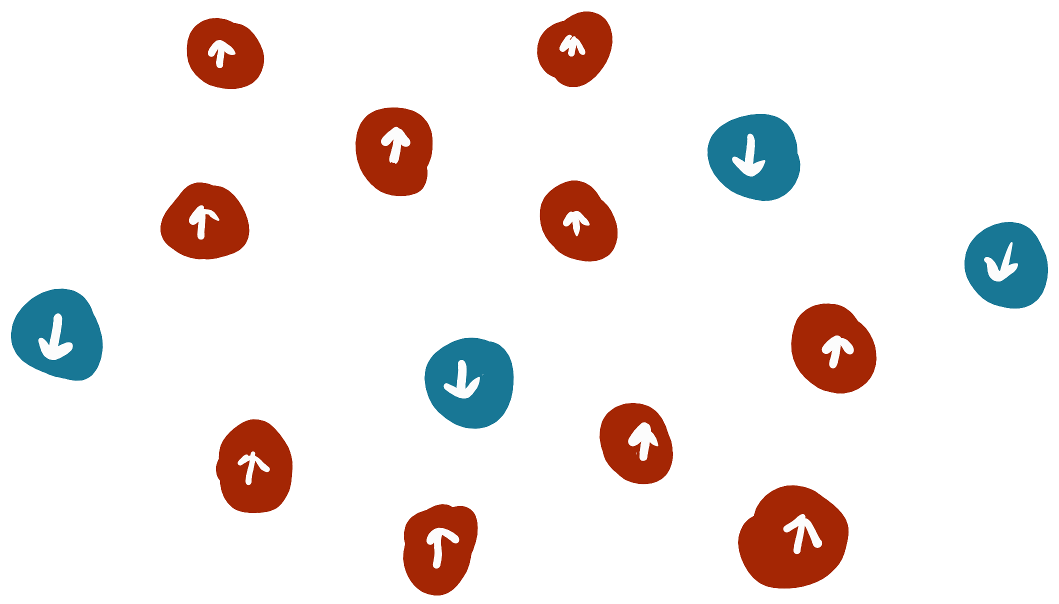
spin-polarized fermions at unitarity: a complex Langevin study

[Berger, Loheac, LR, Ehmann, Braun, Drut *arXiv:1907.10183*]
[LR, Loheac, Drut, Braun *Phys. Rev. Lett.* 121, 173001, 2018]



Lukas Rammelmüller, TU Darmstadt

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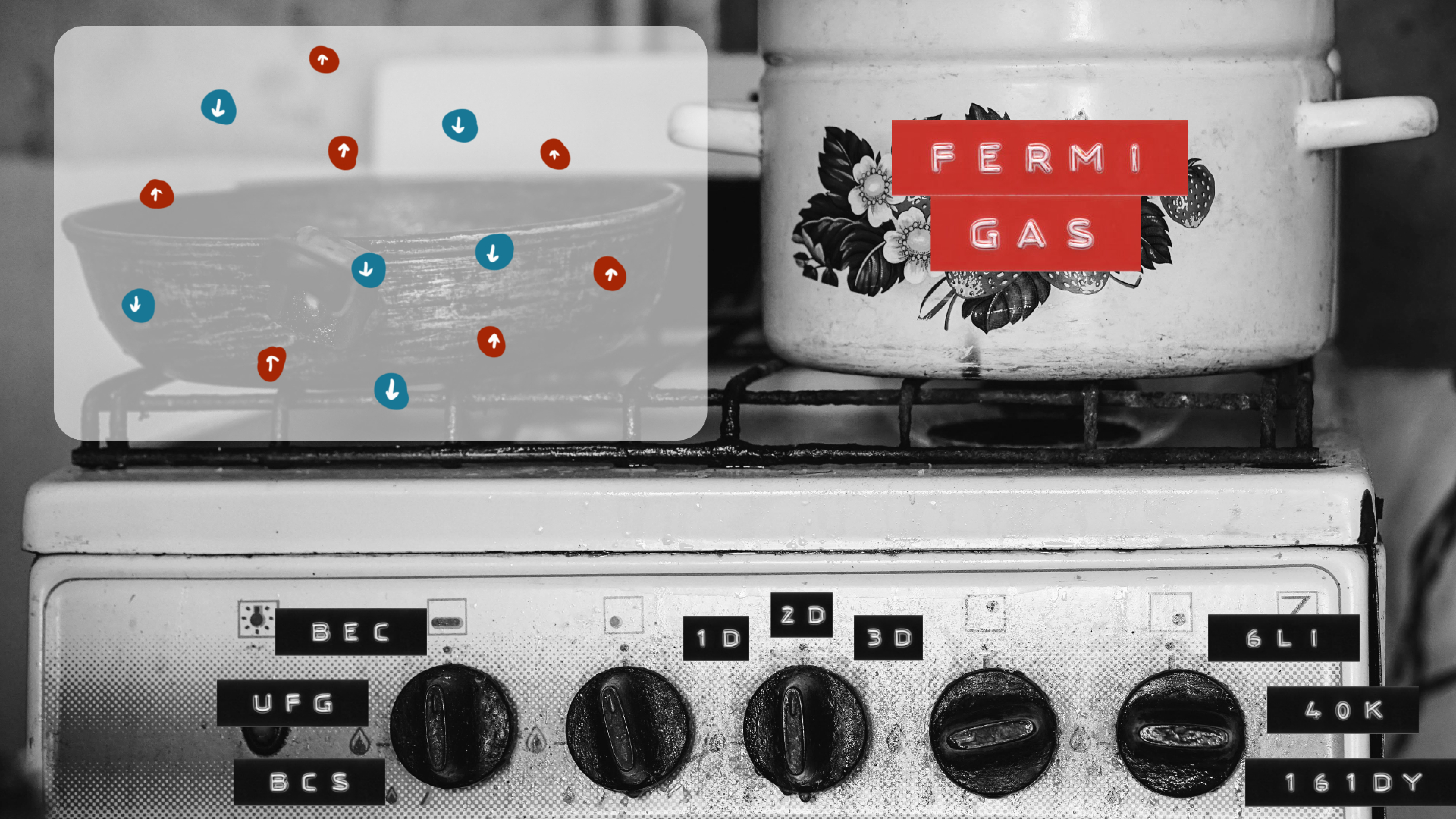
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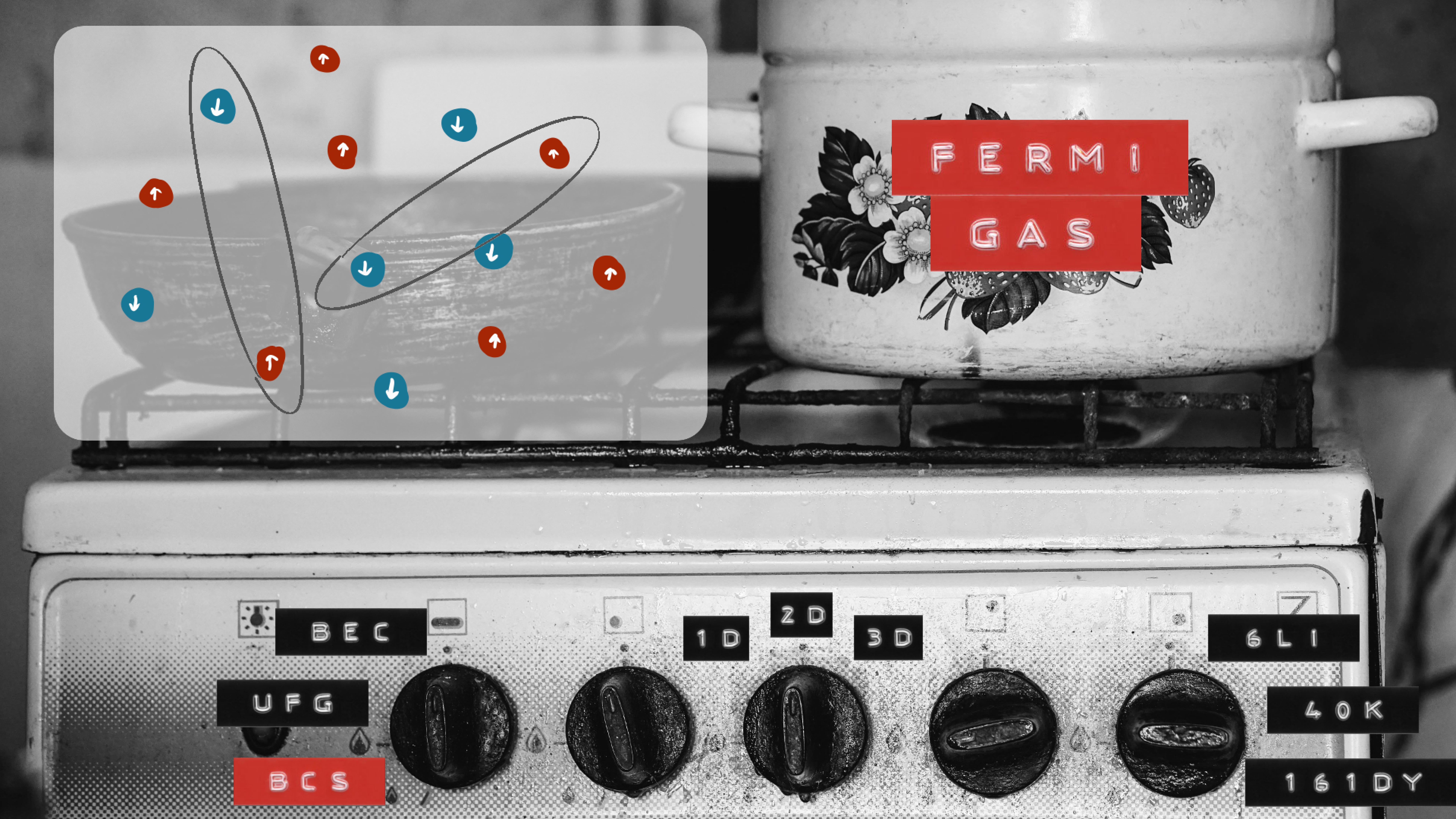
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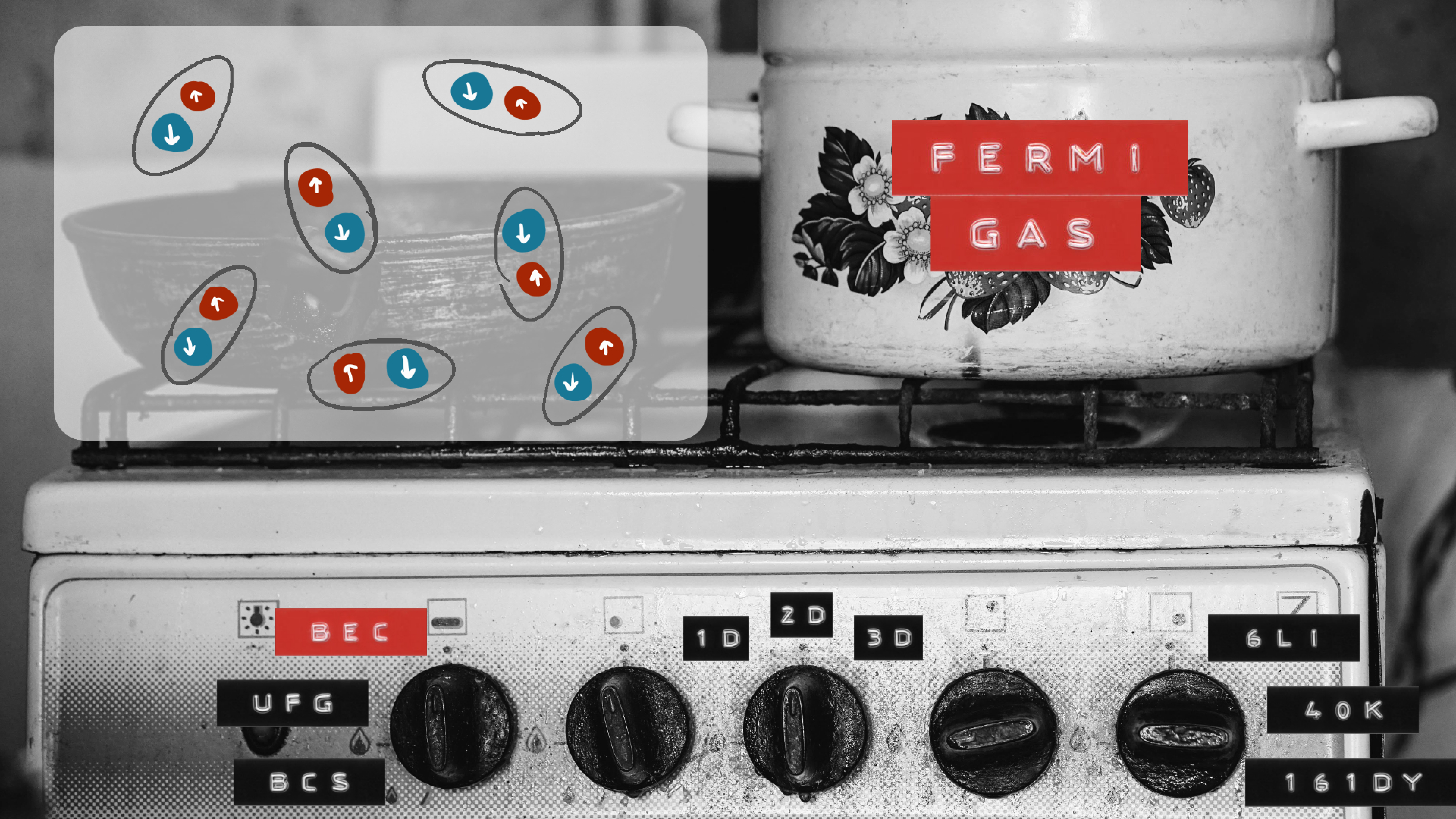
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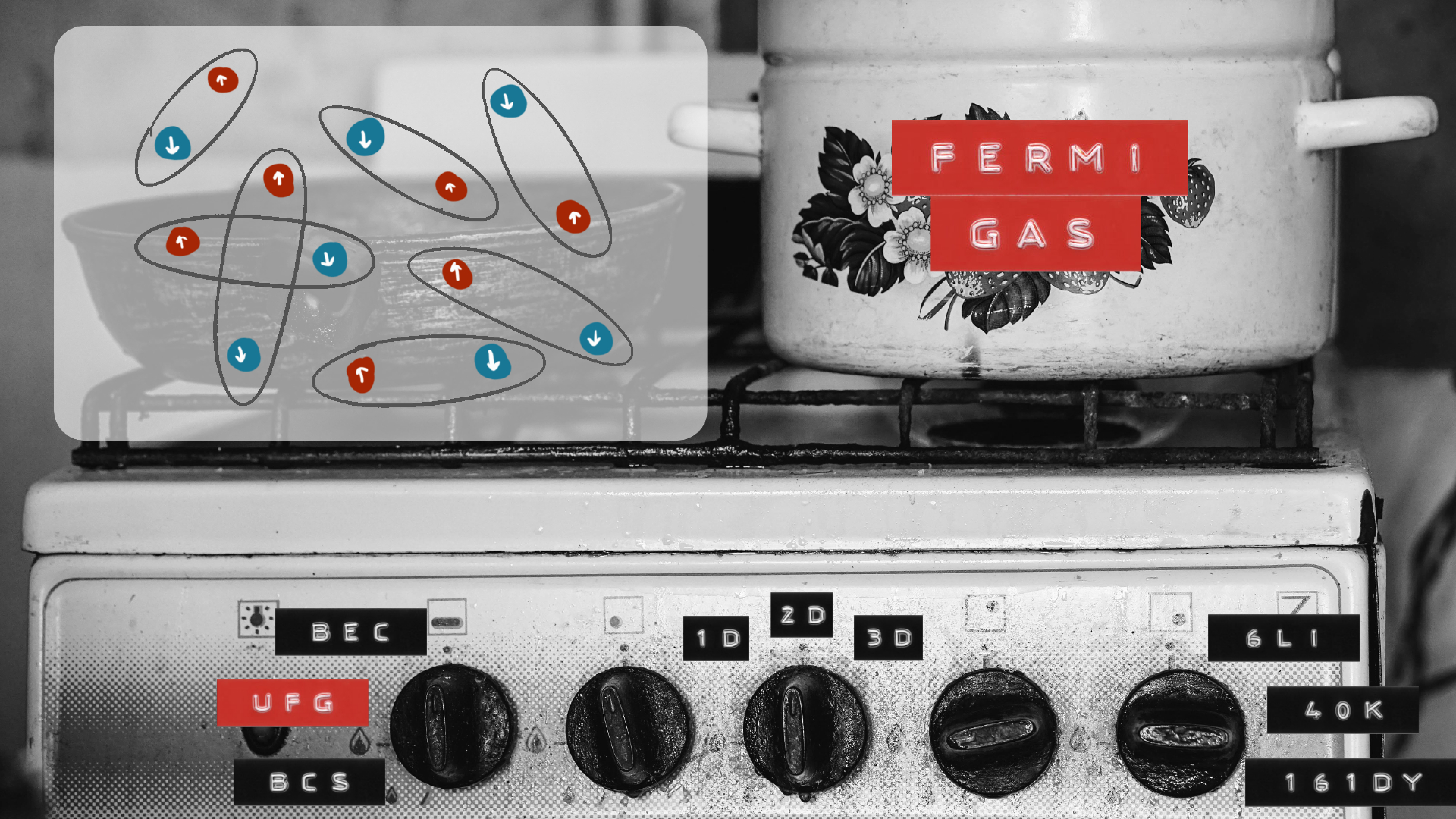
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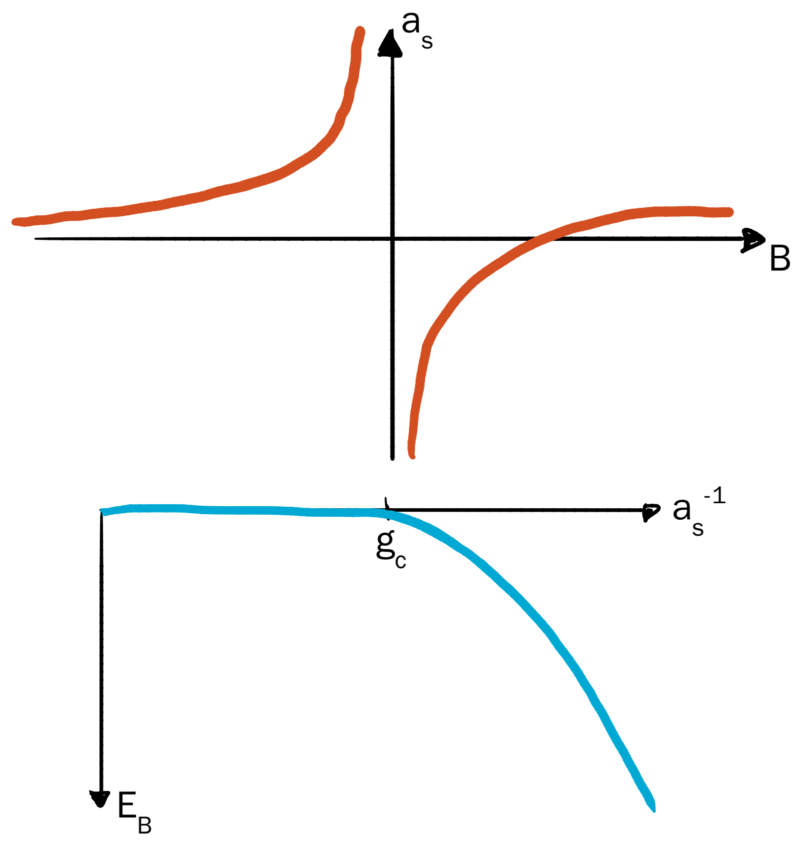
the unitary Fermi gas (UFG)

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

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



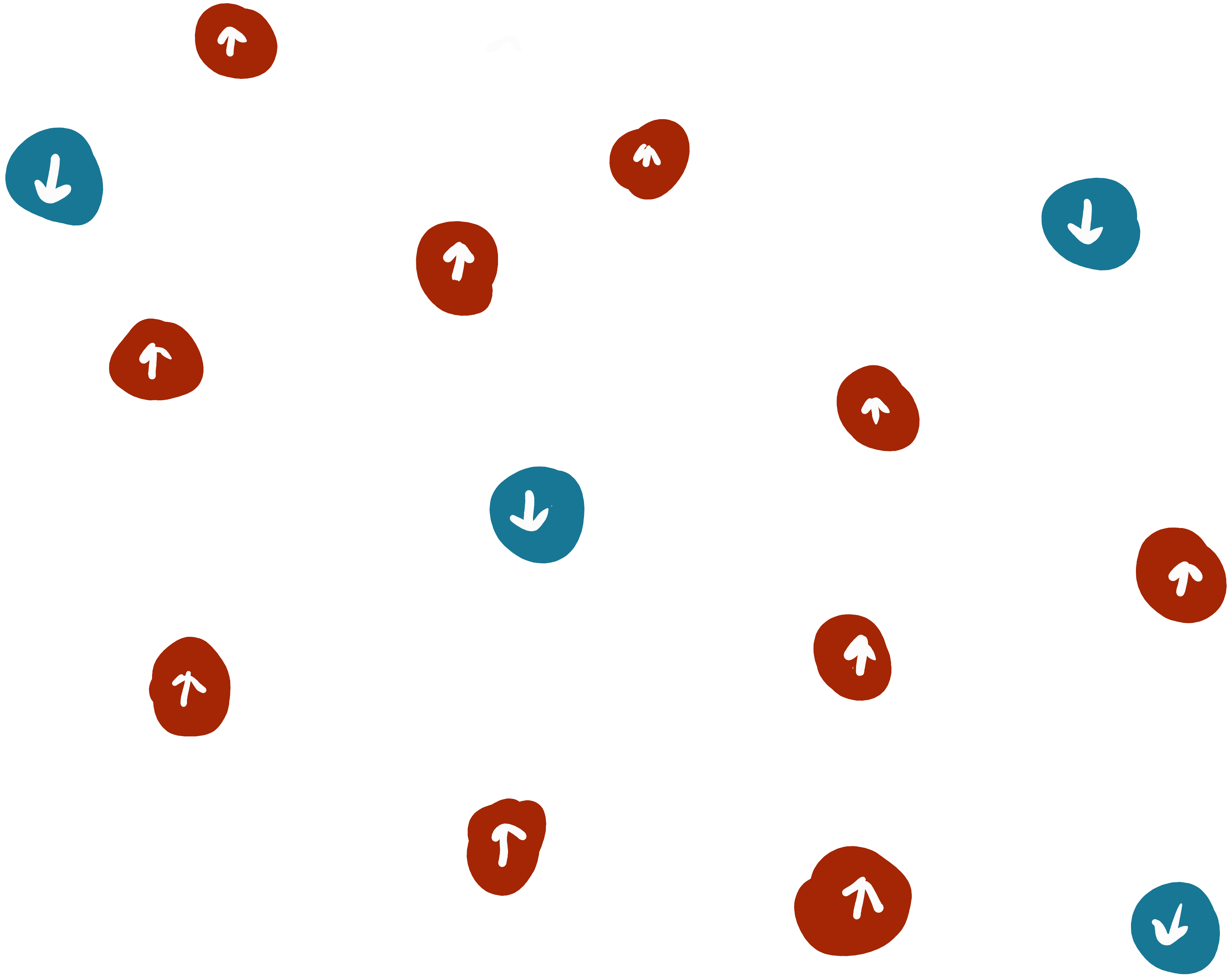
density & temperature are the **only** dimensionful scales in the system

universal scaling functions:

$$E = E_{FG}\, f_E(n, T)$$

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 reminder on **stochastic quantization & CL**

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

part II

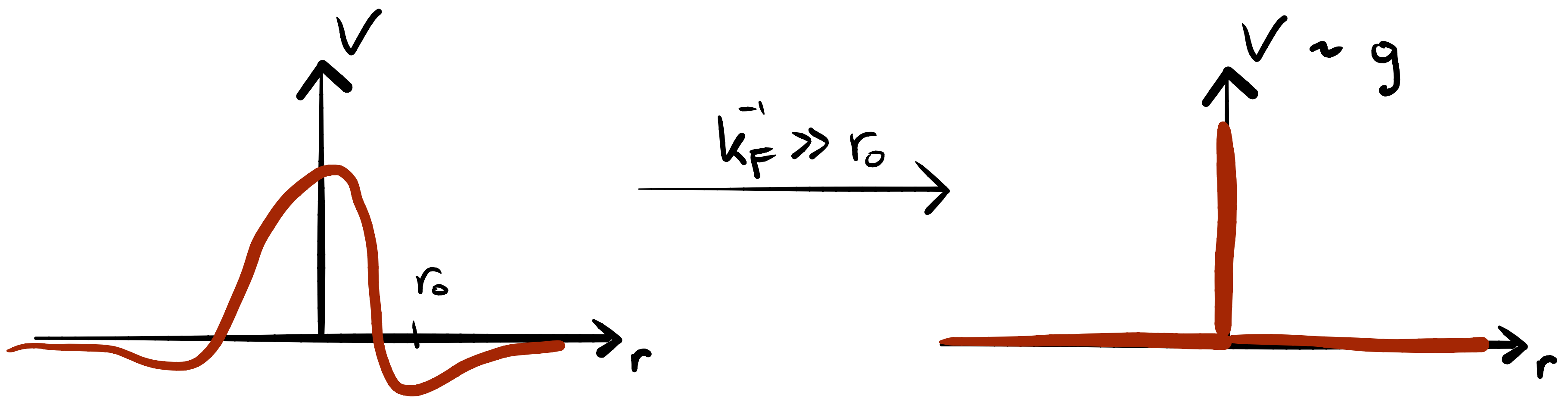
unitary fermions with finite polarization

(equations of state & thermodynamic response)

fermions with contact interaction

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

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



what do we need to compute?

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

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

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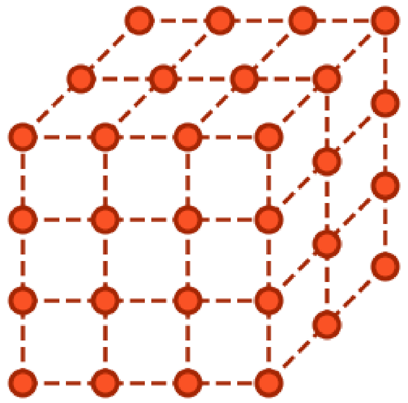

+ Trotter decomposition

+ 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; Zhang '13]

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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(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):

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

stochastic quantization

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

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ficticious Langevin time
(not physical)

stochastic quantization

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

random walk governed by

Langevin equation (Brownian motion):

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

ficticious 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?

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

how can stochastic quantization help us to study fermions?

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

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

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

the path integral & complex actions

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

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; Berger et al. '19]

complex probablities

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

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

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

complex probablities & possible issues

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

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**

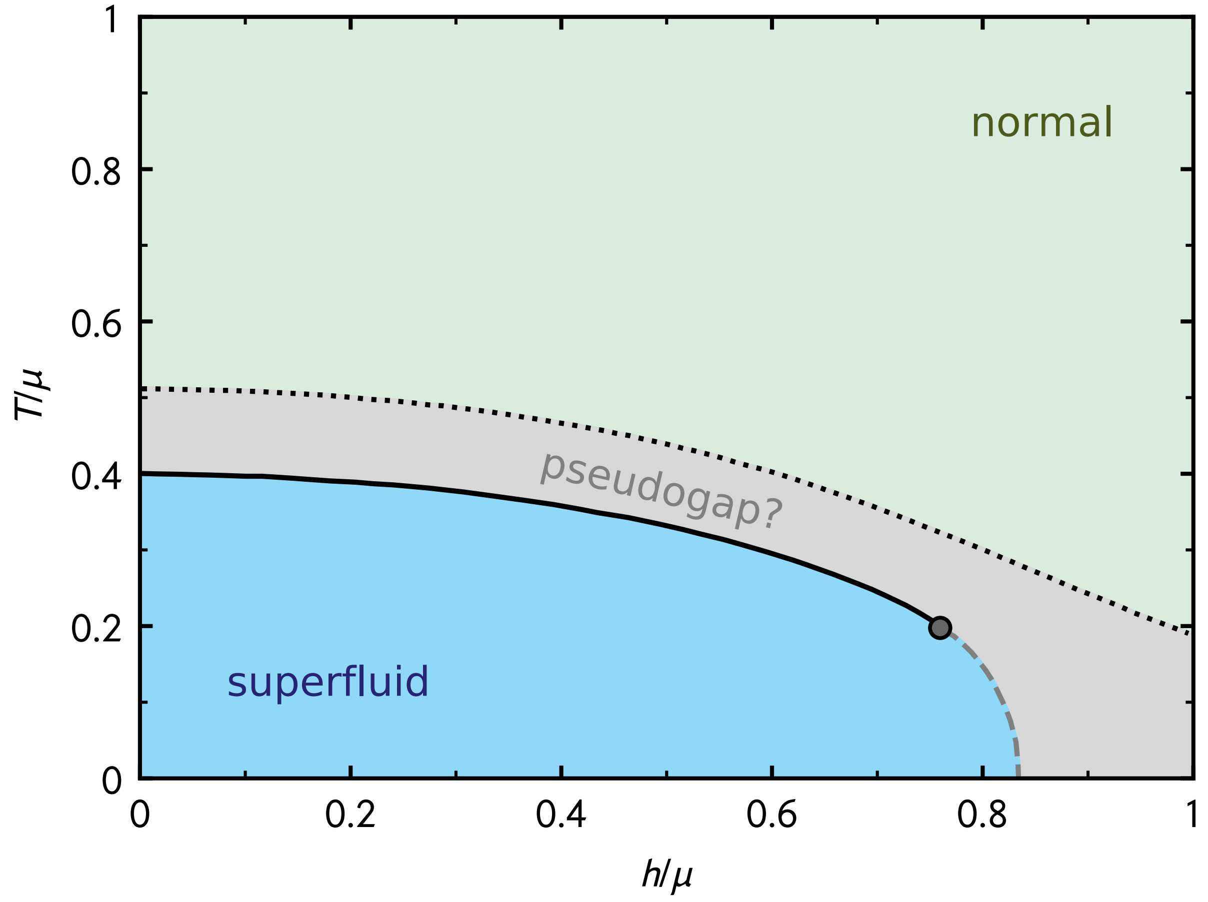
complex Langevin provides a way
to **evade sign problems** in some cases

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

recent review: [Berger et al. arXiv:1907.10183]

the unitary Fermi gas at finite temperature

[LR, Loheac, Drut, Braun '18]



[fRG phase diagram: Boettcher et. al '15]

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

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

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

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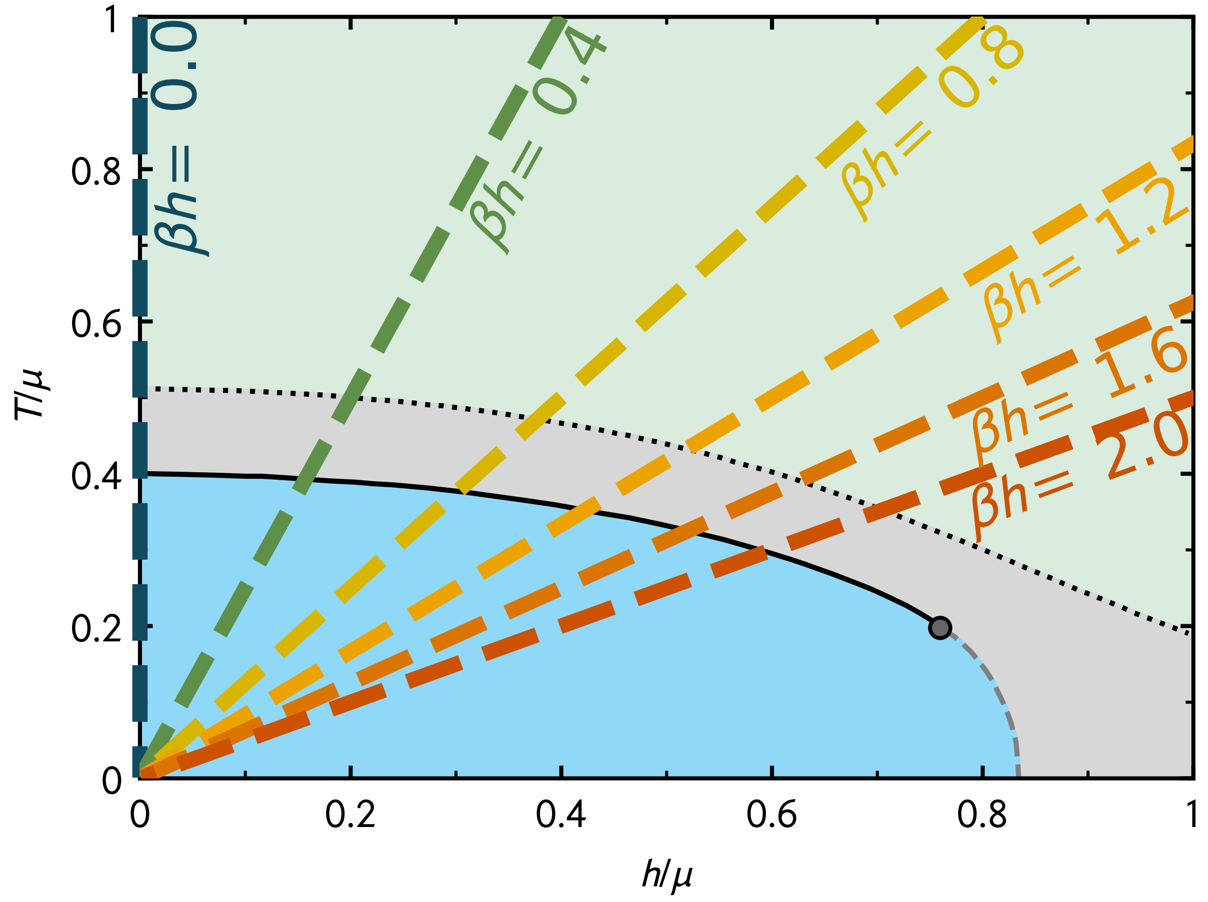

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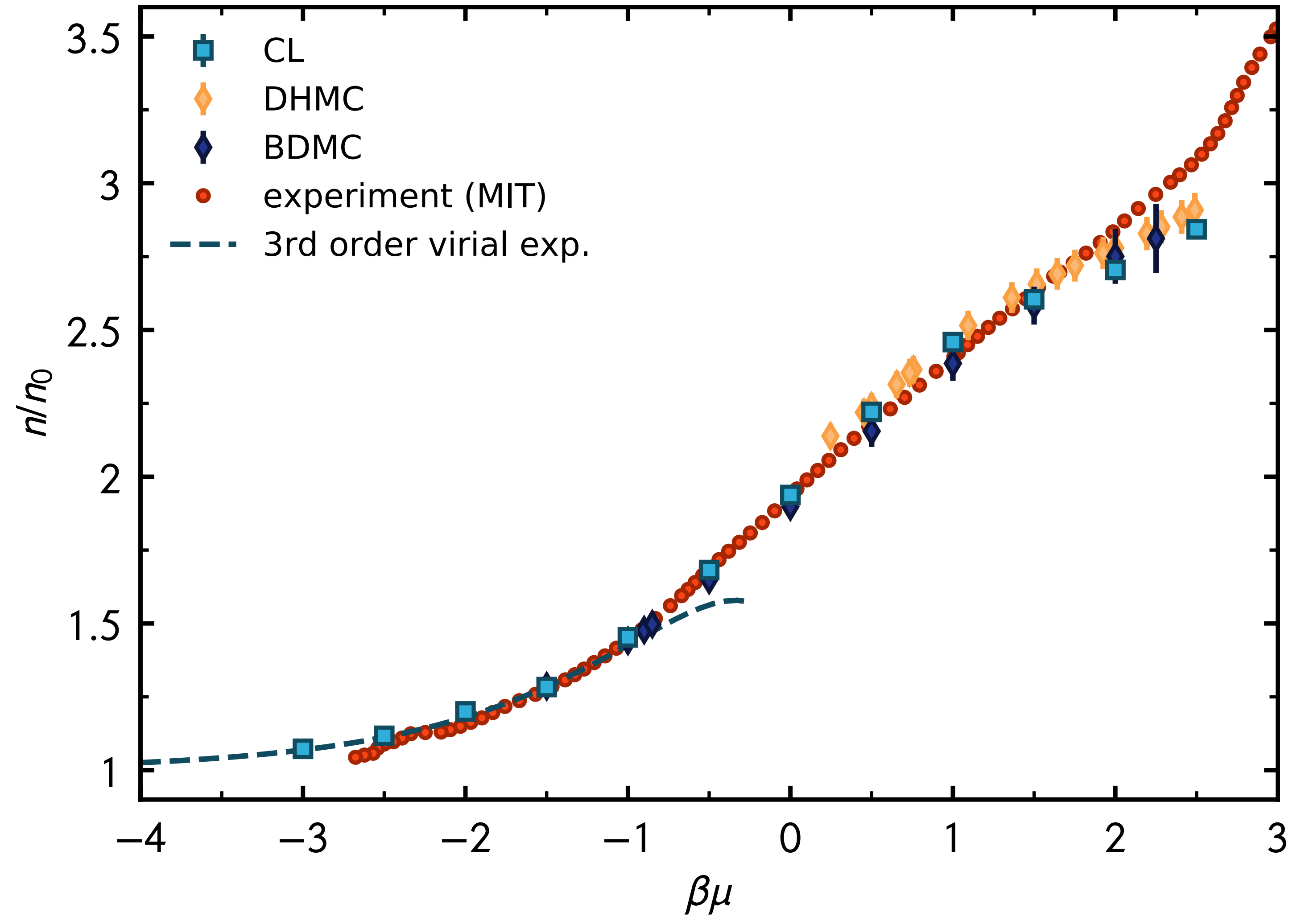
density equation of state

[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]



classical regime

$k_B T$ dominates

quantum regime

E_F dominates

density equation of state

[LR, Loheac, Drut, Braun '18]

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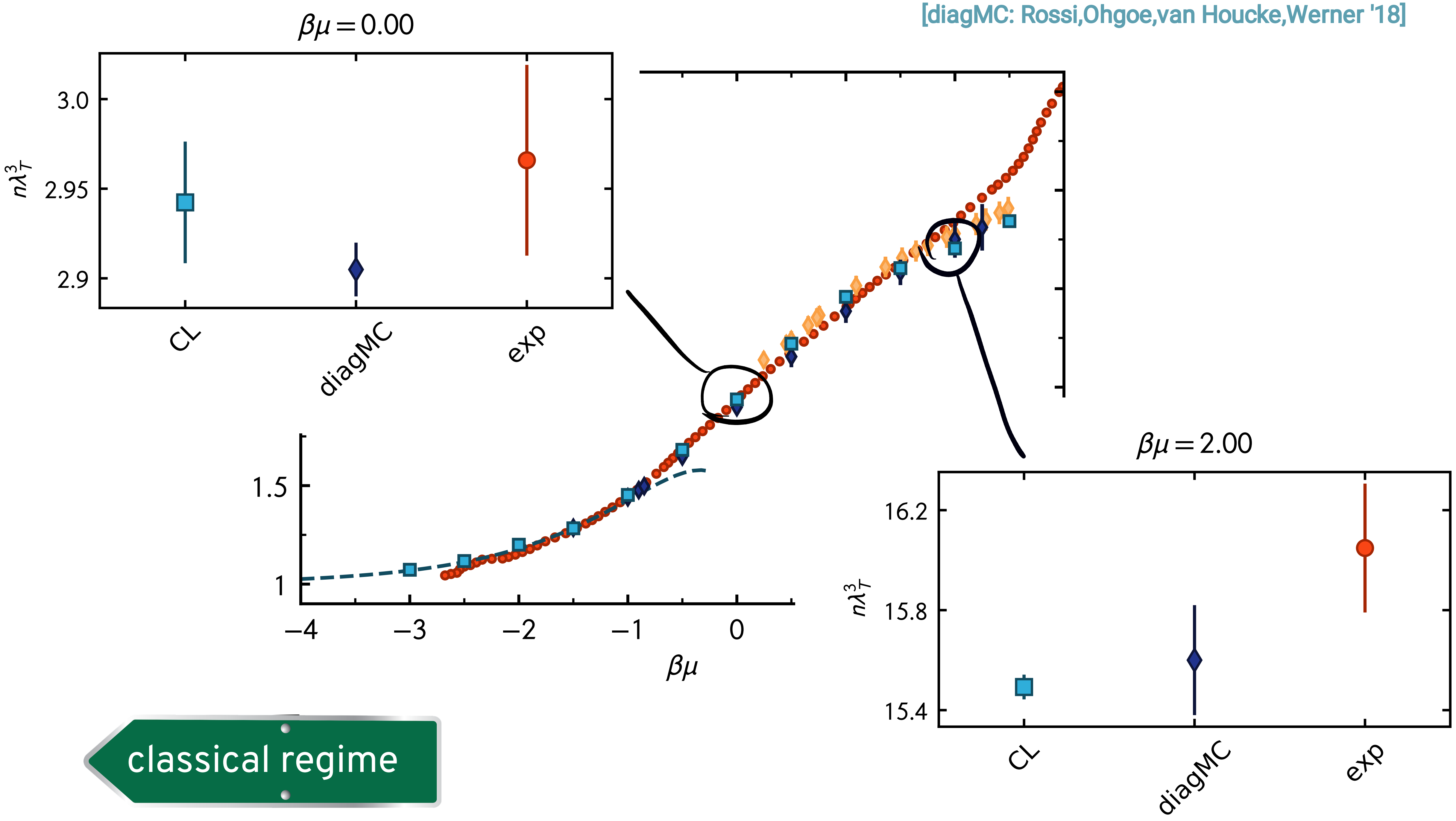

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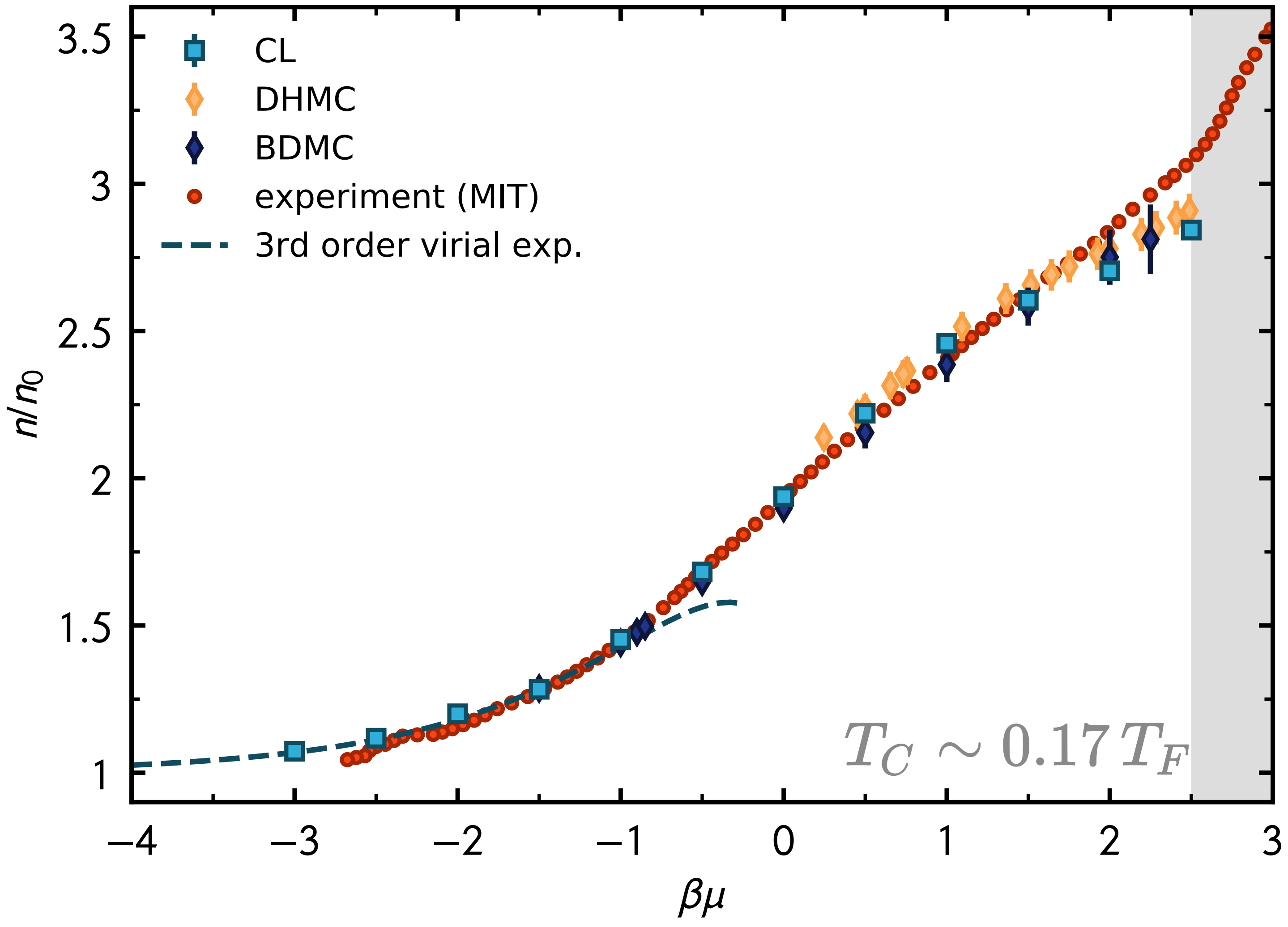
good agreement with experiment and other methods!

CL results:

finite lattice $V = 11^3$



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

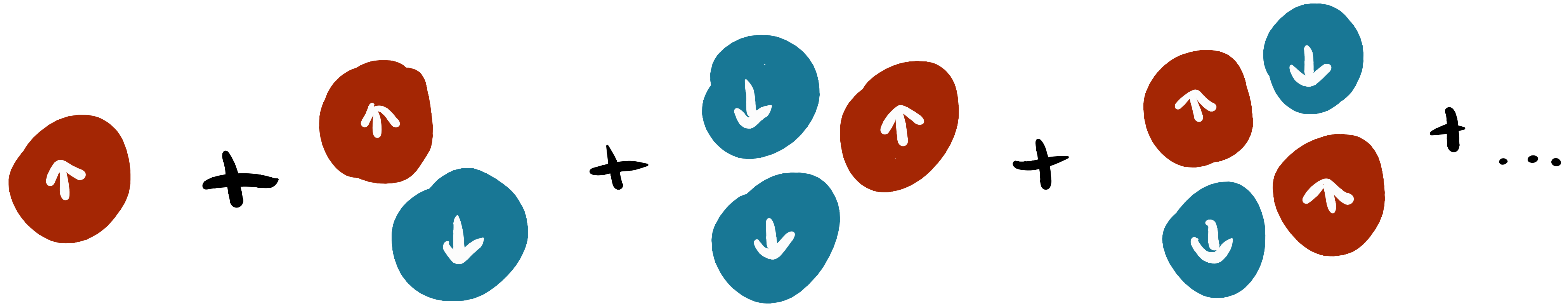
[Liu '13]

dilute gases: few-body correlations dominate

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

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

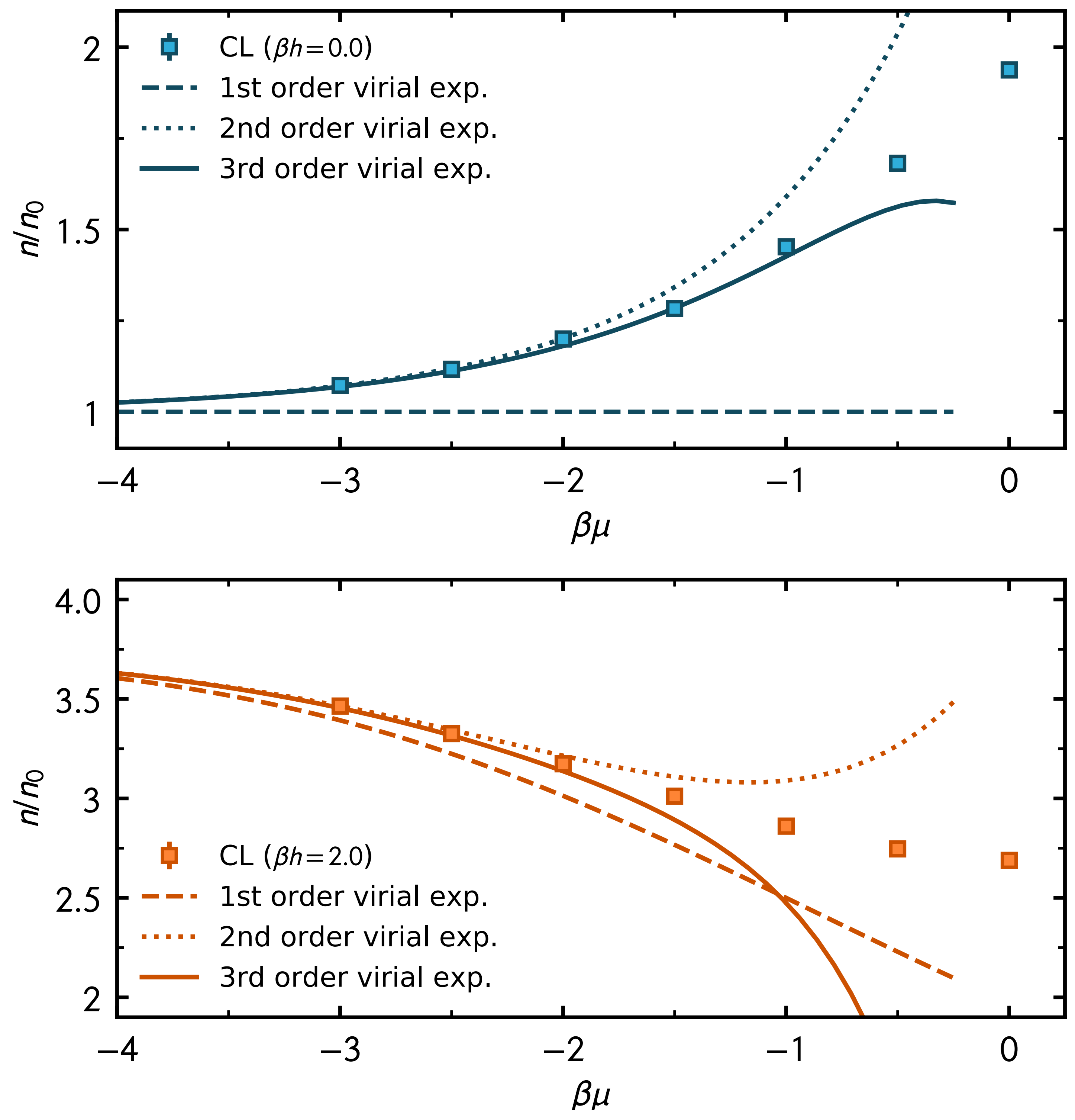
$$\ln \mathcal{Z} = Q_1 \sum_n z^n b_n$$



density EOS (virial regime)

[LR, Loheac, Drut, Braun '18]

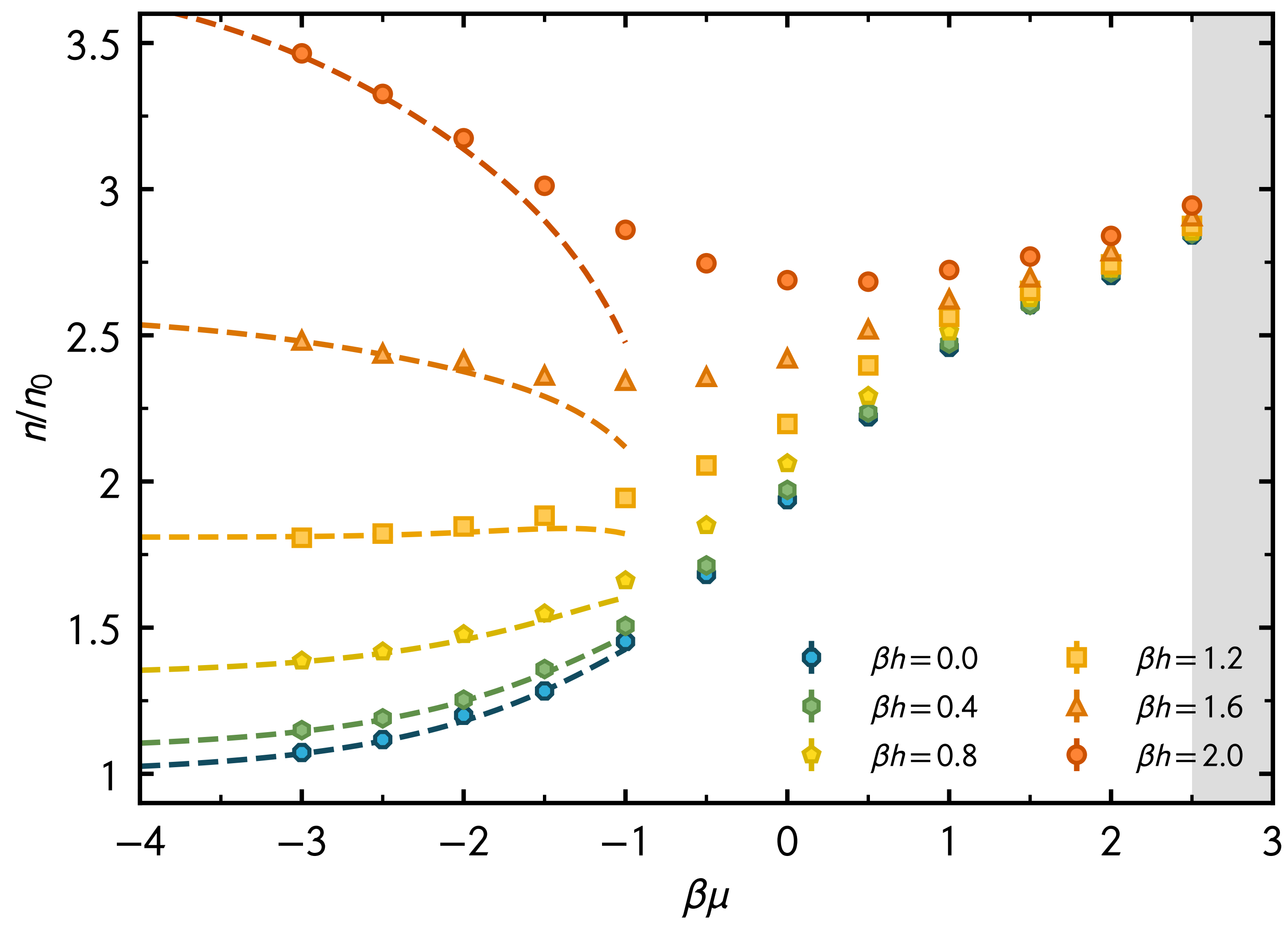
VE approaches the CL results order-by-order



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**

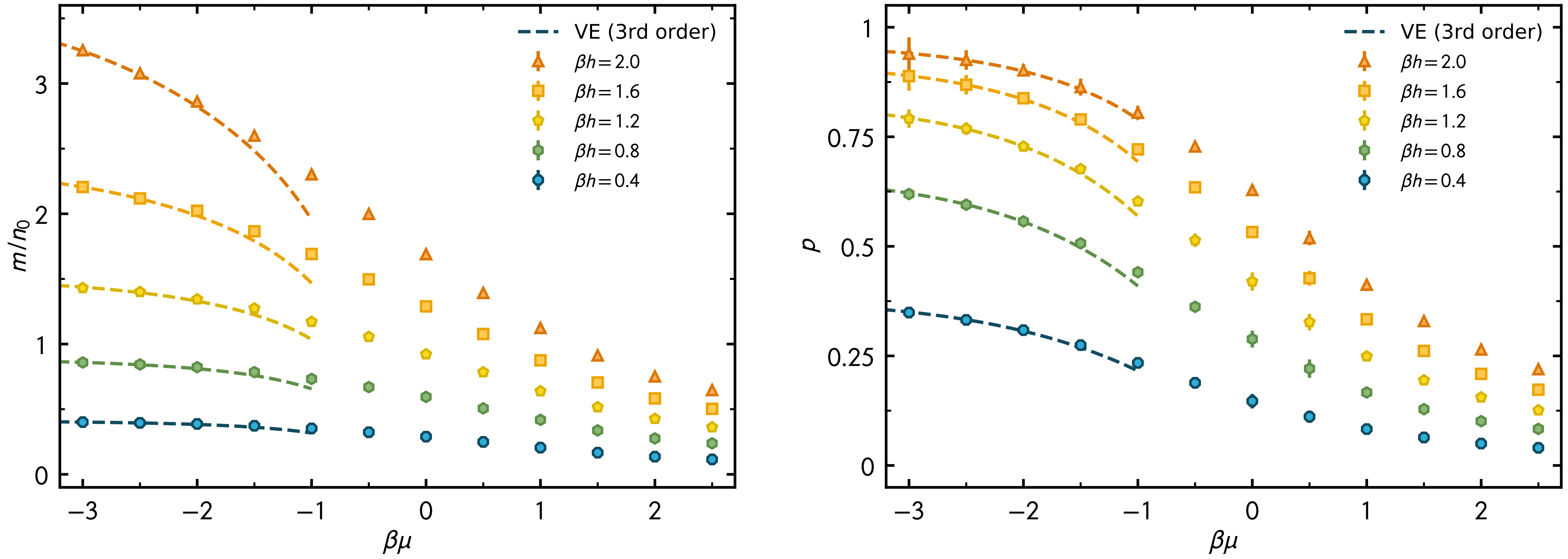
experimentally testable prediction

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

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

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

thermodynamic response

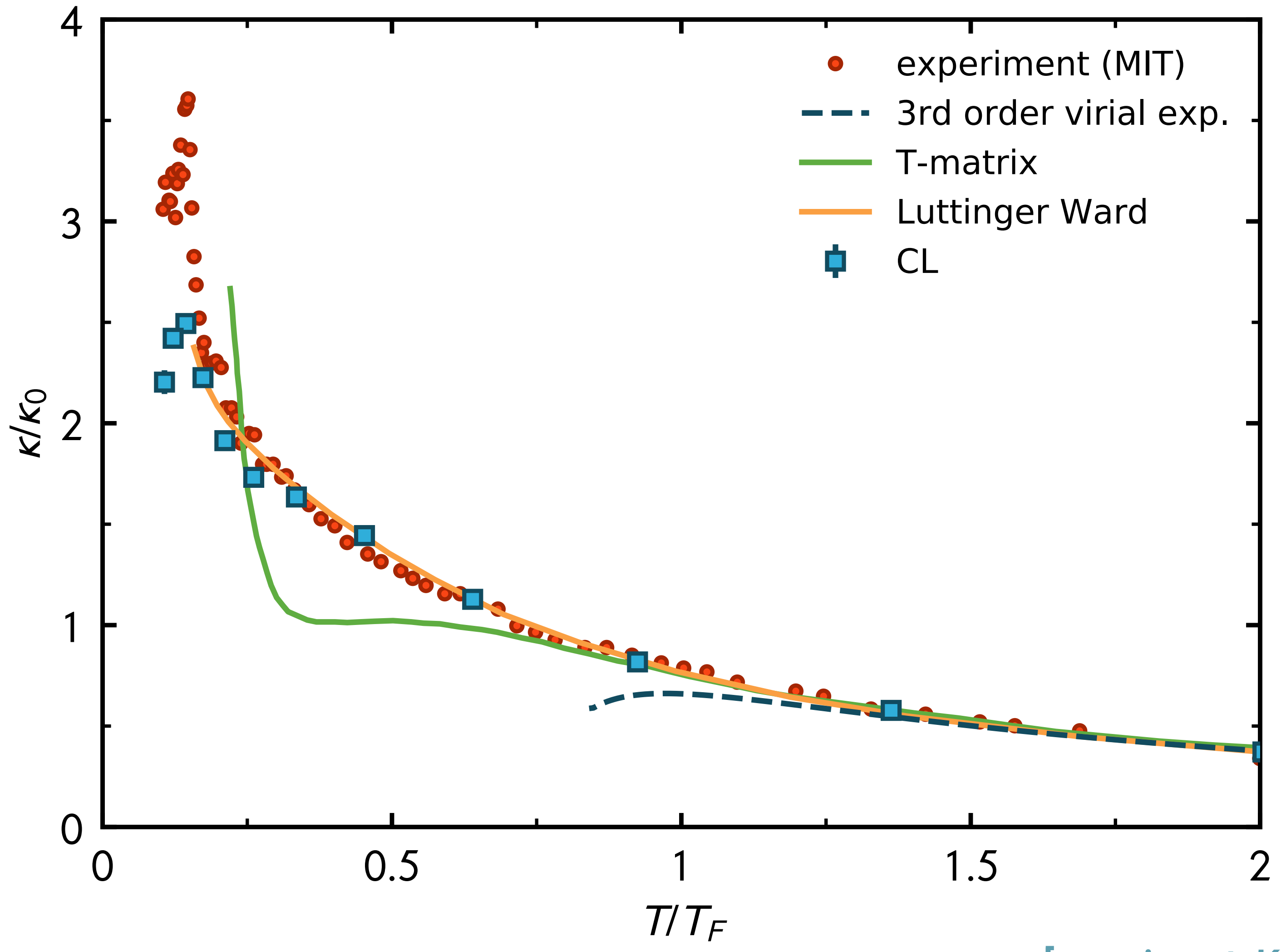
$$\kappa = \frac{1}{n}\left(\frac{\partial n}{\partial P}\right)_{T,V,h}$$

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

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]
[T-matrix: Pantel et al. '14]

compressibility (unpolarized)

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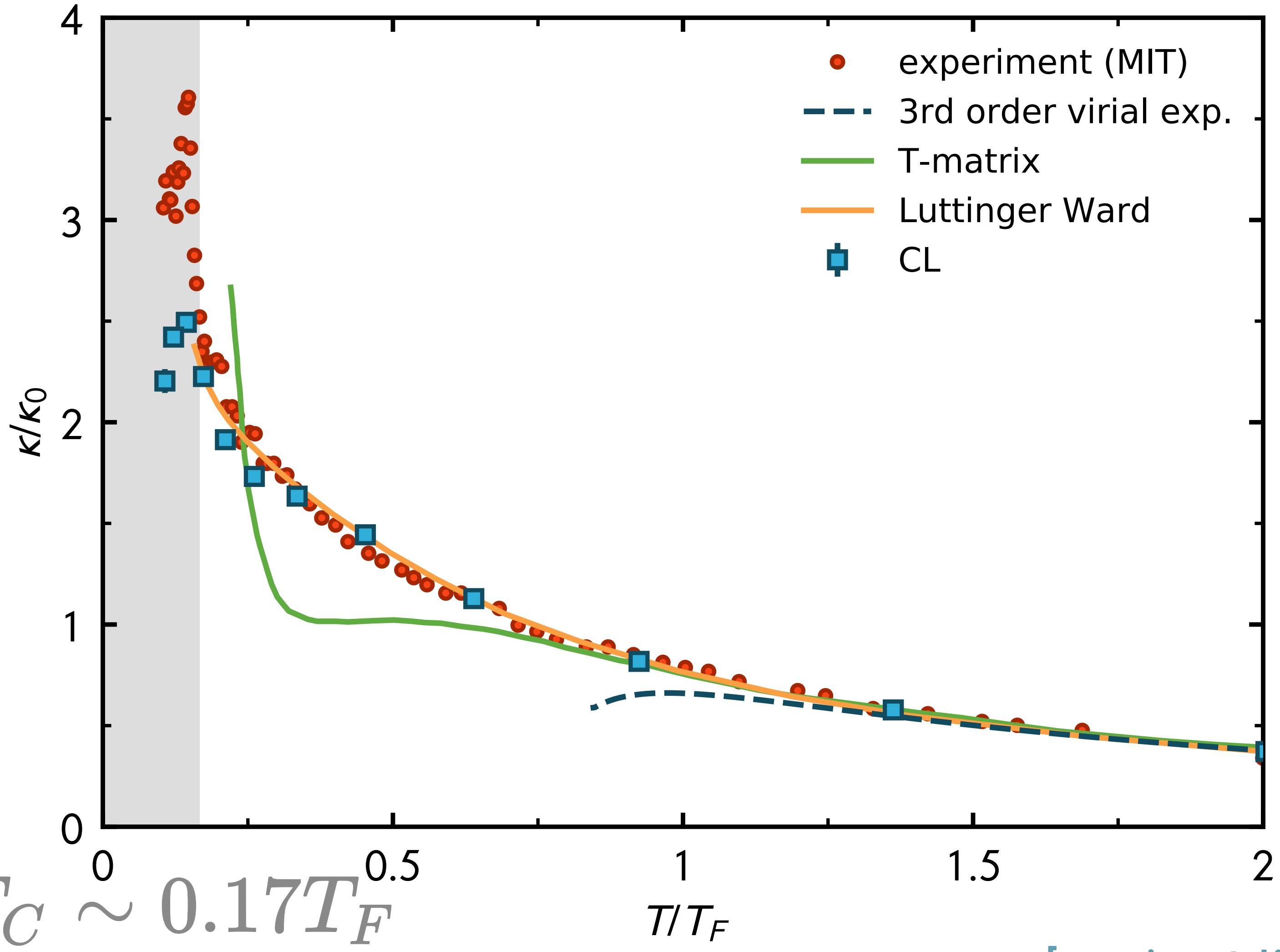
$$\kappa = \frac{1}{n}\left(\frac{\partial n}{\partial P}\right)_{T,V,h} = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_{T,V,h}$$

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



$T_C \sim 0.17 T_F$

features of curve recovered with CL

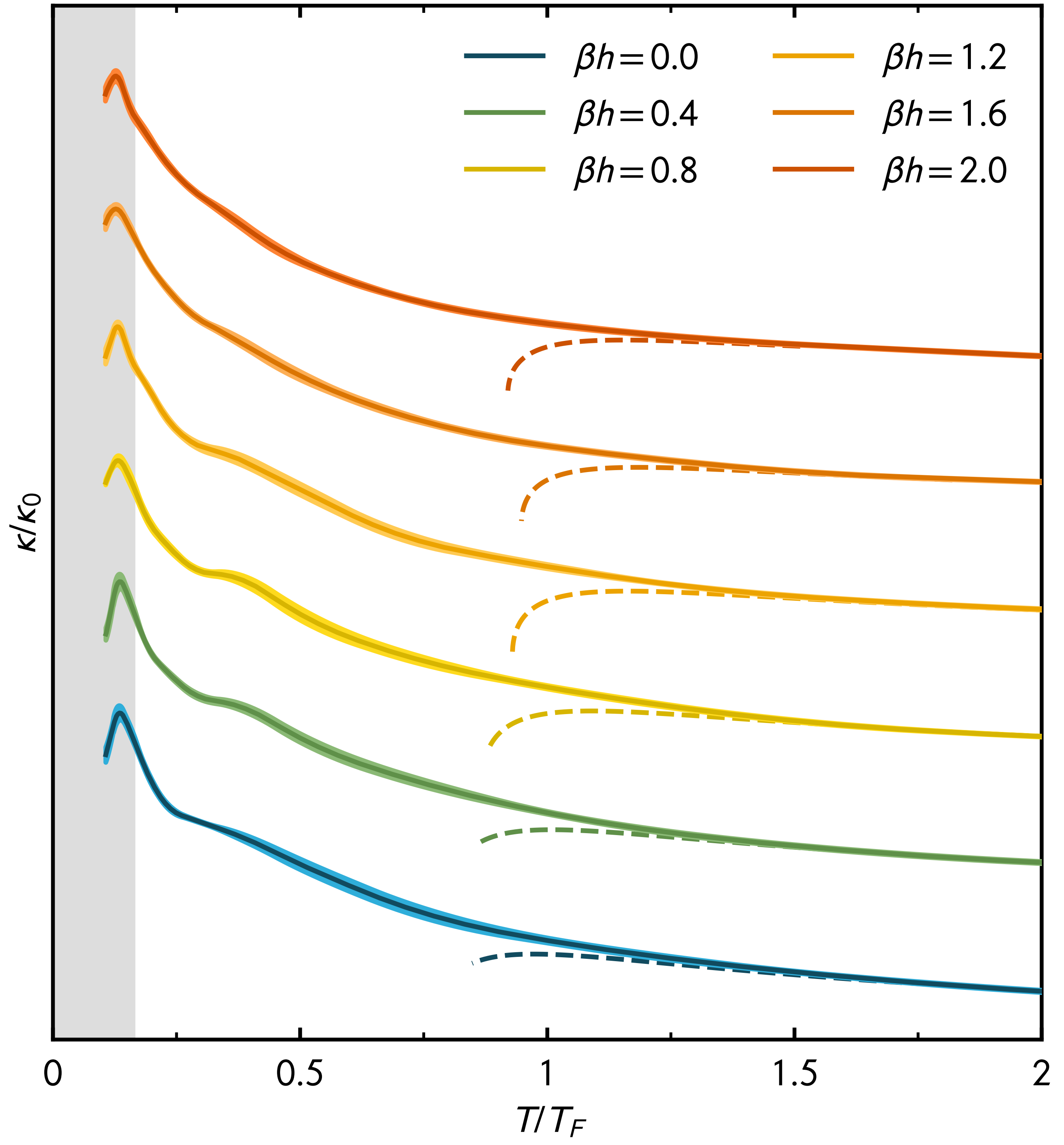
quantitative disagreement at low temperatures

[experiment: Ku,Sommer,Cheuck,Zwierlein '12]
[Luttinger-Ward: Enns,Haussmann '12]
[T-matrix: Pantel et al. '14]

compressibility for polarized systems

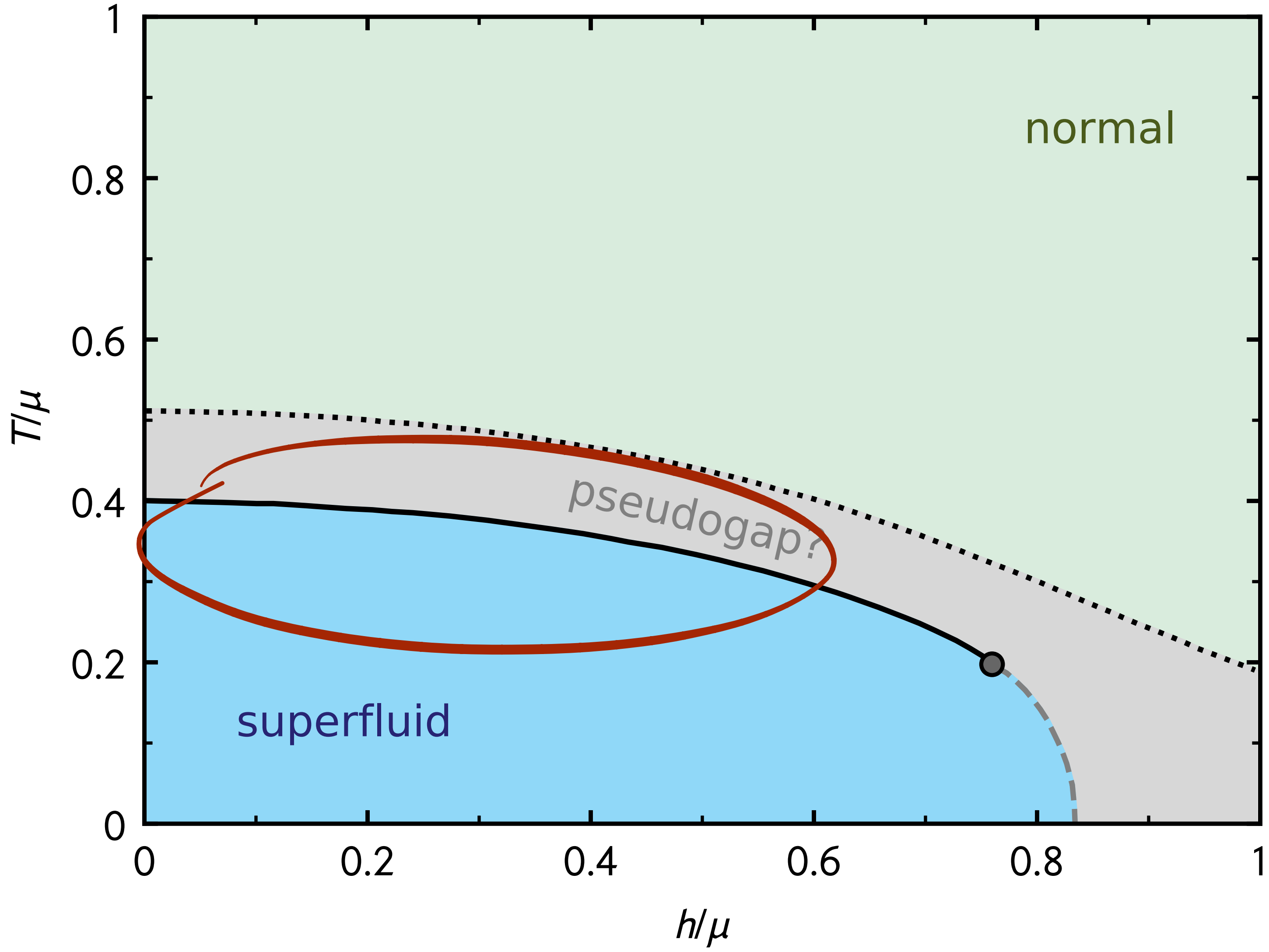
[LR, Loheac, Drut, Braun '18]

weak dependence of the critical temperature on polarization indicated



challenging to extract precise T_C

UFG phase diagram



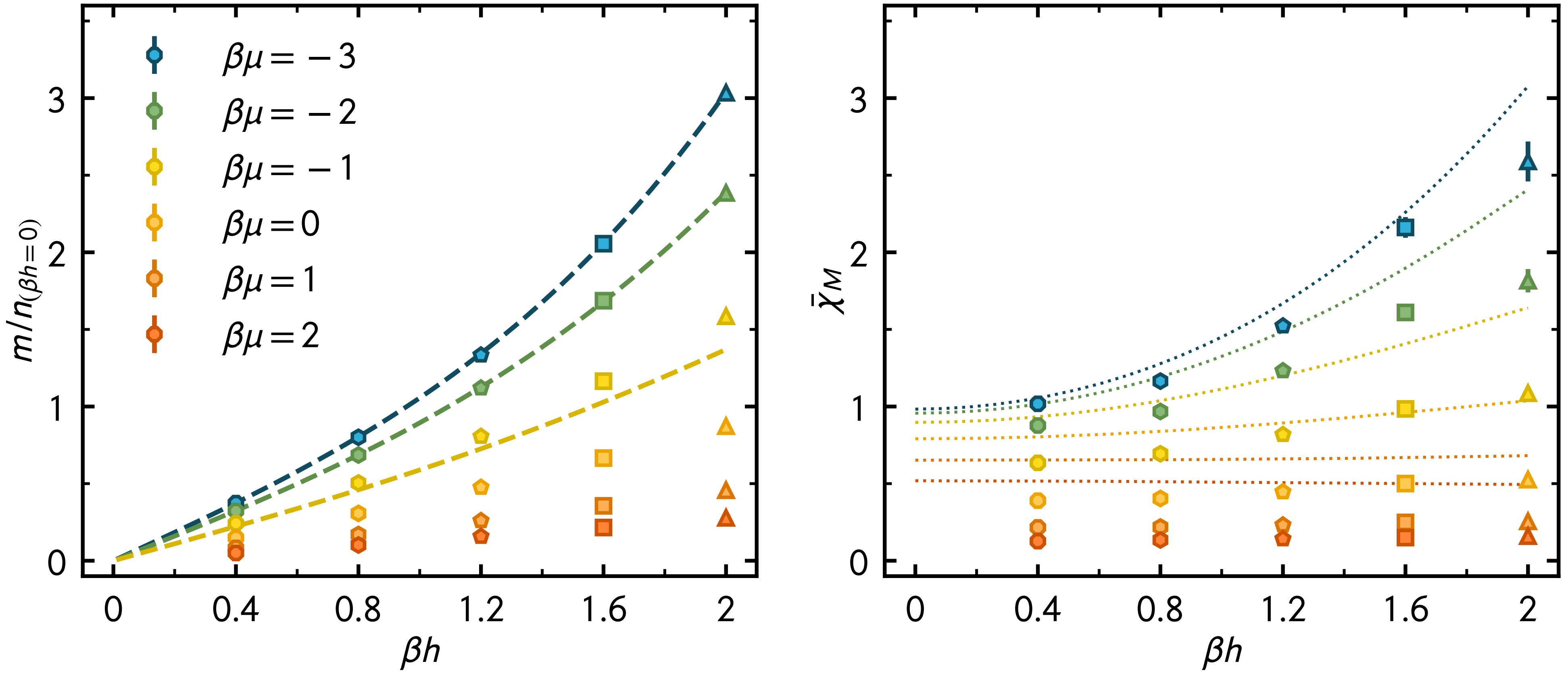
$$\mu = \frac{\mu_\uparrow + \mu_\downarrow}{2}$$
$$h = \frac{\mu_\uparrow - \mu_\downarrow}{2}$$

[fRG: Boettcher et. al '15]

spin susceptibility

[LR, Loheac, Drut, Braun '18]

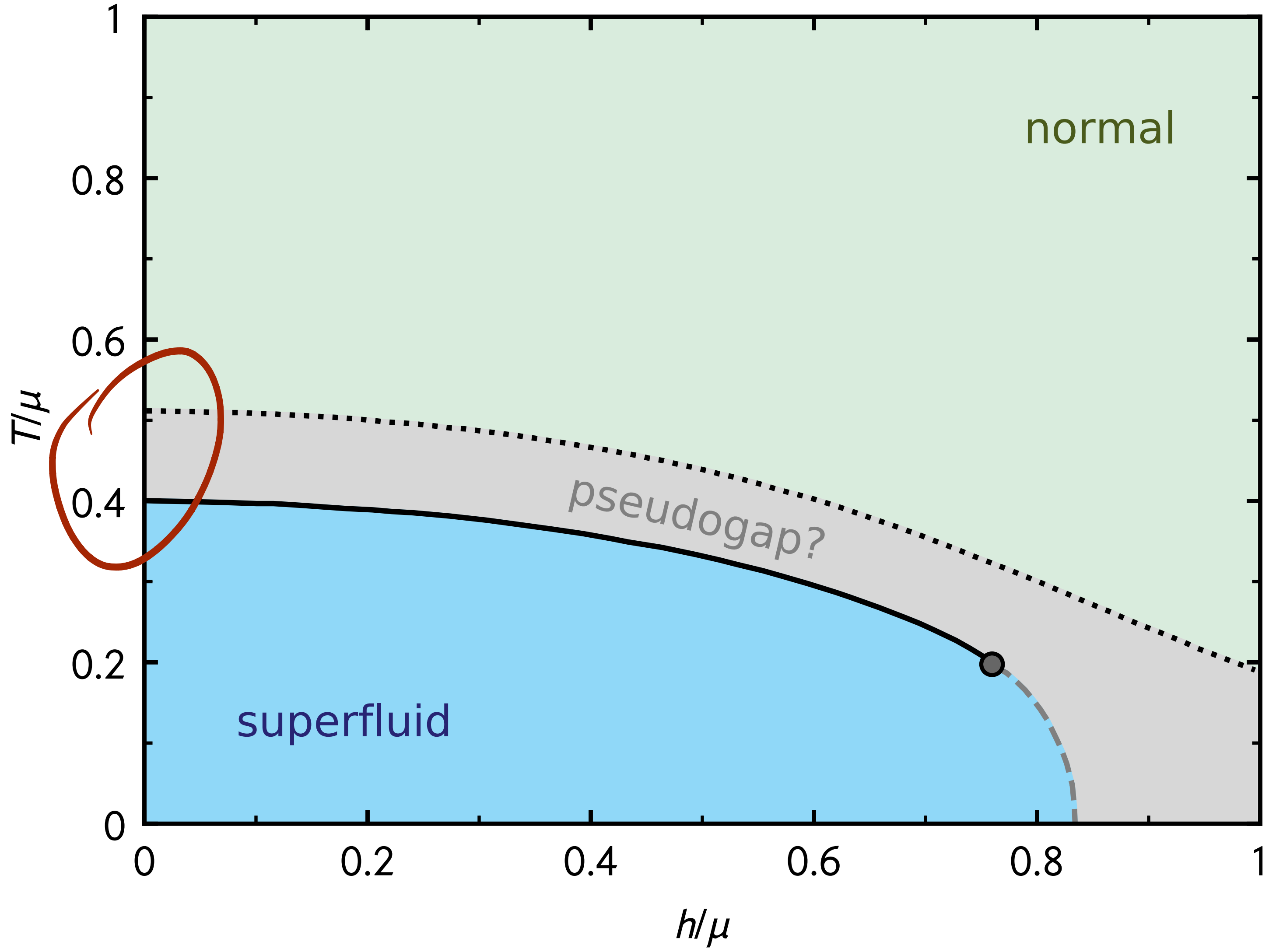
$$\chi = \left(\frac{\partial m}{\partial h}\right)_{T,V,\mu}$$



Pauli susceptibility field independent at low field and temperature

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

UFG phase diagram (sketch)



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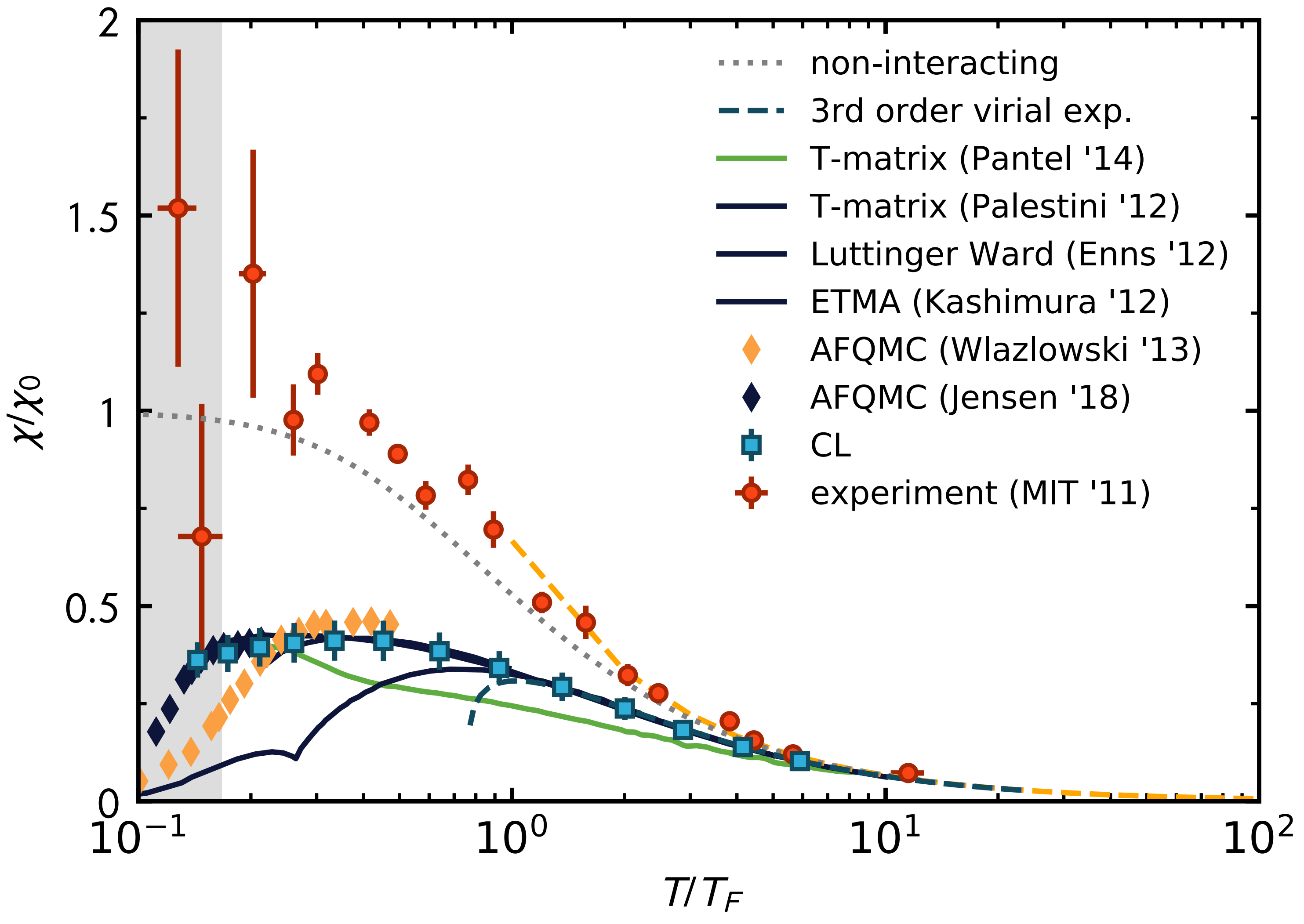
[fRG: Boettcher et. al '15]

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]

magnetic susceptibility (unpolarized)

[LR, Loheac, Drut, Braun in preparation]

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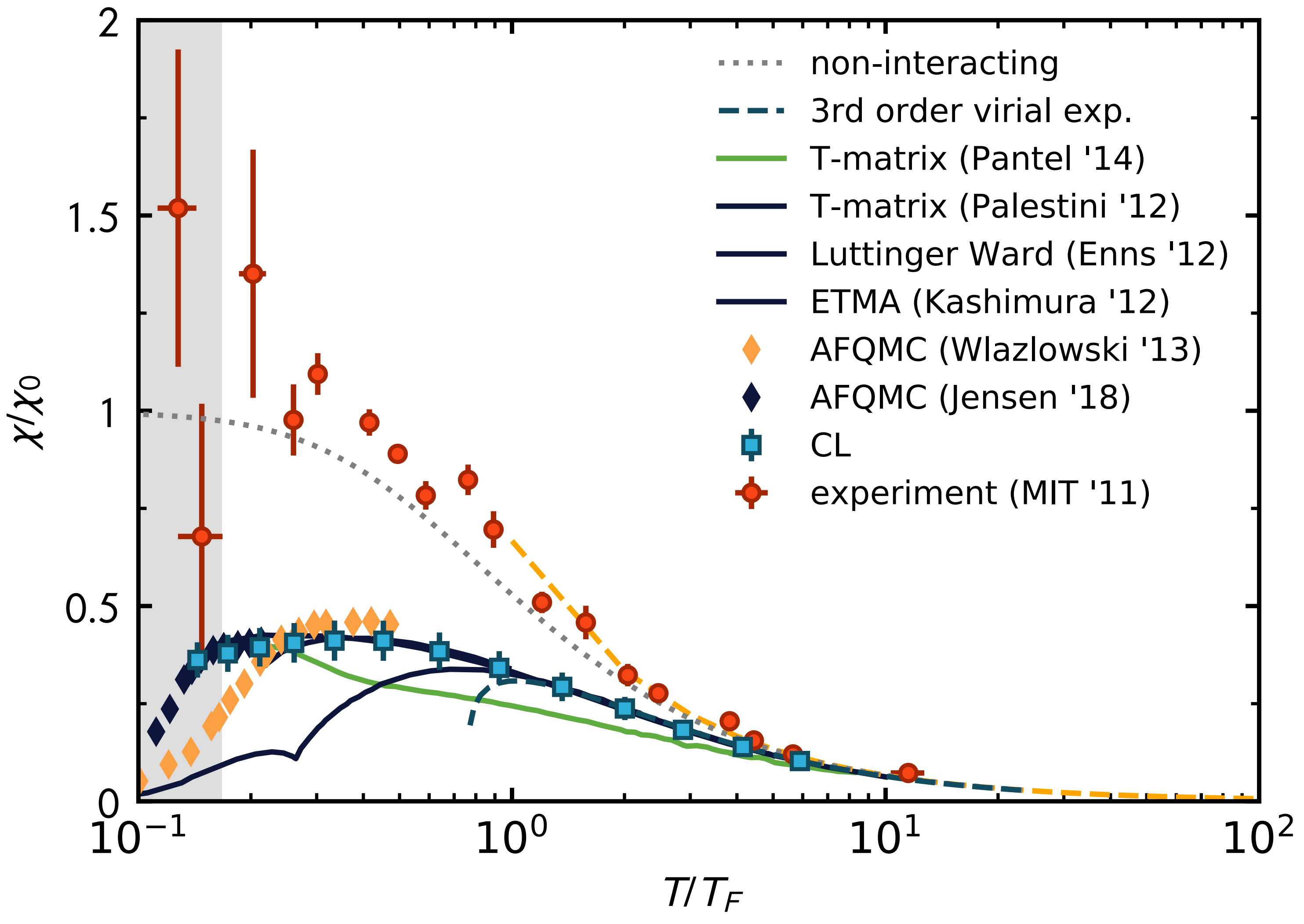

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Pseudogap:
suppression of χ at $T > T_C$

[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

recap

complex Langevin is a valuable tool
to study ultracold Fermi gases
(it works quite well)

team CL

Jens Braun Florian Ehmann


Joaquin Drut Andrew Loheac


LR


Josh McKenney Casey Berger

TU Darmstadt

UNC Chapel Hill