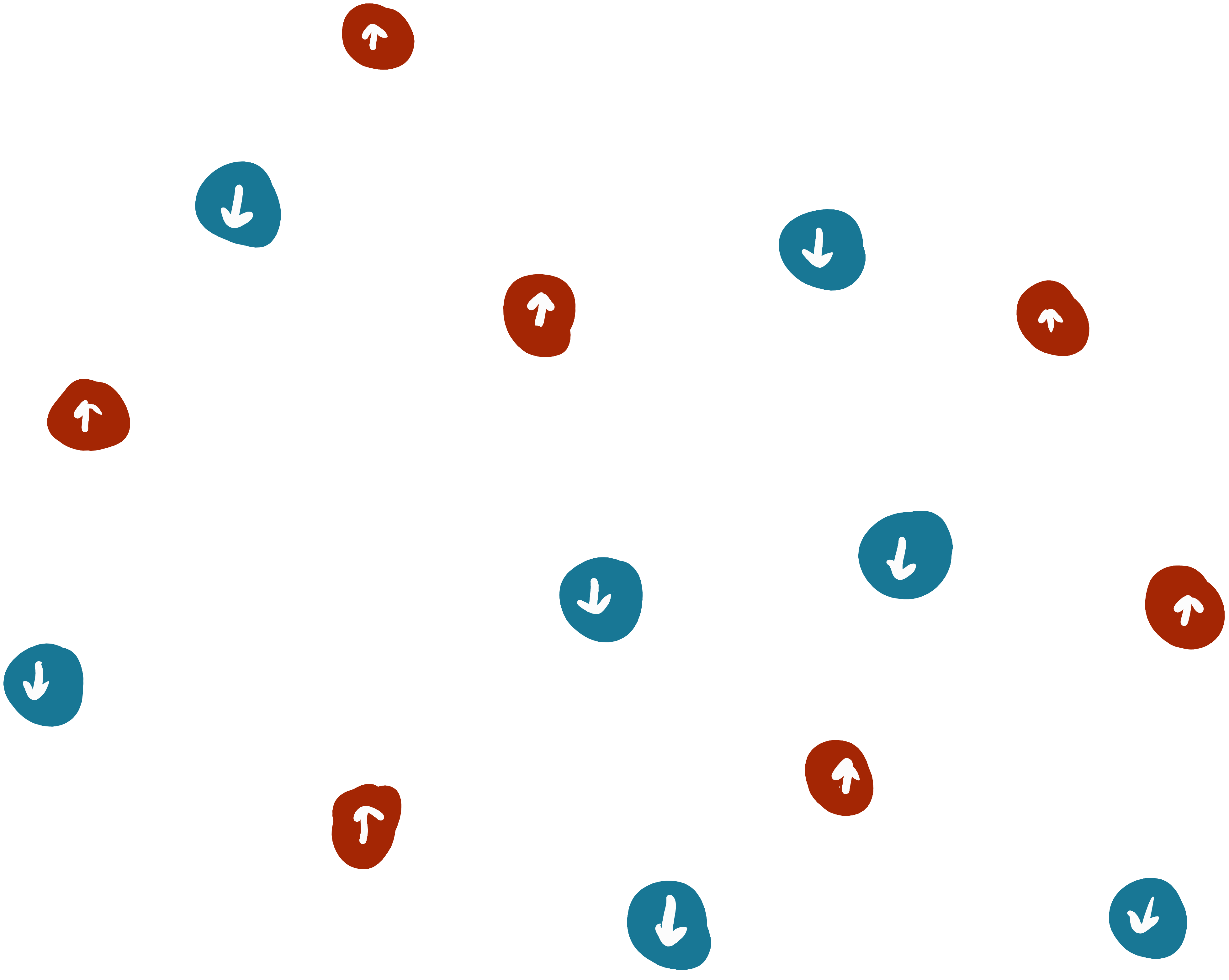
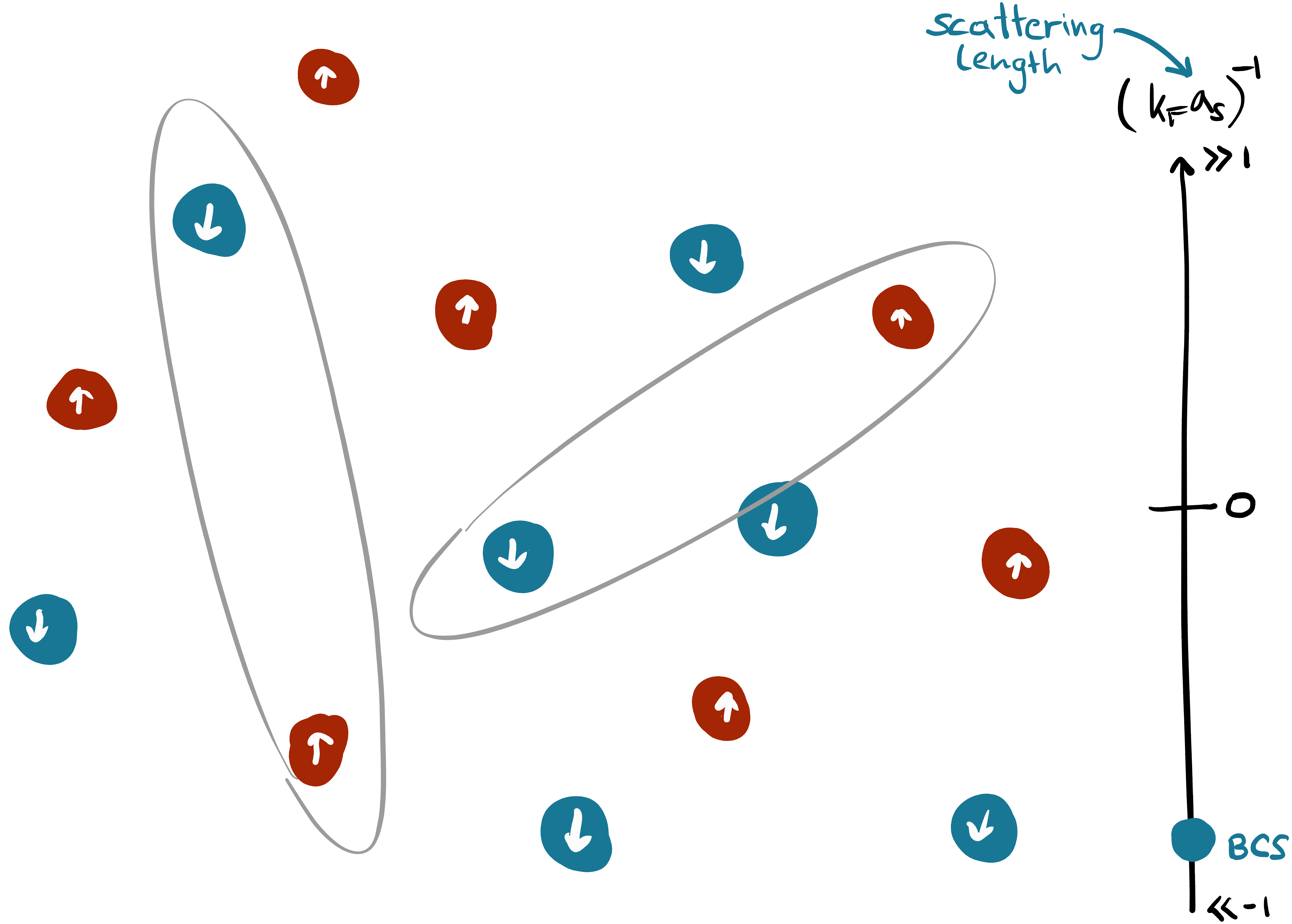
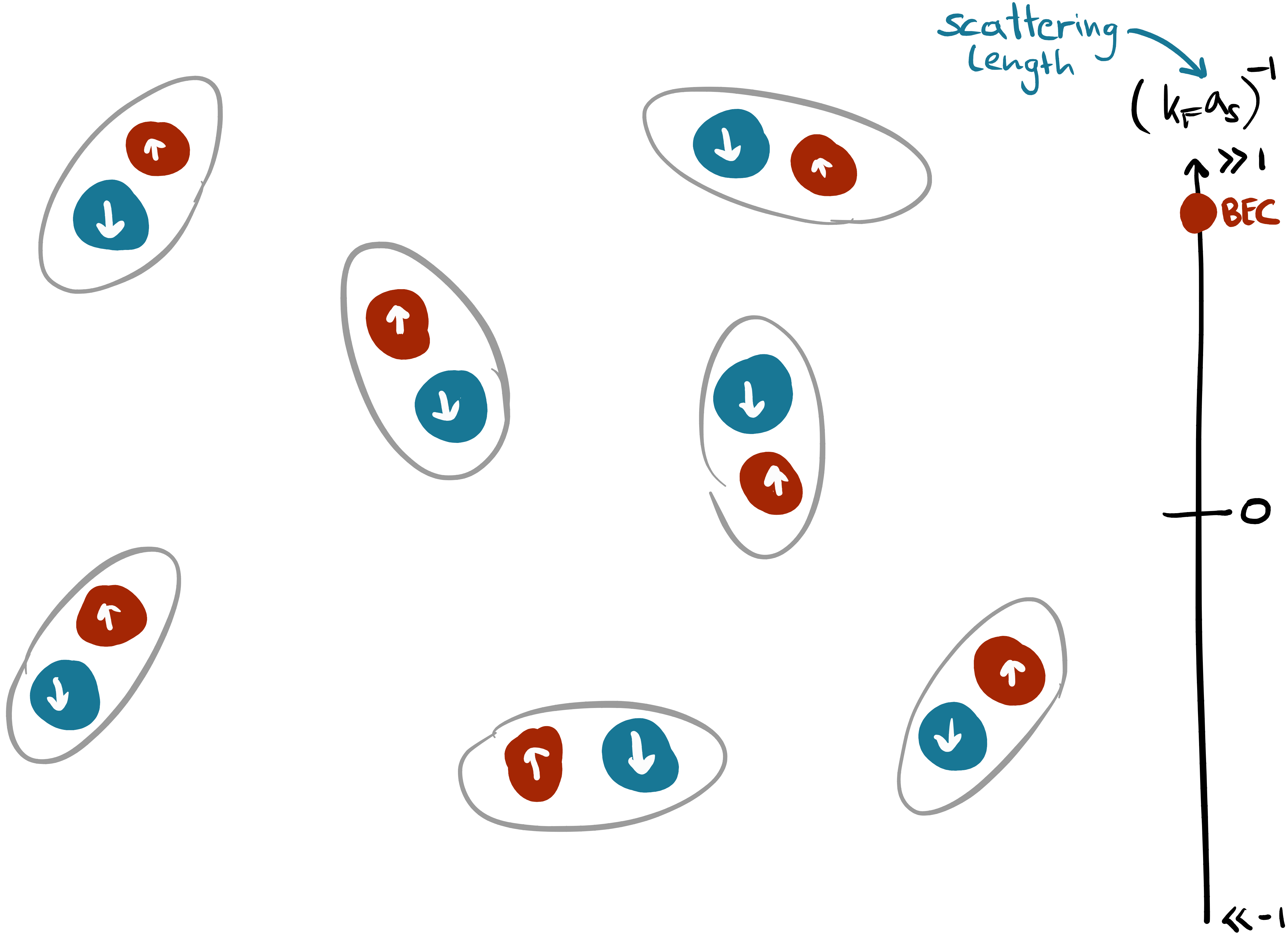
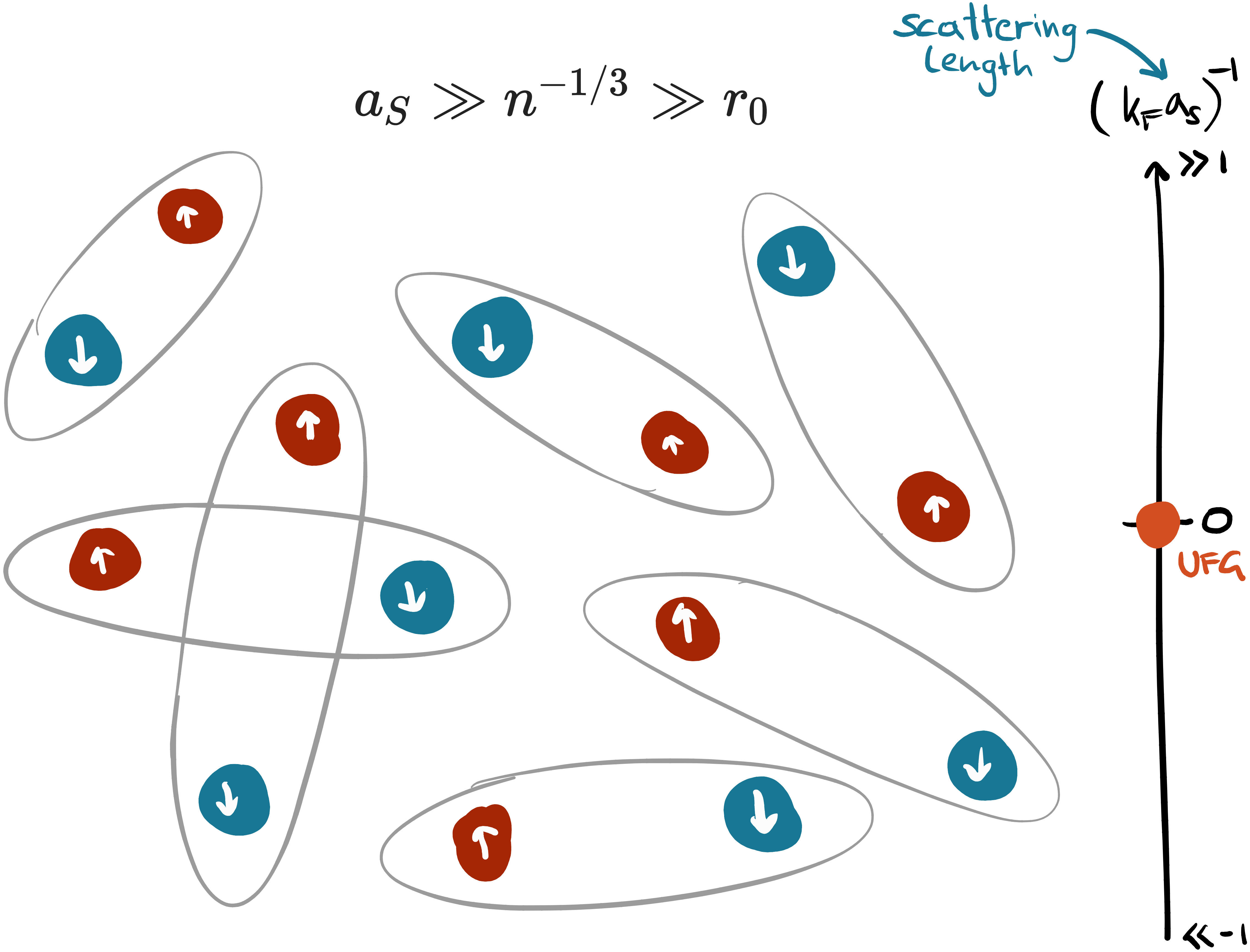


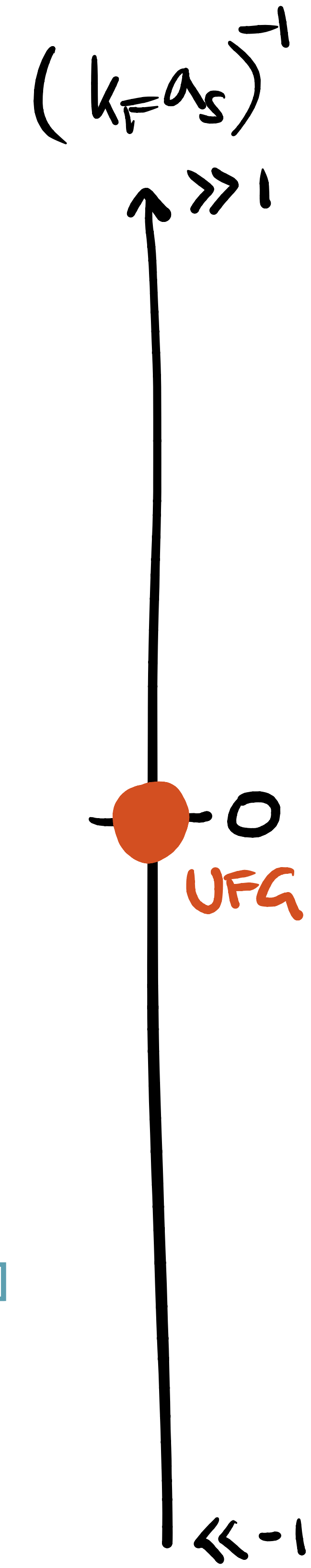

scattering length
$(k_F a_s)^{-1}$
$\gg 1$
0
BCS
$\ll -1$


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]



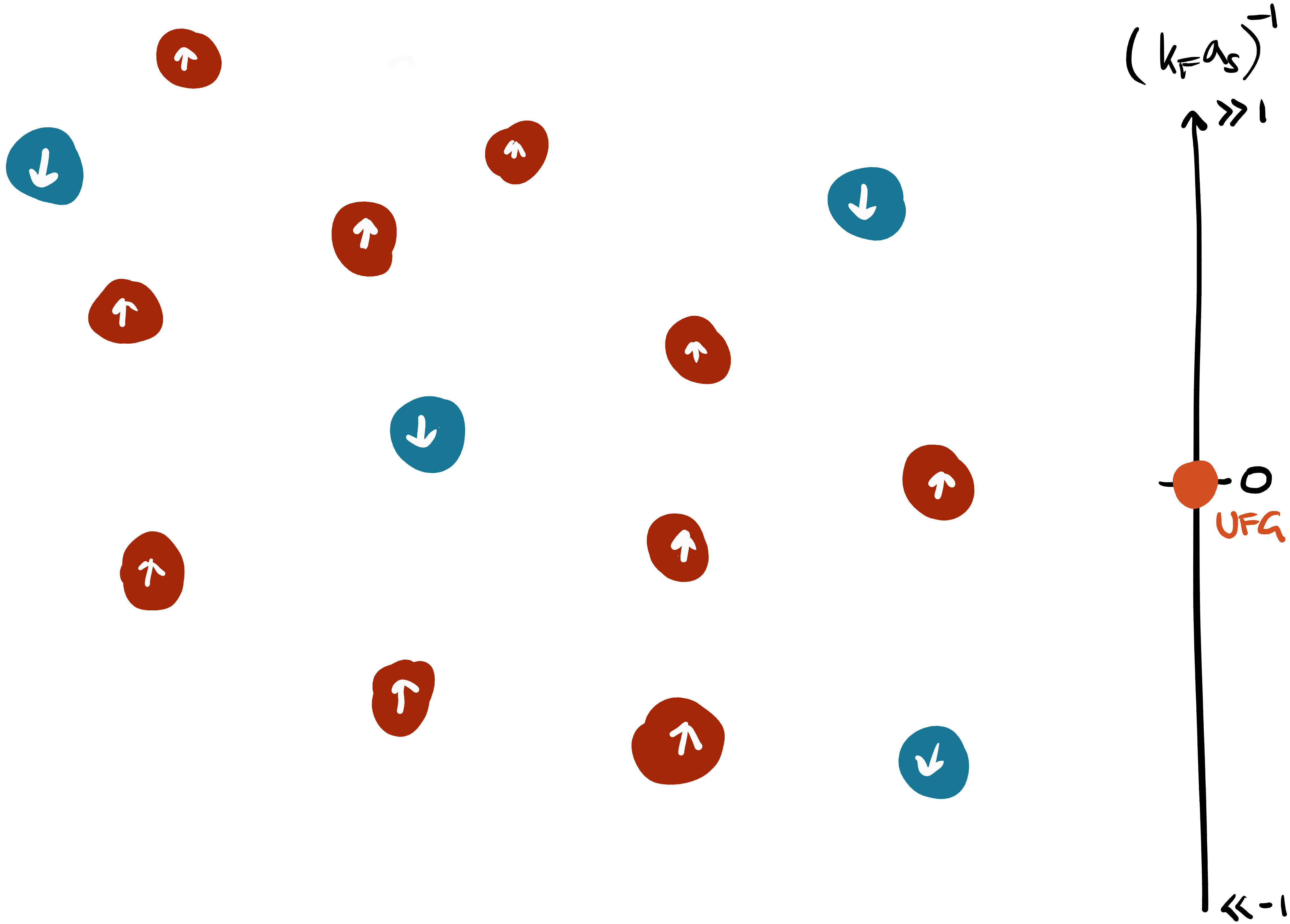
density & temperature are the **only** dimensionful scales in the system

universal scaling functions:

$$E = E_{FG}\ f_E(\beta\mu)$$
$$P = P_{FG}\ f_P(\beta\mu)$$
$$\cdots$$

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]

agenda

part I

quick intro to **stochastic quantization & CL**

(what is it & how can it help us for fermions?)

part II

unitary fermions with finite polarization

(equations of state & thermodynamic response)

part III

correlation functions & pairing at finite polarization

(one-dimensional systems, preliminary)

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)

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):

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

ficticous Langevin time (not physical)

noise term

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

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

the Langevin method

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

discretization

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

(Markov chain)

statistical evaluation

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

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

how can stochastic quantization help us to study fermions?

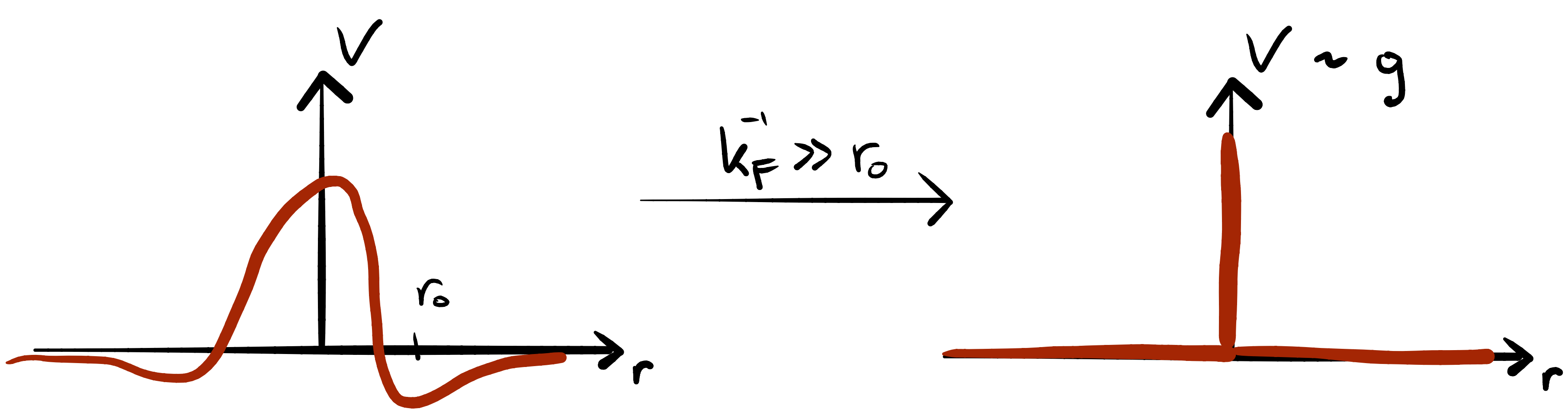
fermions with contact interaction

kinetic part

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

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

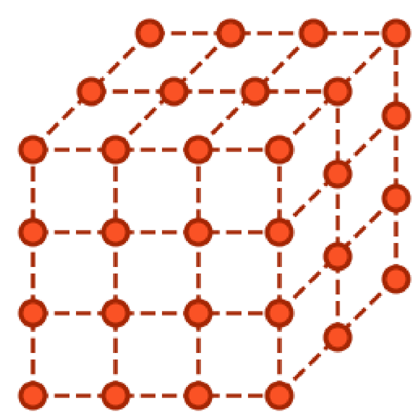
interaction part



what do we need to compute?

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

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



+ 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 & 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:

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

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

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

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

$$\int \mathcal{D}\phi \; P[\phi]O[\phi] \stackrel{?}{=} \int \mathcal{D}\phi_{\mathrm{R}}\mathcal{D}\phi_{\mathrm{I}} \; P[\phi_{\mathrm{R}} + \mathrm{i}\phi_{\mathrm{I}}]O[\phi_{\mathrm{R}} + \mathrm{i}\phi_{\mathrm{I}}]$$

guaranteed convergence if PDF decays
fast enough and $S[\phi]$ is holomorphic

[Aarts,Seiler,Stamatescu '10; Aarts,James,Seiler,Stamatescu '11]

non-analyticities in the action

- zeros in measure ($\det M = 0$)
- could lead to ergodicity issues (bottlenecks)

[Aarts,Seiler,Sexty,Stamatescu '17]

non-vanishing boundary terms

- convergence to wrong limits possible
- behavior must be monitored

[Scherzer,Seiler,Sexty,Stamatescu '19]

recap:
stochastic quantization & CL

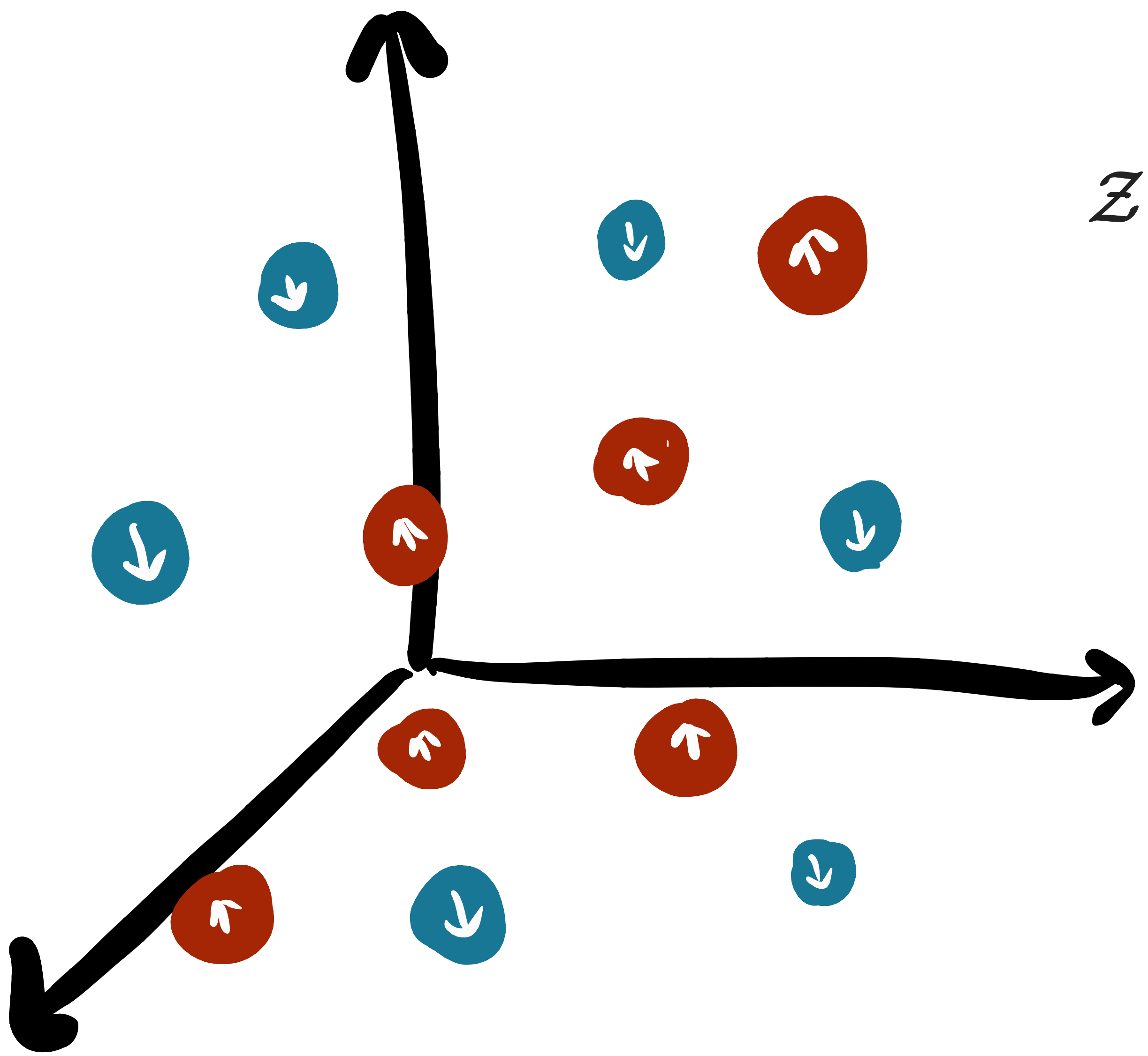
SQ: interpret **Euclidean field theories**
as equilibrium limit of a ficticious **random process**
(allows us to build a **Markov chain**)

complex Langevin provides a way
to **evade sign problems** in some cases

however: not guaranteed to work a-priori
and the **behavior needs to be monitored carefully**

the unitary Fermi gas at finite temperature

[LR, Loheac, Drut, Braun '18]



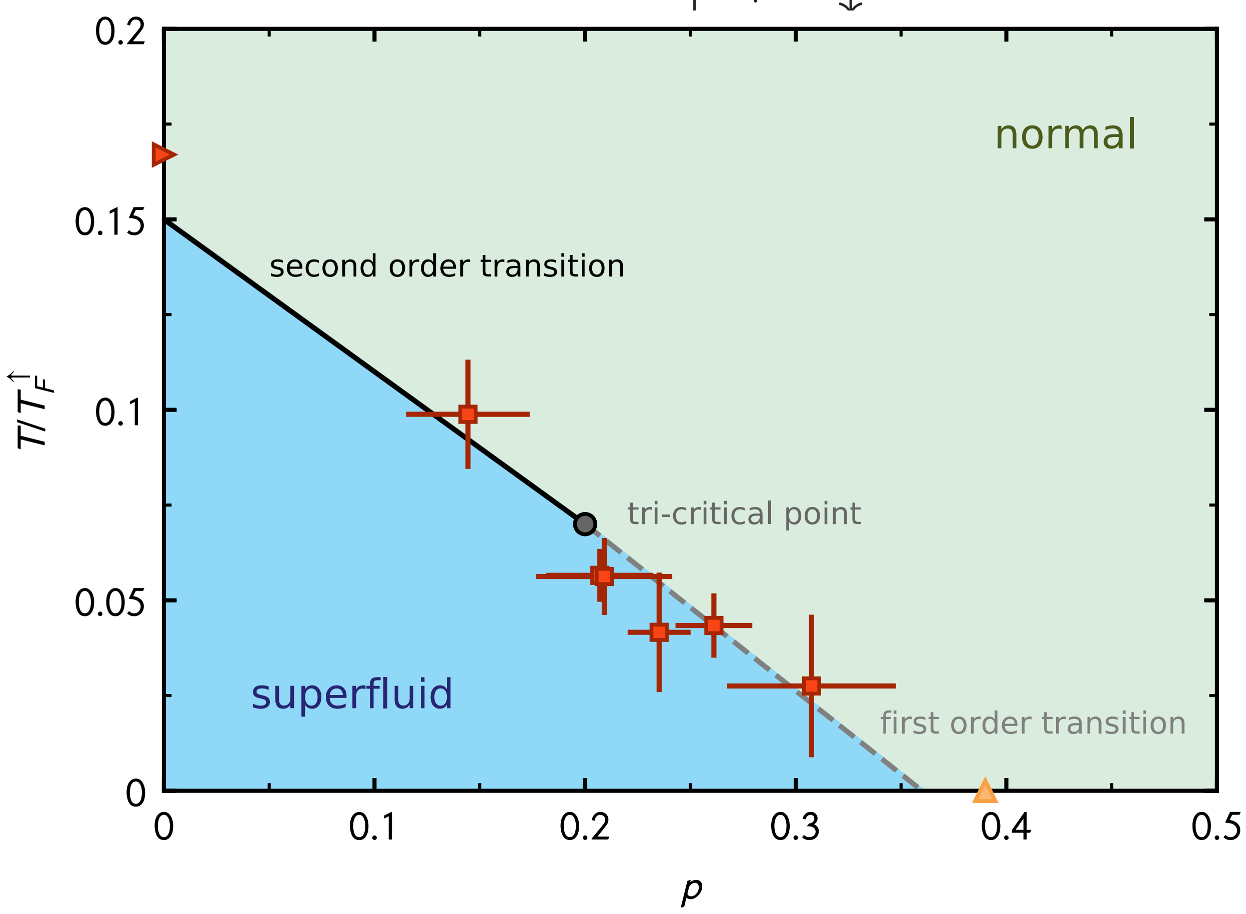
$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu_\uparrow \hat{N}_\uparrow - \mu_\downarrow \hat{N}_\downarrow)}\right]$$
$$= \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu \hat{N} - h\hat{M})}\right]$$

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

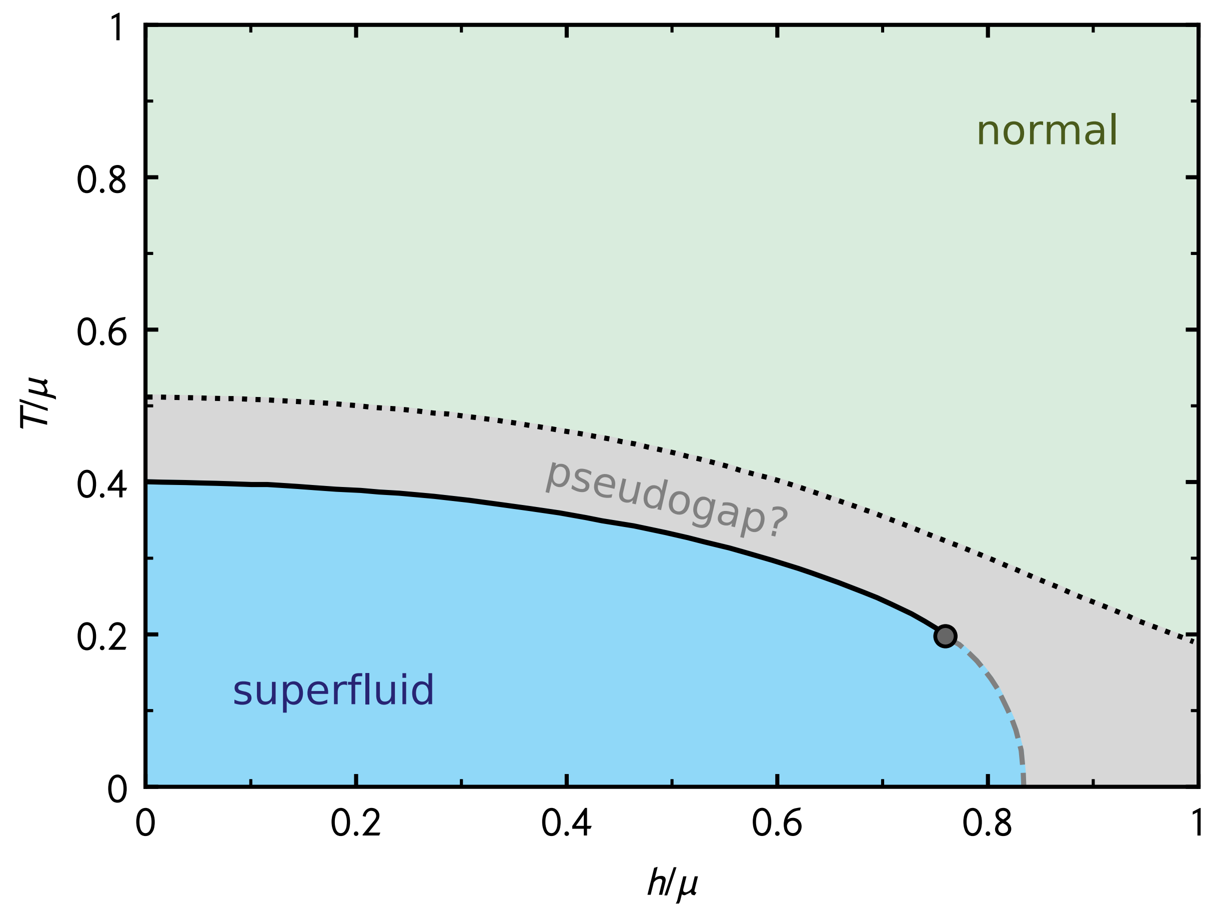
computationally challenging (but feasible)

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]
[zero-temperature PD: Bausmerth,Recati,Stringari '09]

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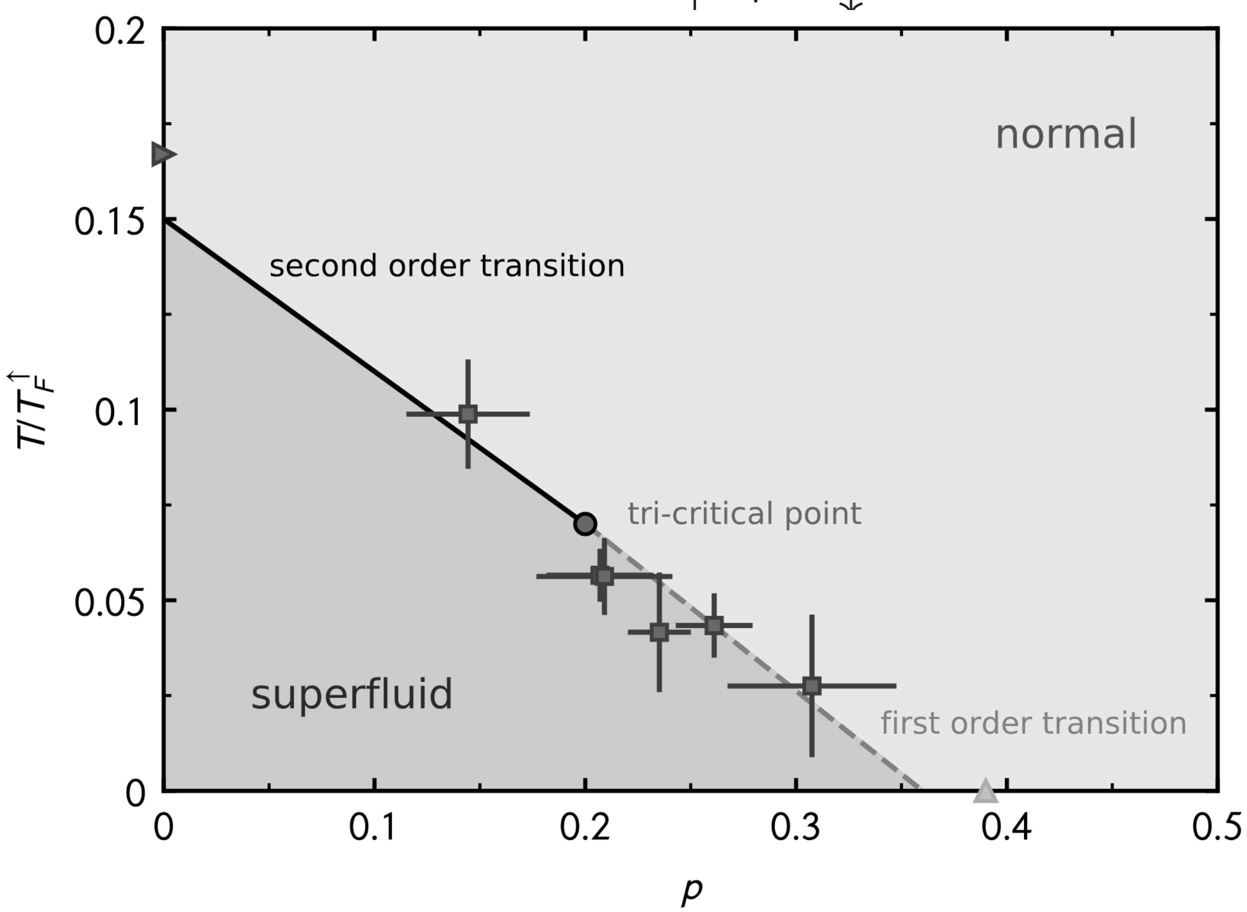

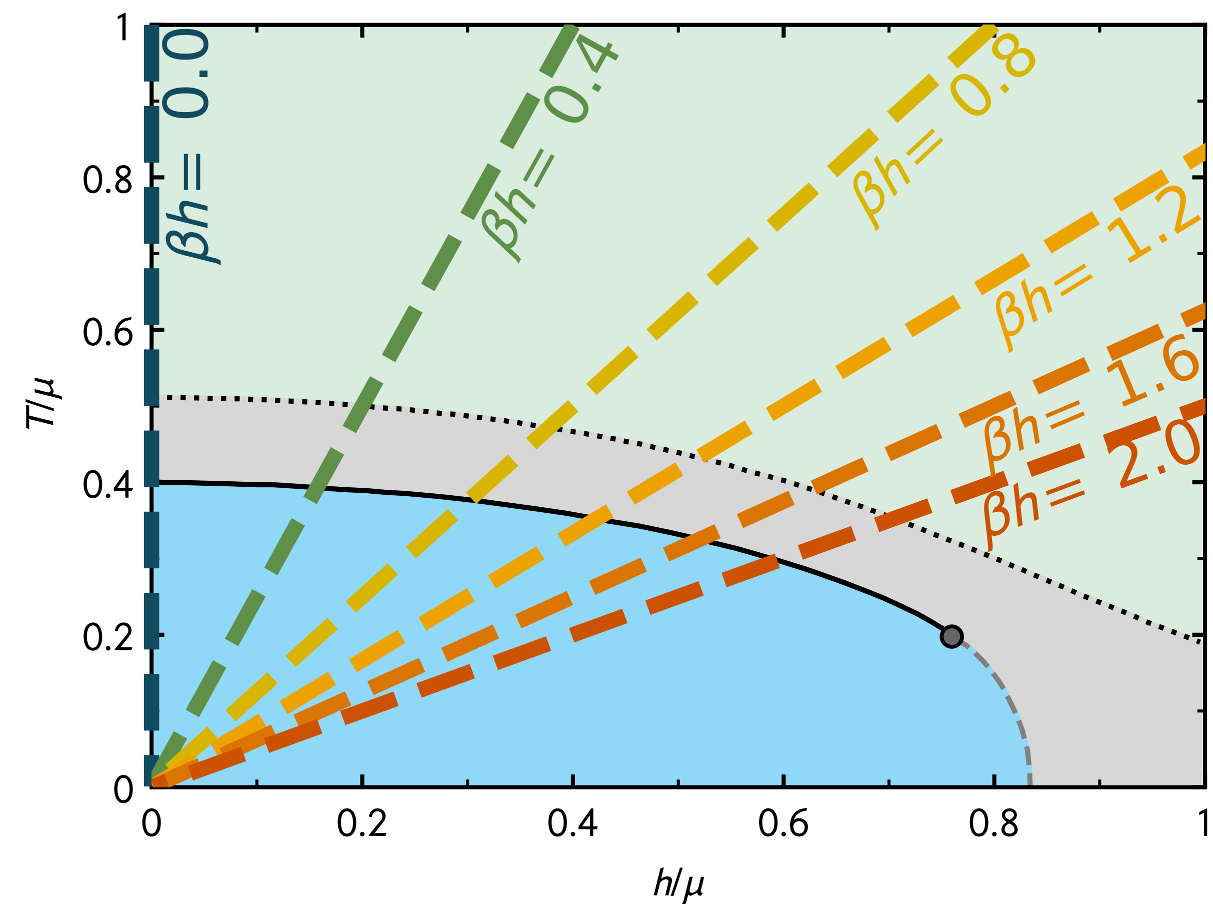

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density equation of state

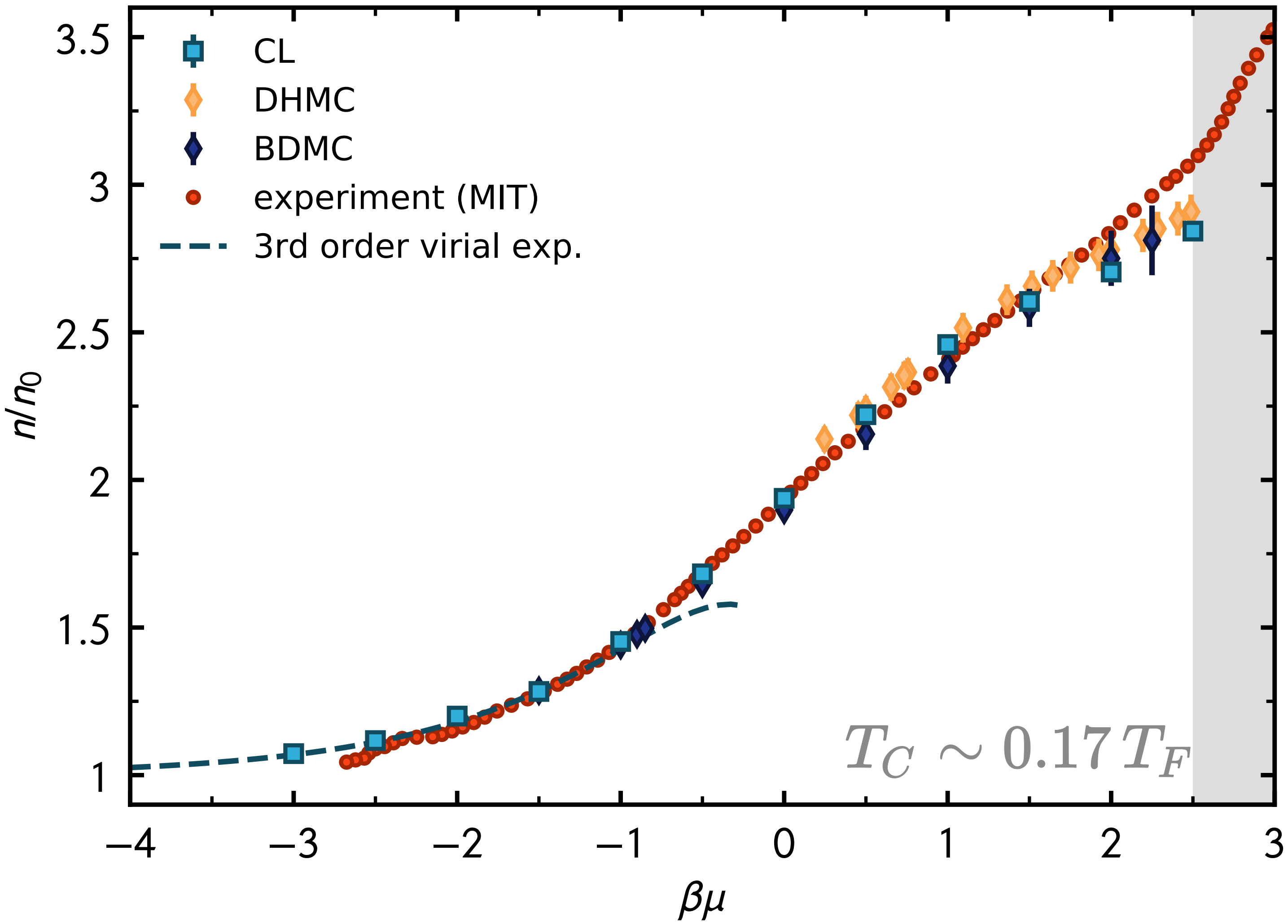
[LR, Loheac, Drut, Braun '18]

[experiment/BDMC: van Houcke et al. '12]
[DHMC: Drut,Lähde,Wlazlowski,Magierski '12]
[diagMC: Rossi,Ohgoe,van Houcke,Werner '18]

good agreement with experiment and other methods!

CL results:

finite lattice $V = 11^3$



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

classical regime

$k_B T$ dominates

quantum regime

E_F dominates

interlude: the virial expansion

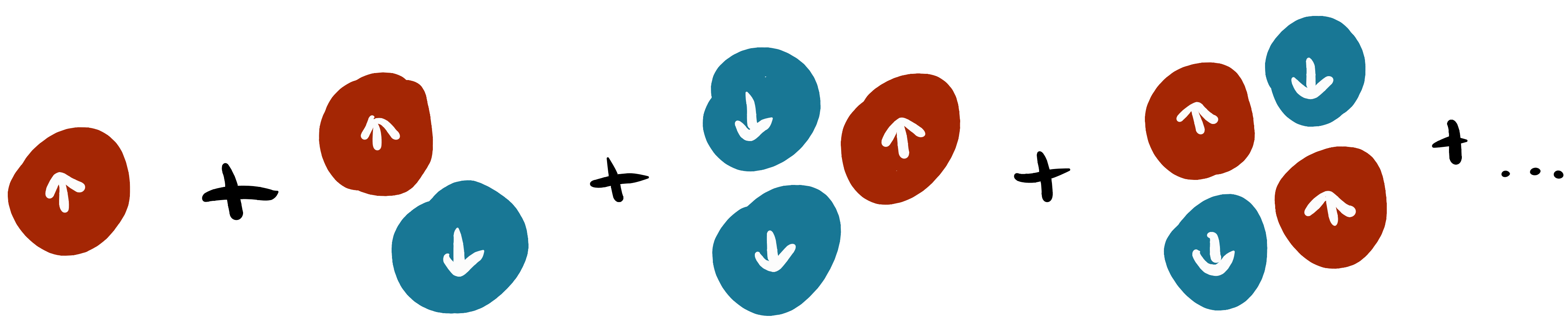
[Liu '13]

dilute gases: few-body correlations dominate

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

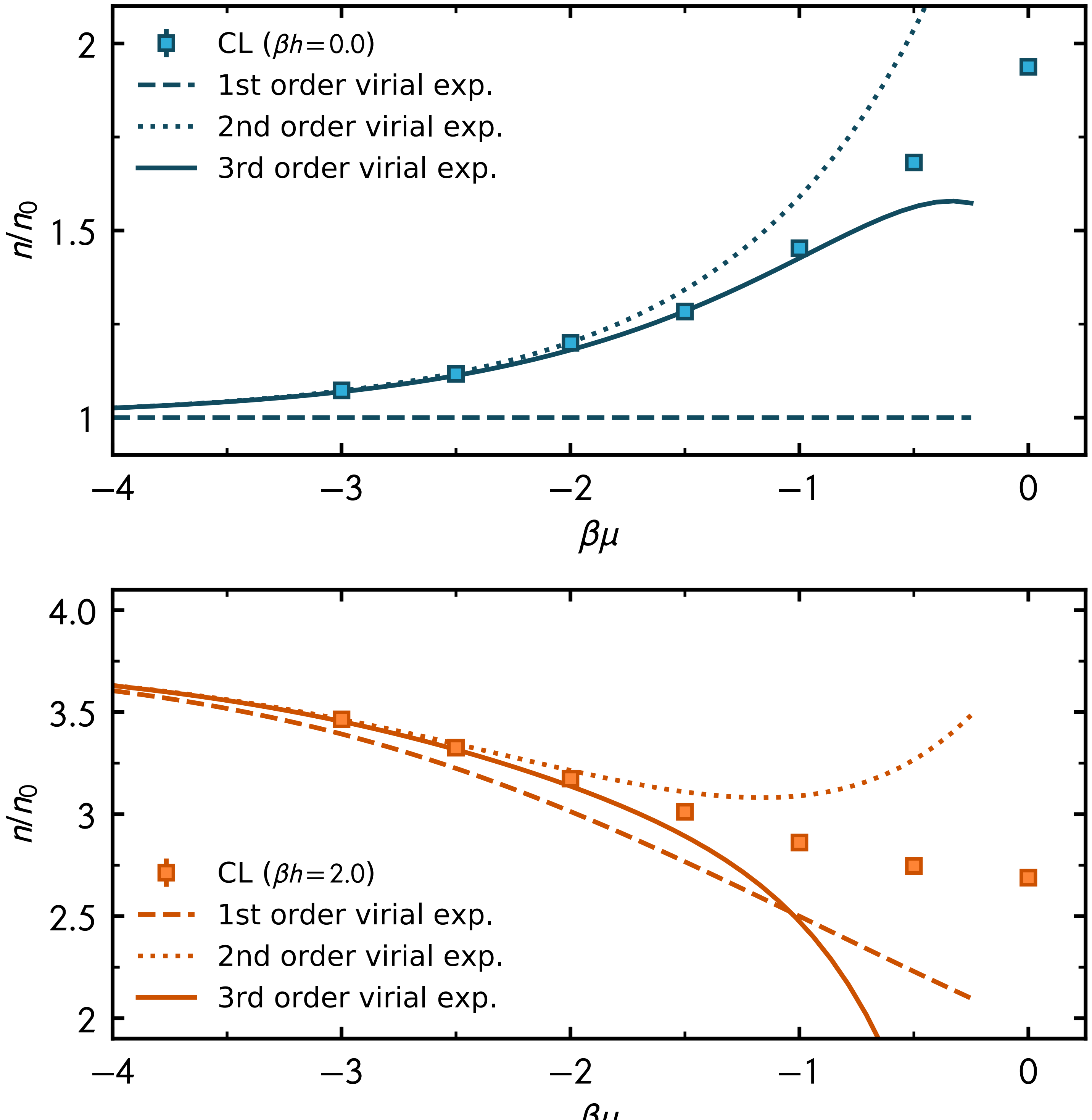
$$z = e^{\beta\mu}$$

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



density EOS (virial regime)

[LR, Loheac, Drut, Braun '18]

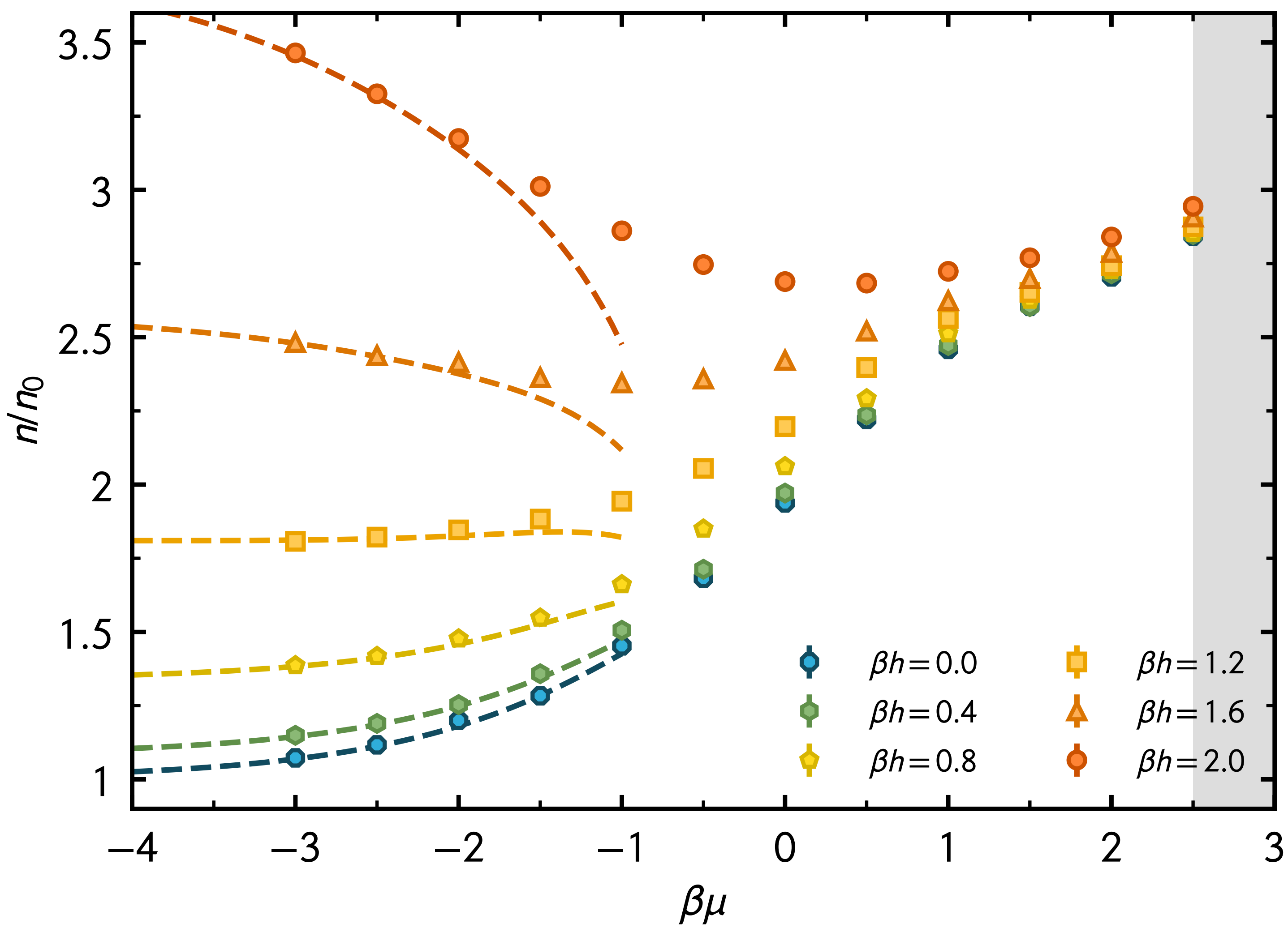


VE approaches the CL results order-by-order

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**

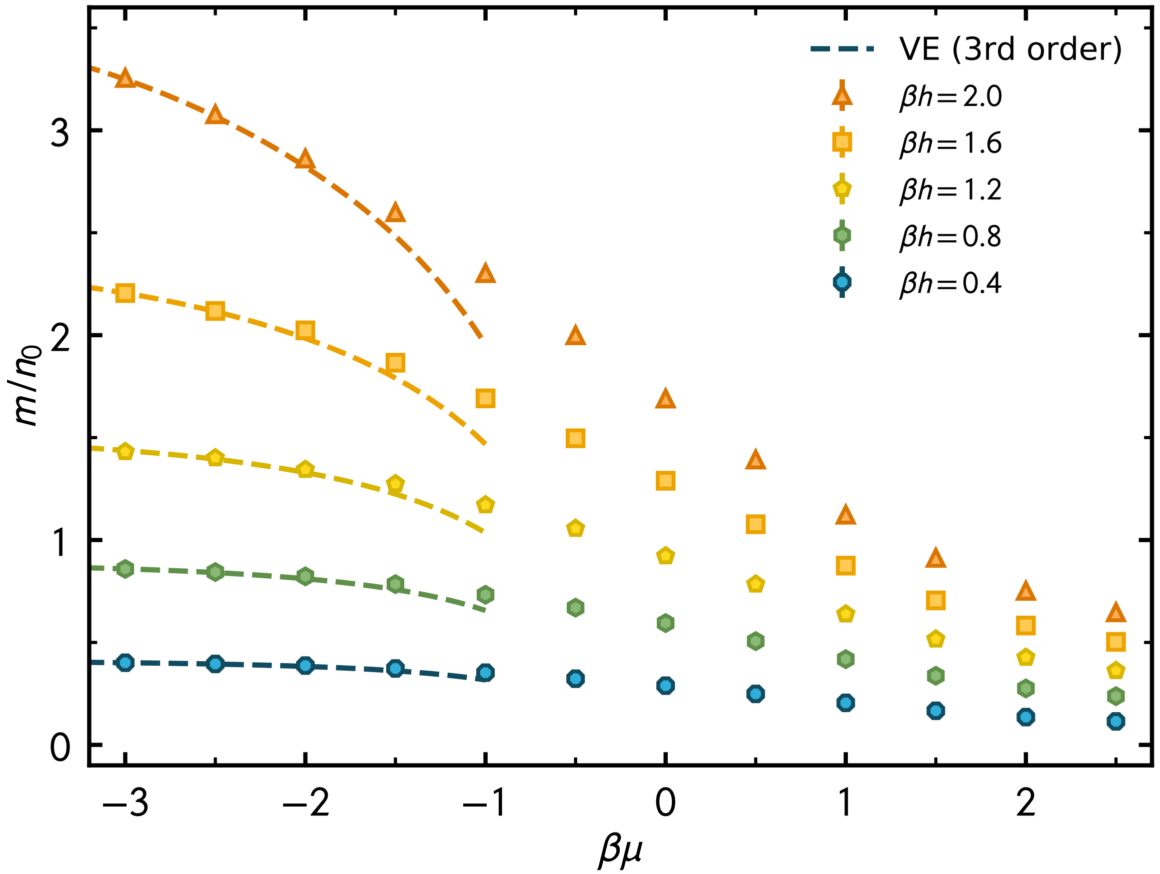
experimentally testable prediction

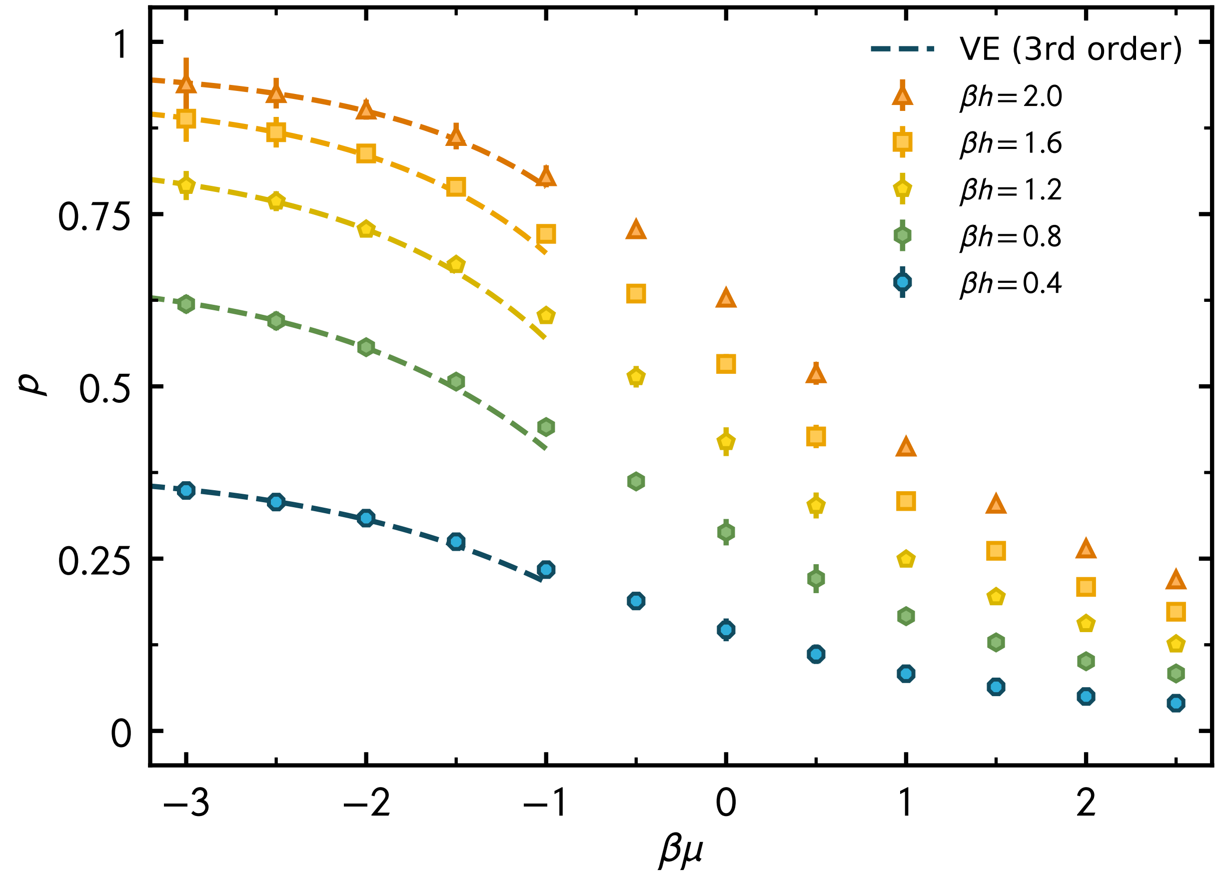
magnetization & polarization

[LR, Loheac, Drut, Braun '18]

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

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





textbook thermodynamics

$$n = \frac{\partial \ln \mathcal{Z}}{\partial(\beta\mu)}$$

$$m = \frac{\partial \ln \mathcal{Z}}{\partial(\beta h)}$$

pressure & energy

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

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

thermodynamic response

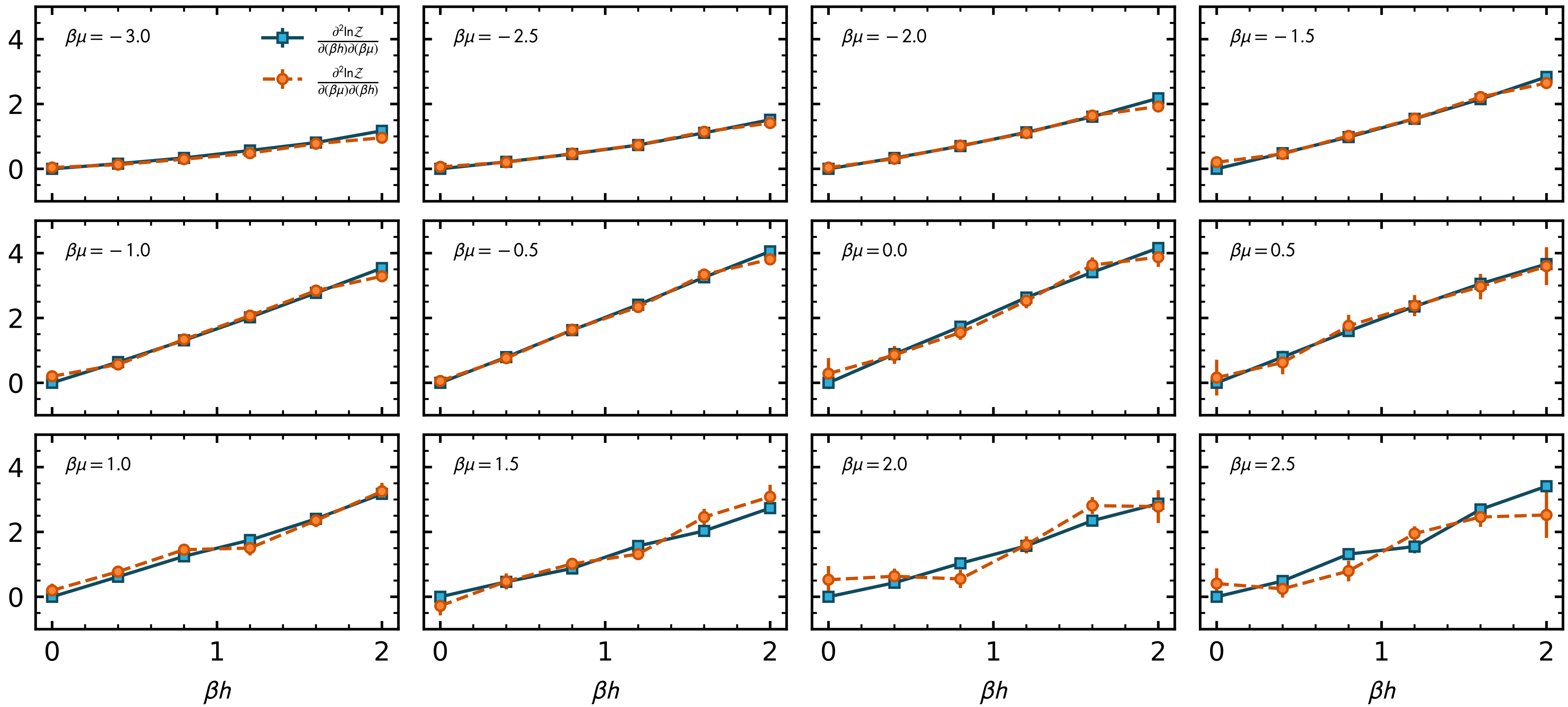
$$\kappa = \frac{1}{n} \left(\frac{\partial n}{\partial P} \right)_{T,V,h}$$

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

Maxwell relations: consistency check

[LR, Loheac, Drut, Braun '18]

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

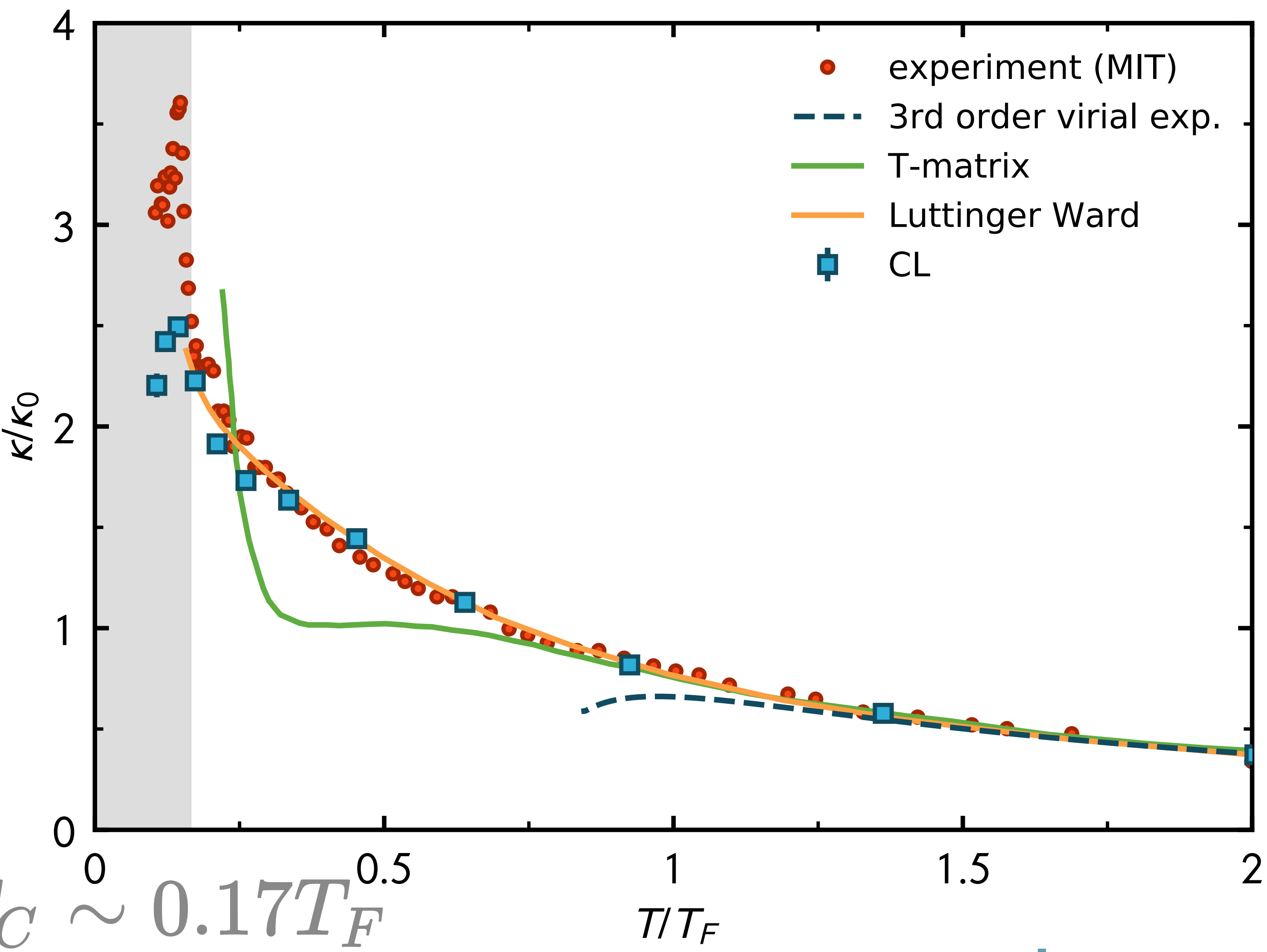


compressibility (unpolarized)

[LR, Loheac, Drut, Braun '18]

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

sudden increase of κ **indicates superfluid phase transition**



$T_C \sim 0.17 T_F$

features of curve recovered with CL

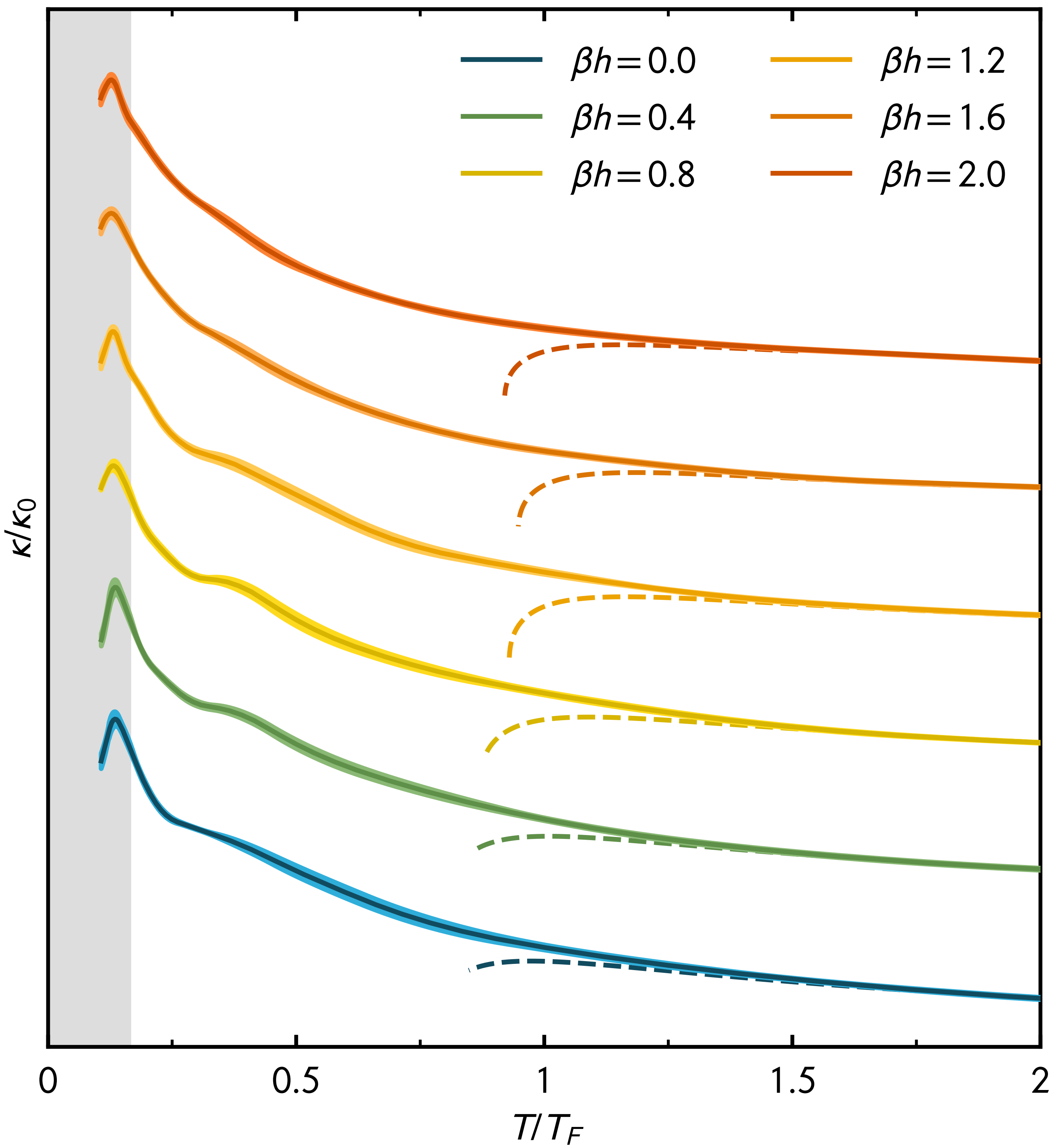
quantitative disagreement at low temperatures

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

compressibility for polarized systems

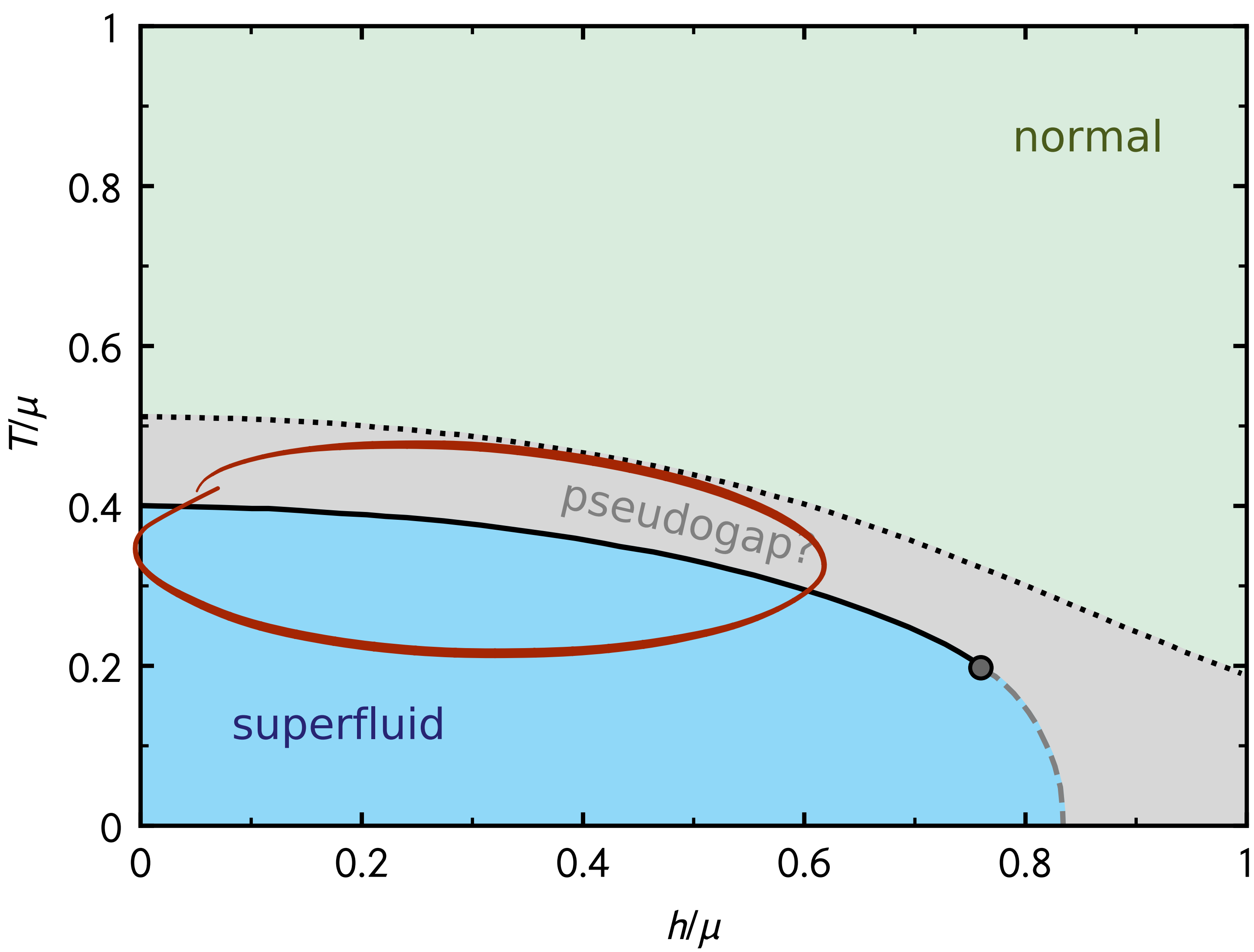
[LR, Loheac, Drut, Braun '18]

weak dependence of the critical temperature on polarization indicated



challenging to extract precise T_C

UFG phase diagram



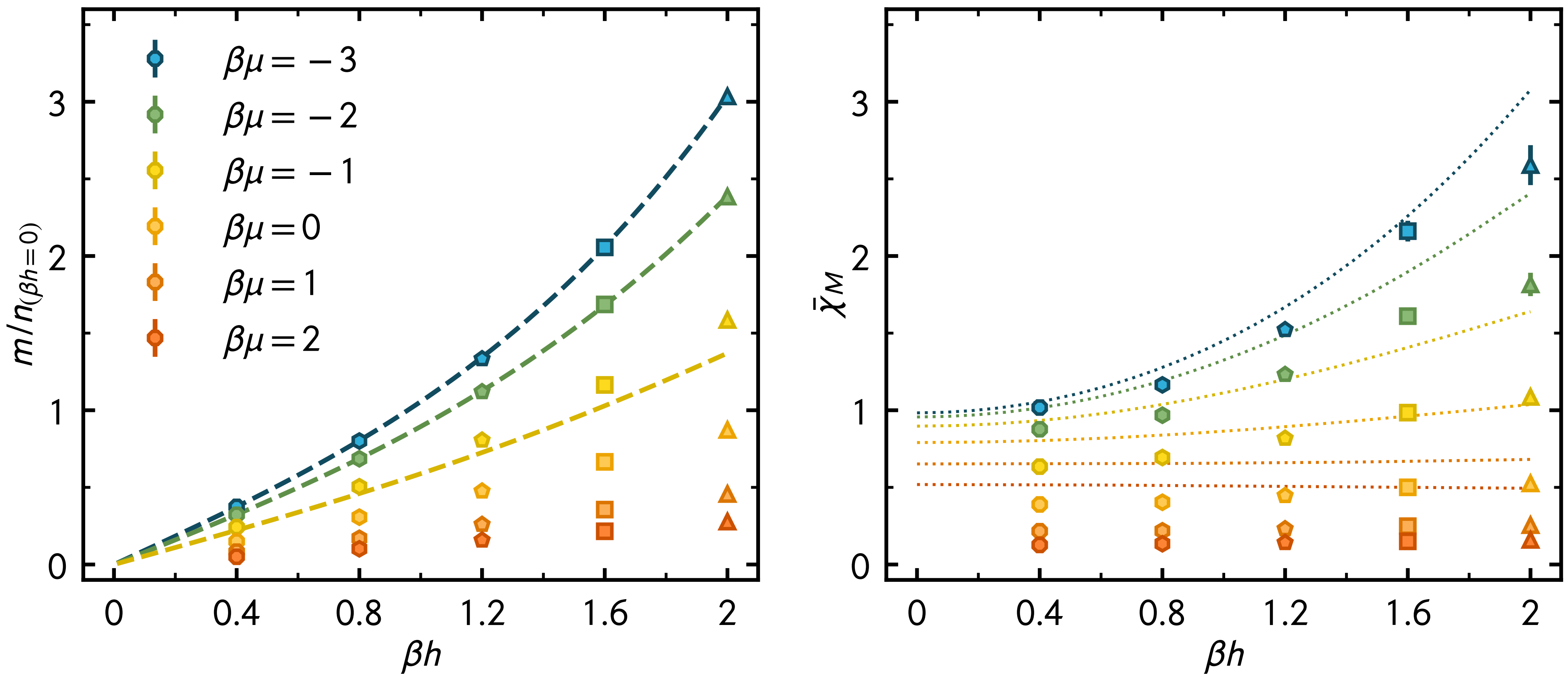
$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$
$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

[fRG: Boettcher et. al '15]

spin susceptibility

[LR, Loheac, Drut, Braun '18]

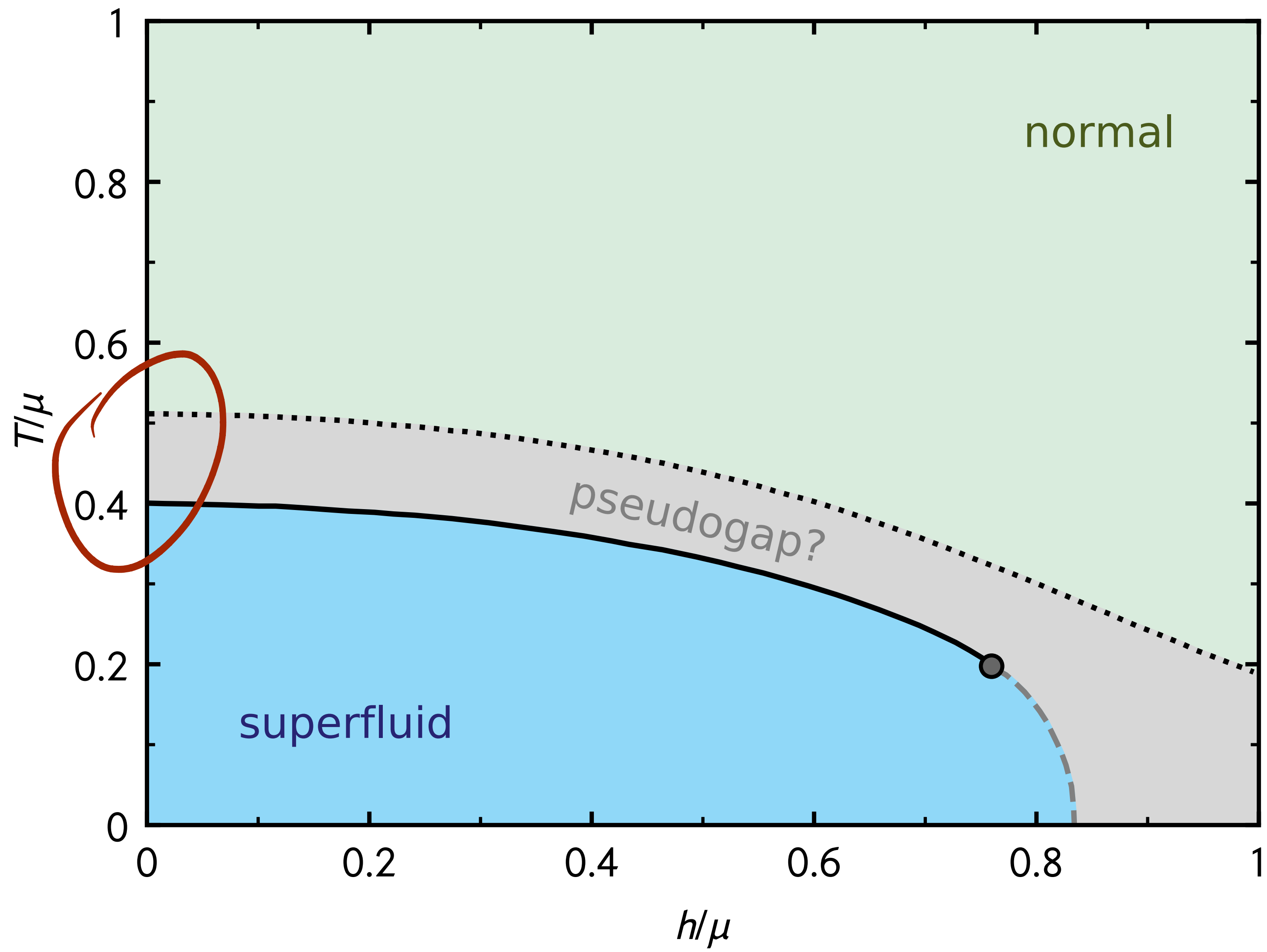
$$\chi = \left(\frac{\partial m}{\partial h}\right)_{T,V,\mu}$$



Pauli susceptibility field independent at low field and temperature

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

UFG phase diagram (sketch)



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

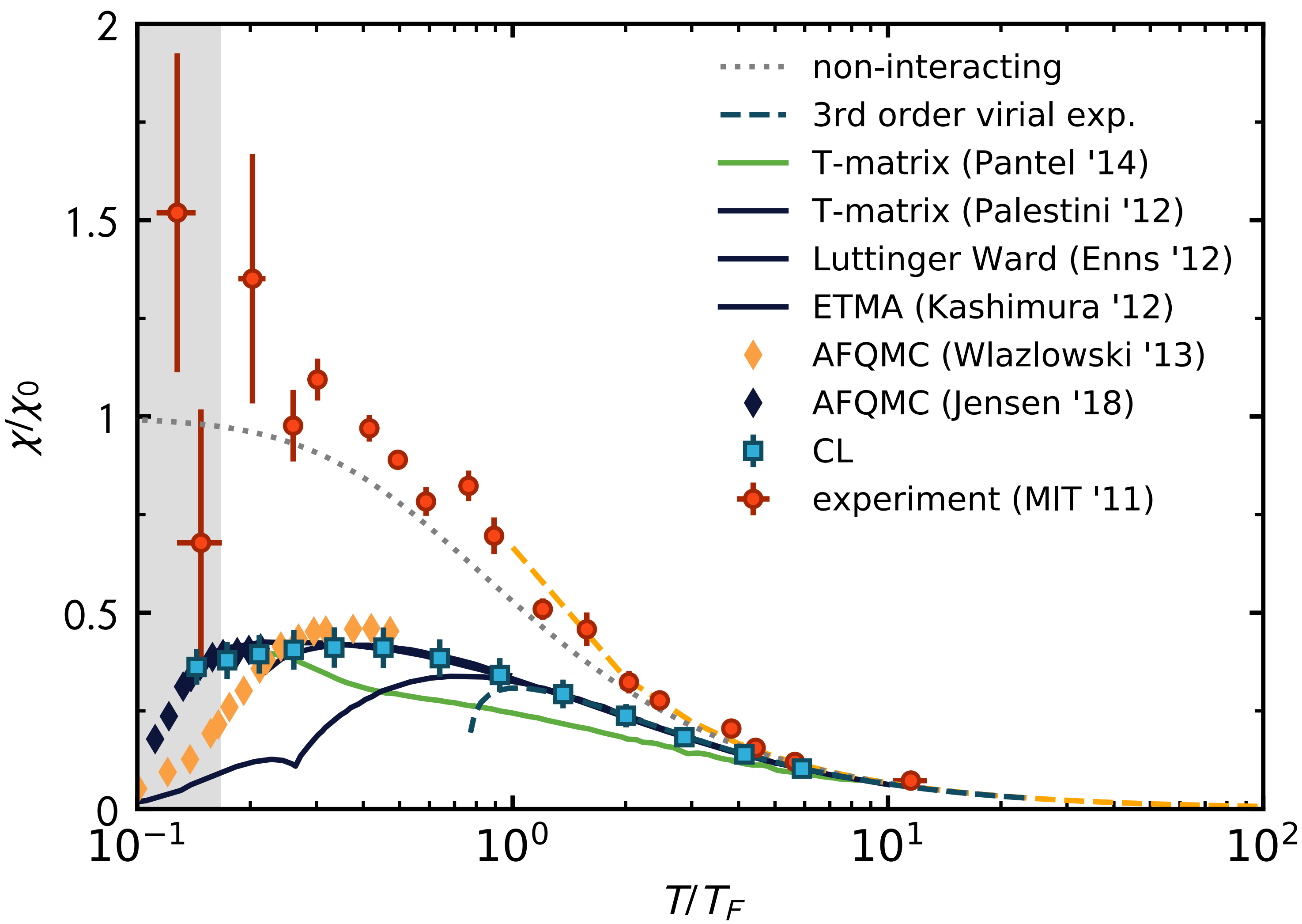
$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

[fRG: Boettcher et. al '15]

magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]

low temperature: discrepancy between experiment and theory



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]

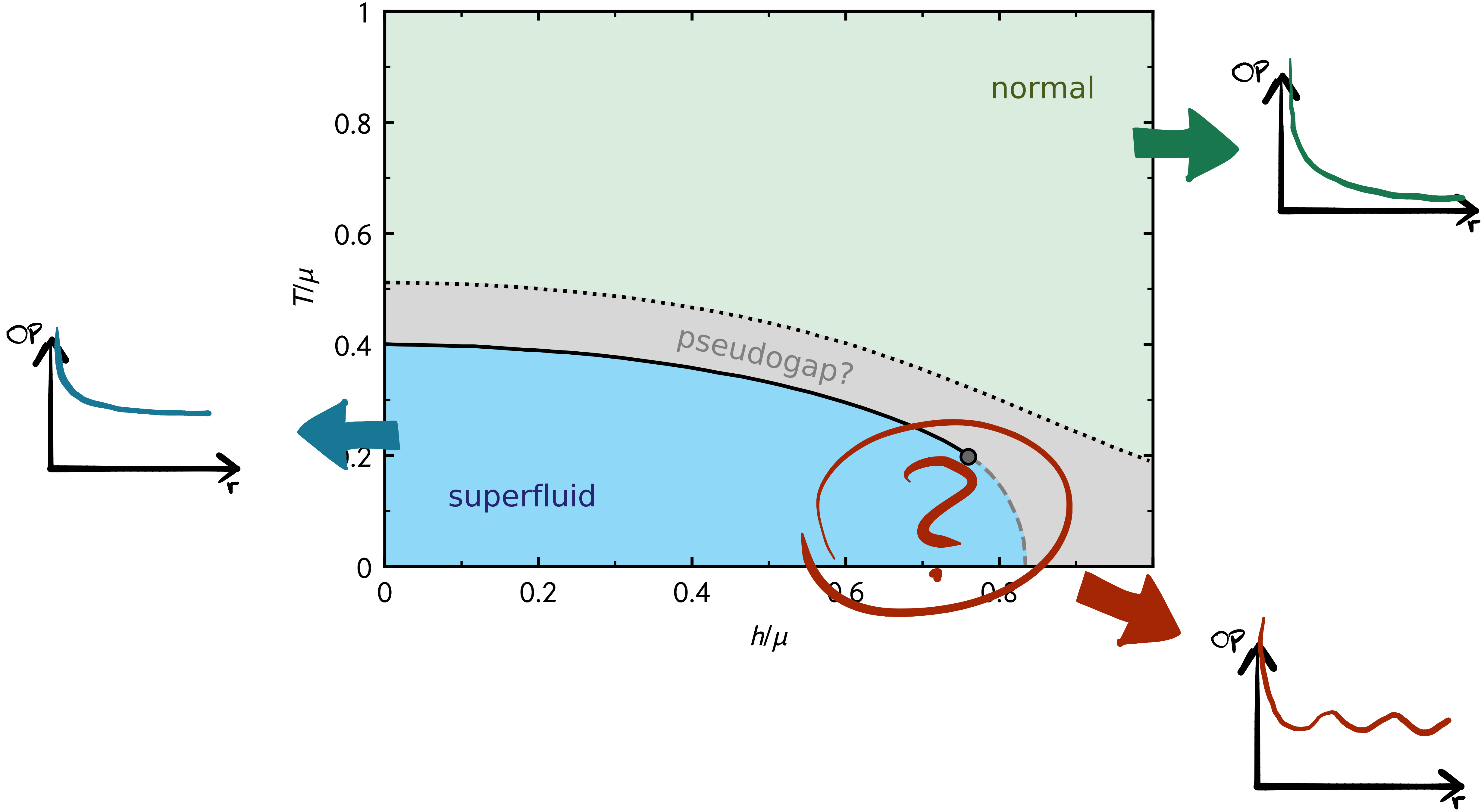
CL: pseudogap possible
T^* and T_C seem to be very close

recap: unitary fermions

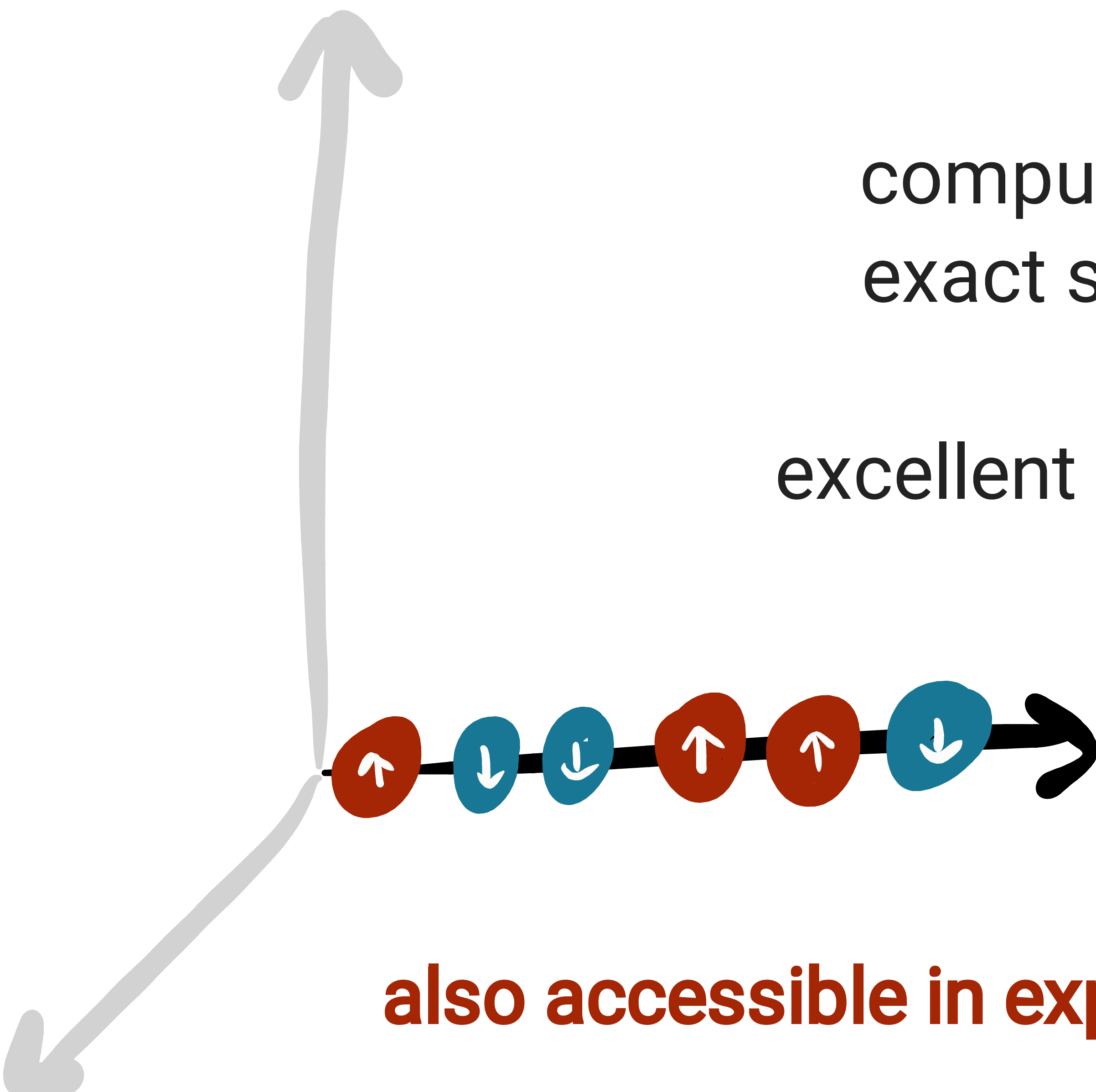
EOS, magnetic properties & response accessible for the unitary Fermi gas at finite temperature and polarization

CL **matches state-of-the art results** from other methods and experiments wherever available

UFG phase diagram (sketch)



one-dimensional systems



computationally cheap &
exact solutions available
=
excellent benchmark systems

also accessible in experiment

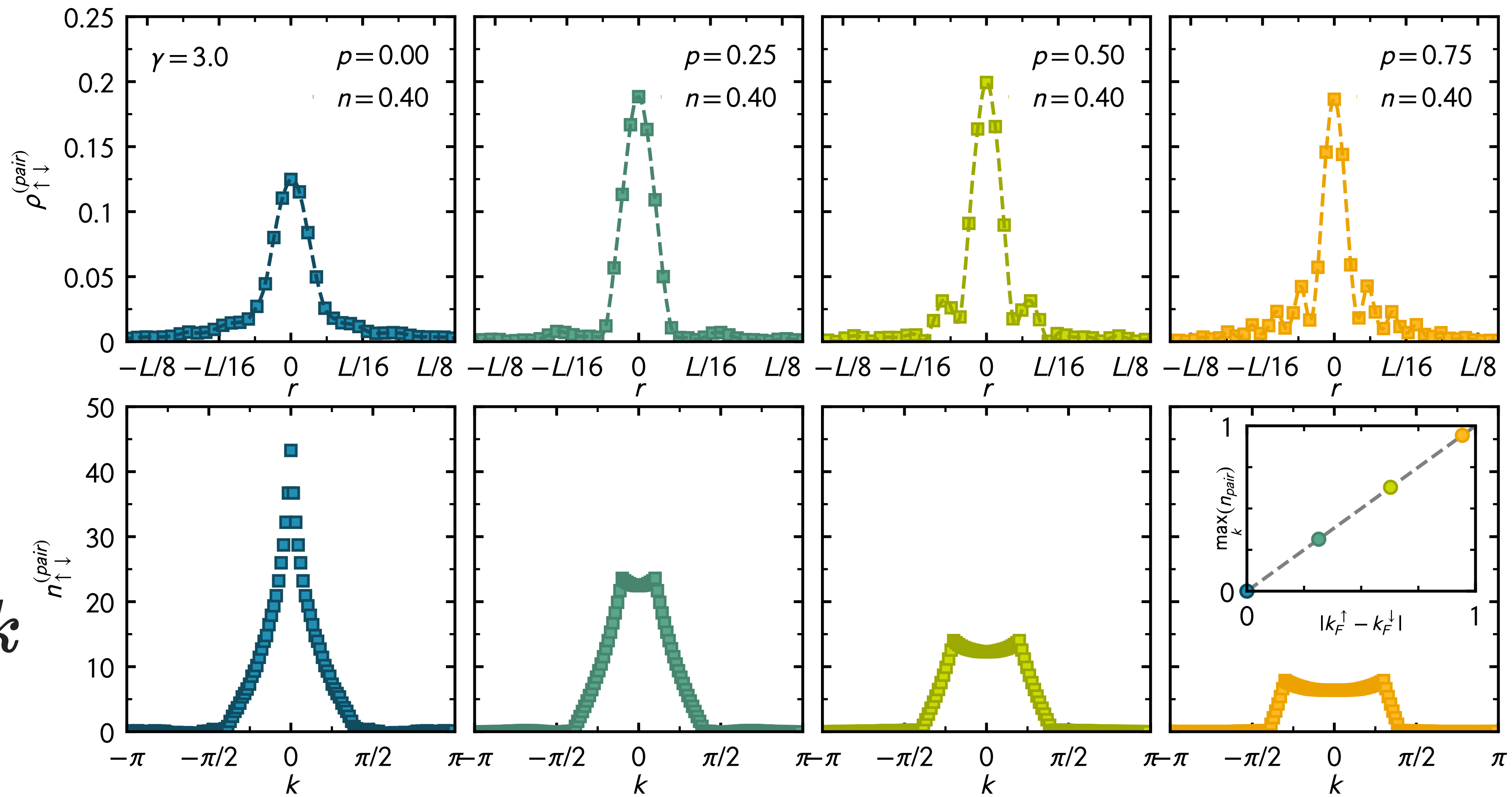
pair correlations

[LR, Drut, Braun in preparation]

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

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

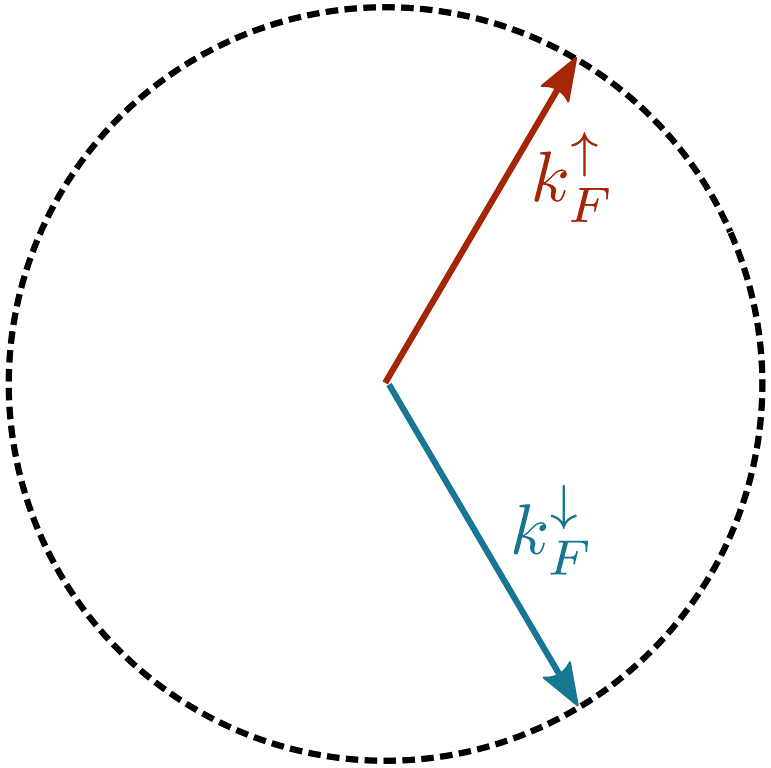
~ likelihood of a pair with momentum k



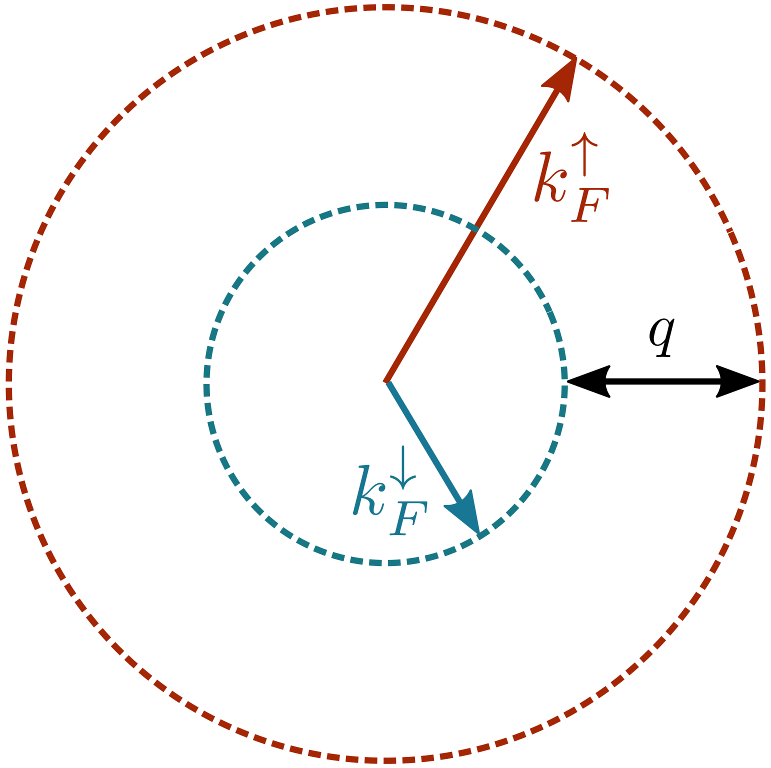
spatially fluctuating order-parameter

off-center peak: hallmark of **FFLO type pairing**

pairing (schematically)



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



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

density-density correlation (shot noise)

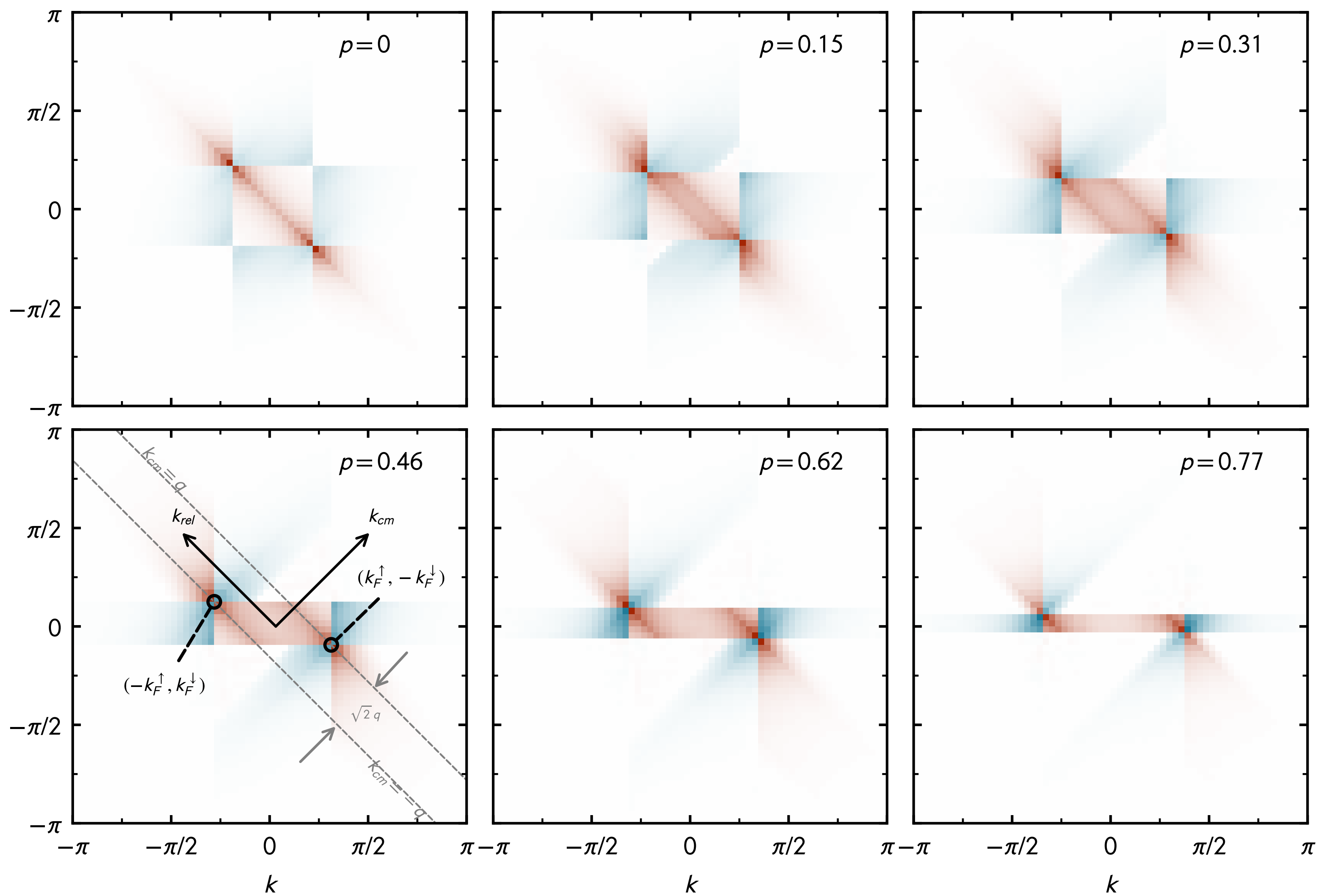
[LR, Drut, Braun in preparation]

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

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

peak positions:

$(\pm k_F^\uparrow, \mp k_F^\downarrow)$



positive correlations: particle-particle

negative correlations: particle-hole

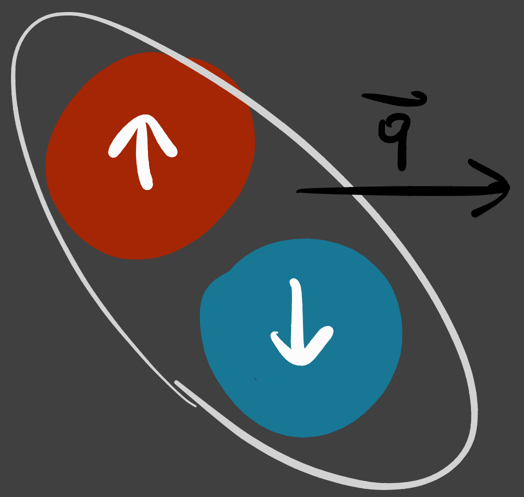
resolution of **internal structure** of fermionic pairs

recap

complex Langevin is a valuable tool to study ultracold Fermi gases

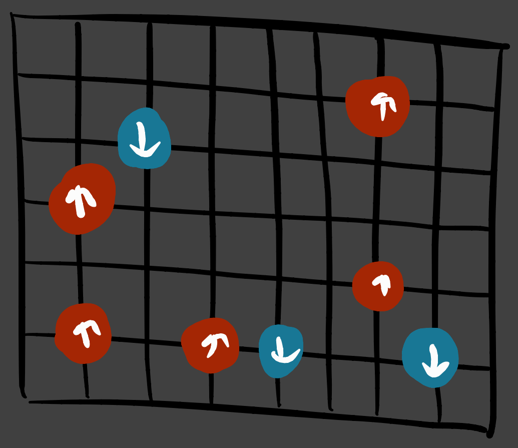
(it works quite well)

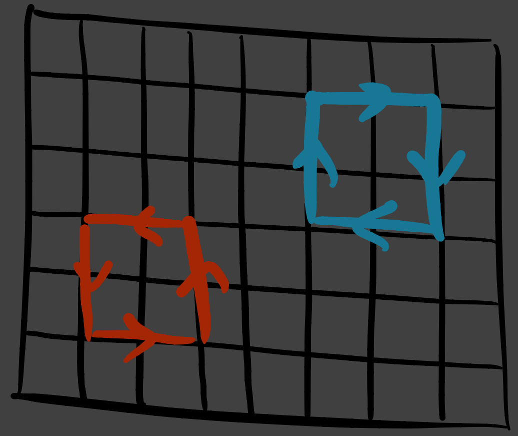
stay tuned!



looking for inhomogeneous phases in the UFG

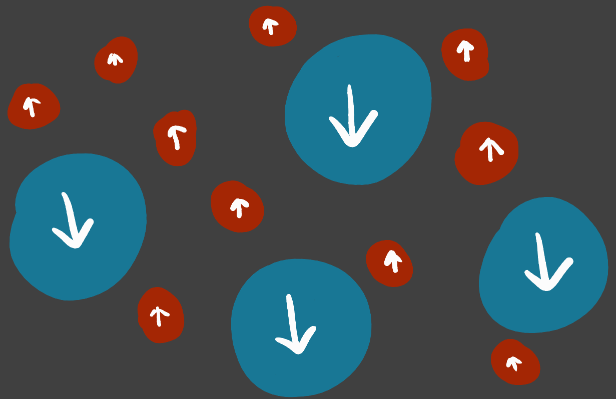
thermodynamics of 2D fermions at finite polarization
[with Josh McKenney, Andrew Loheac & Joaquin Drut, UNC Chapel Hill]





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

effect of mass-imbalance on fermion pair formation



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Jens Braun

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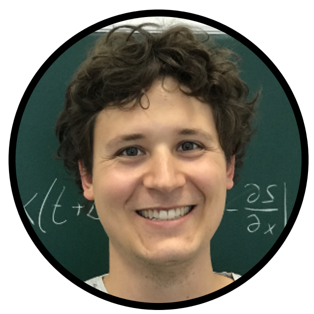

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