Exploring imbalanced Fermi gases with stochastic quantization

Lukas Rammelmüller, LMU Munich

Cold Quantum Coffee, January 28, 2020

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

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MCQST

the plan

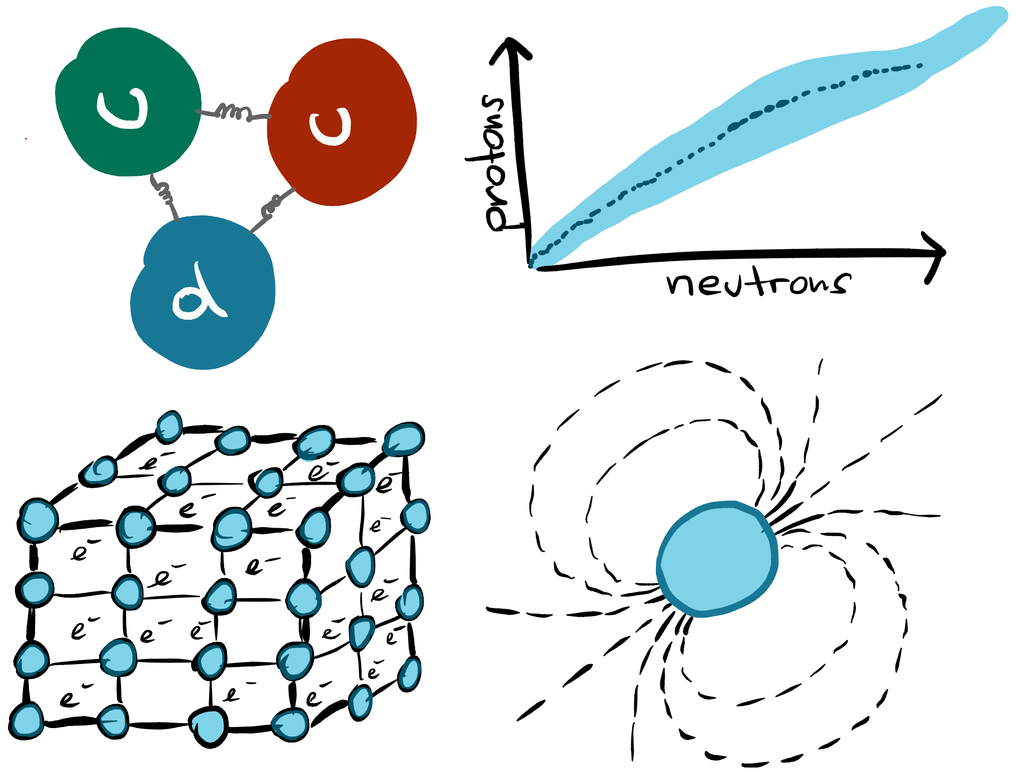
I) motivation: why ultracold fermions?

II) Monte Carlo, the sign problem & complex Langevin in a nutshell

III) some results for 3D and 1D fermions

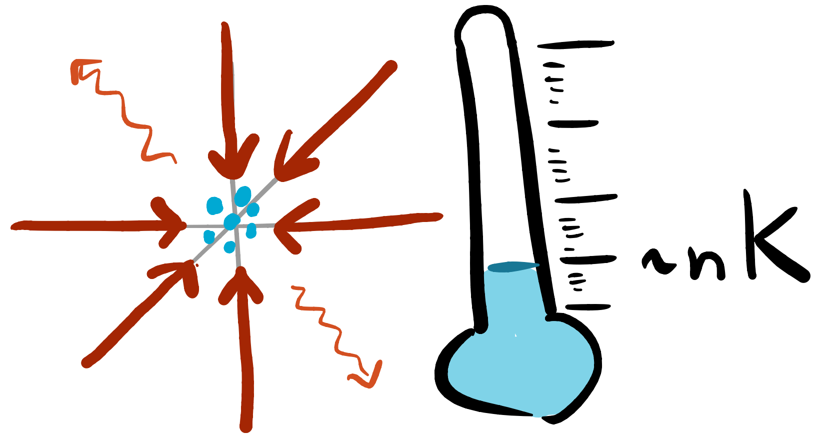
ultracold atoms: a versatile toolbox

[reviews: Bloch,Dalibard,Zerger '08]



we can find strongly correlated systems in nature...

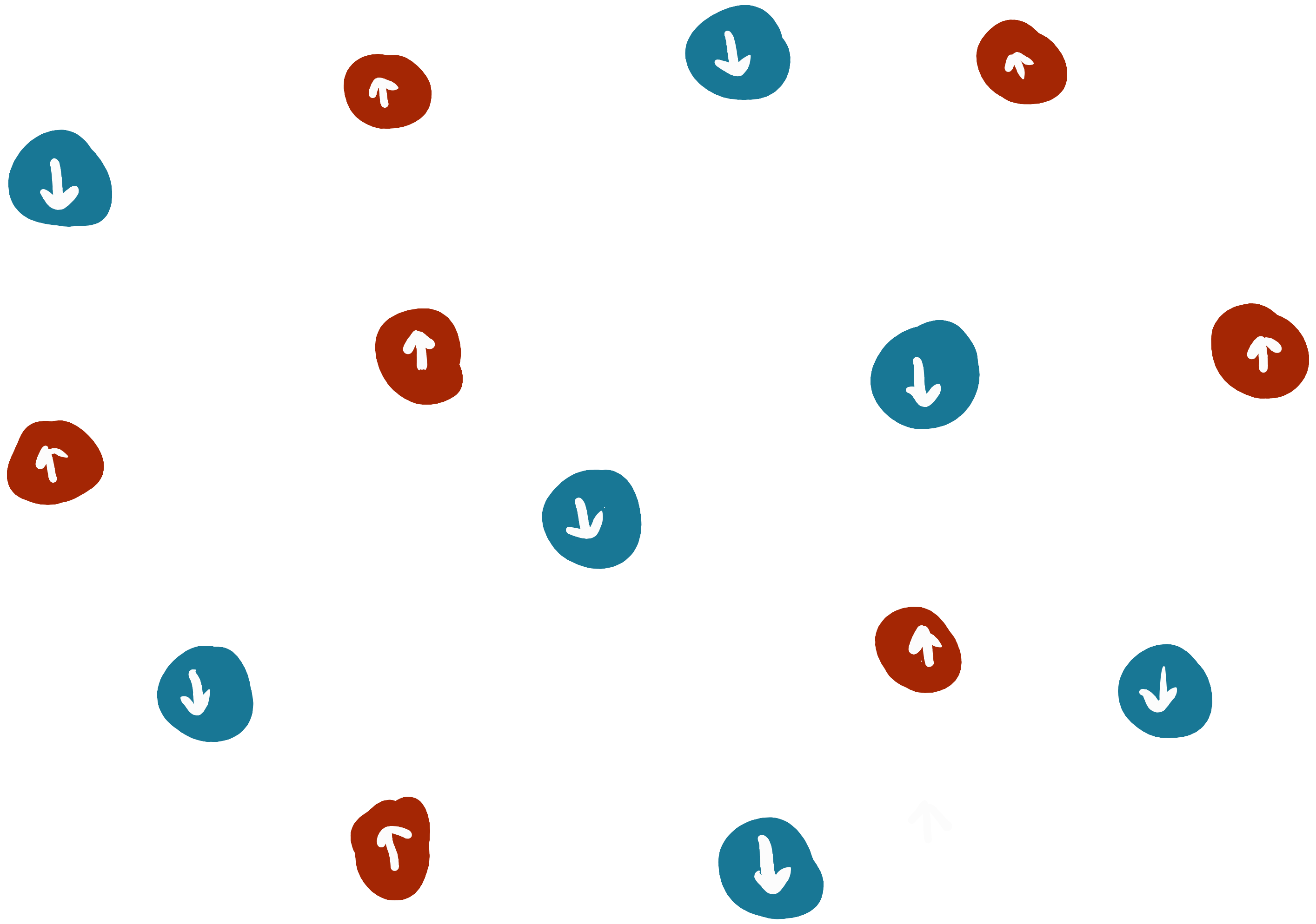
... and study them in the lab!

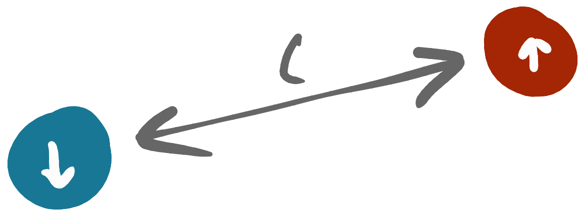


controlled interactions, reduced dimensions, mass/spin imbalance, optical lattices, simulation of gauge theories, ...

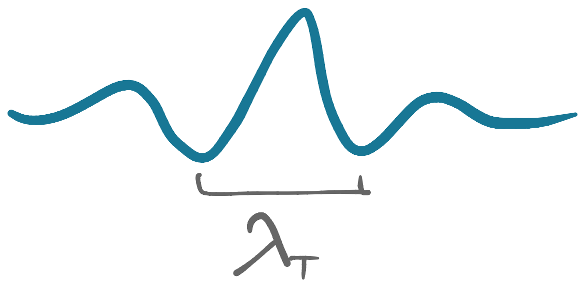
cold & dilute fermions

[reviews: Giorgini,Pitaevskii,Stringari '08; Ketterle,Zwierlein '08]





dilute: $l \gg r_0$

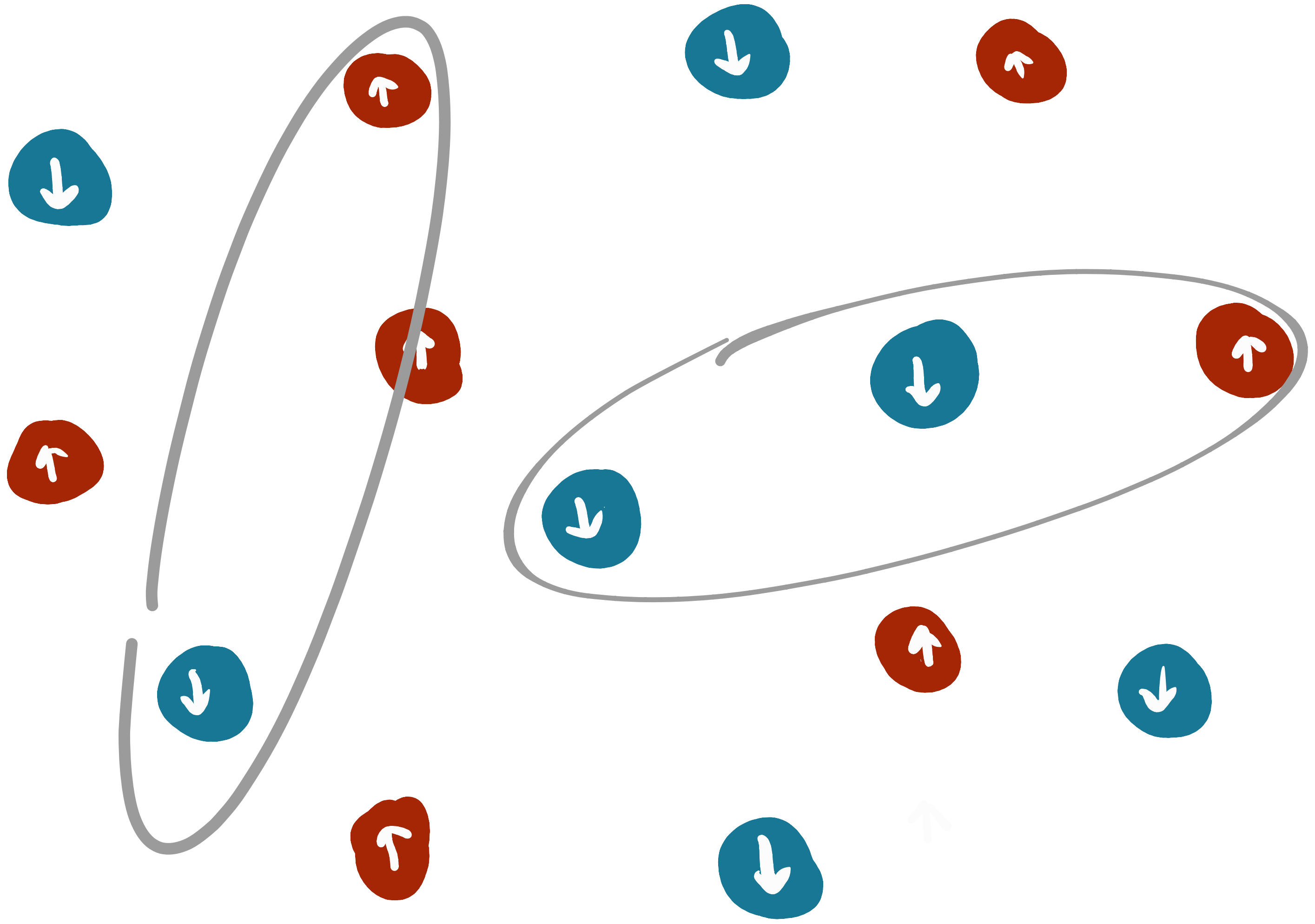


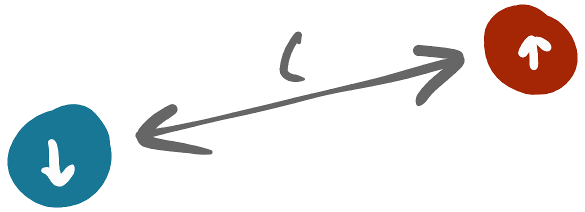
cold: $\lambda_T \gg r_0$

s-wave scattering length fully determines the scattering properties

cold & dilute fermions

[reviews: Giorgini,Pitaevskii,Stringari '08; Ketterle,Zwierlein '08]





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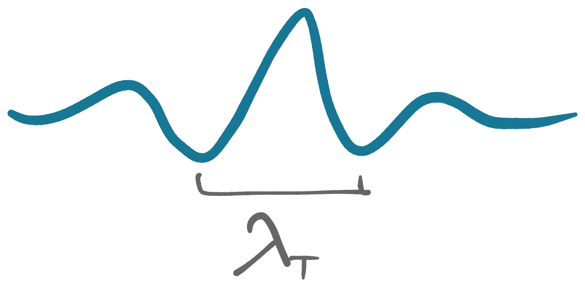

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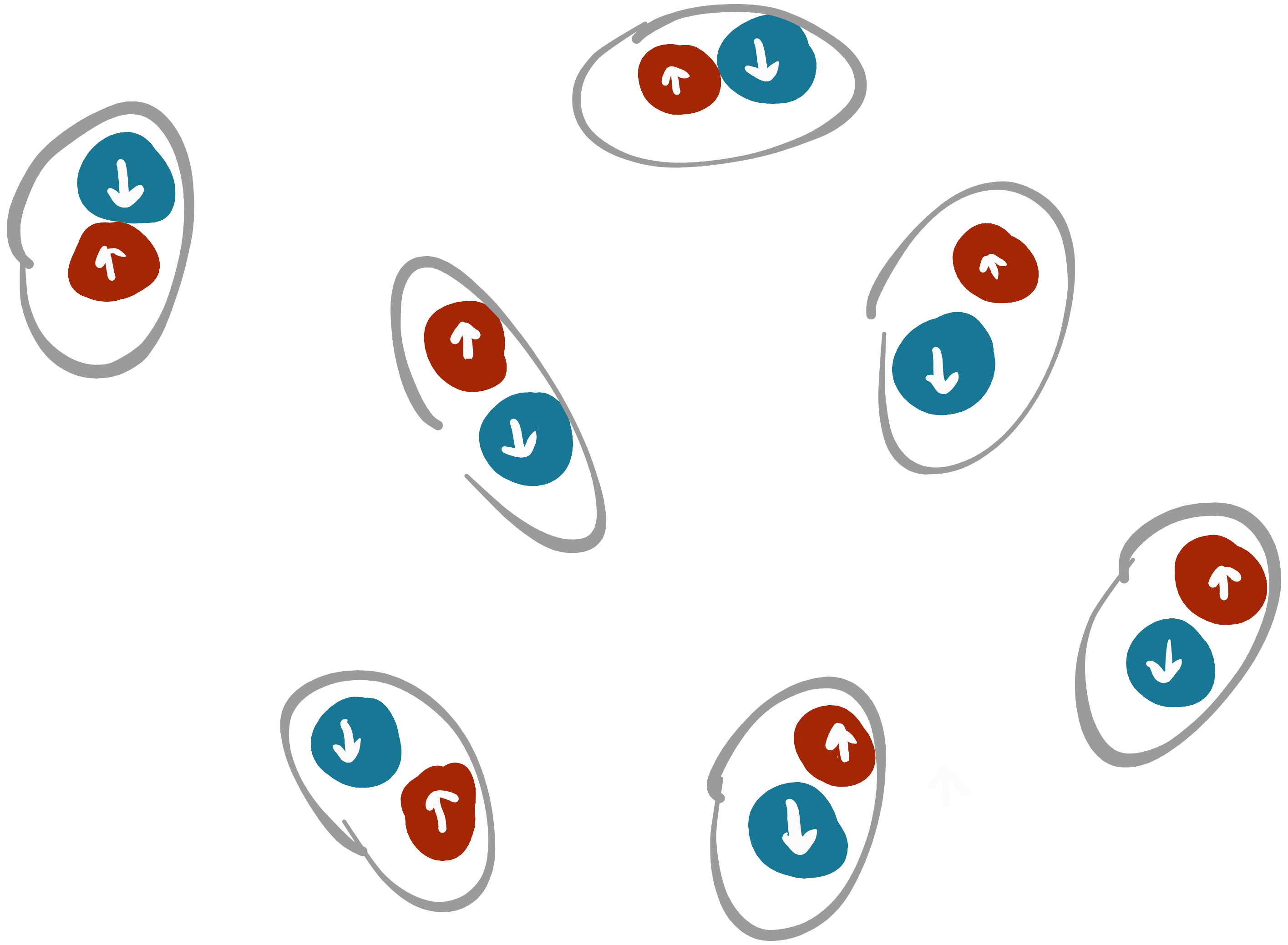

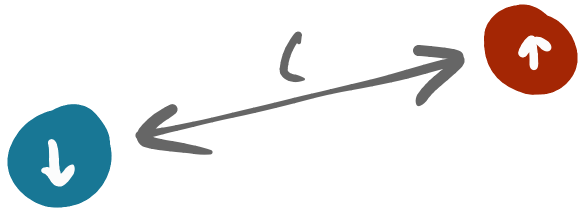

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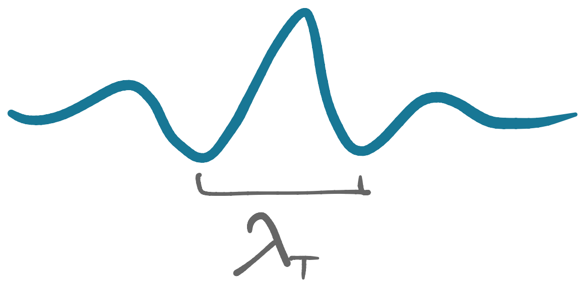

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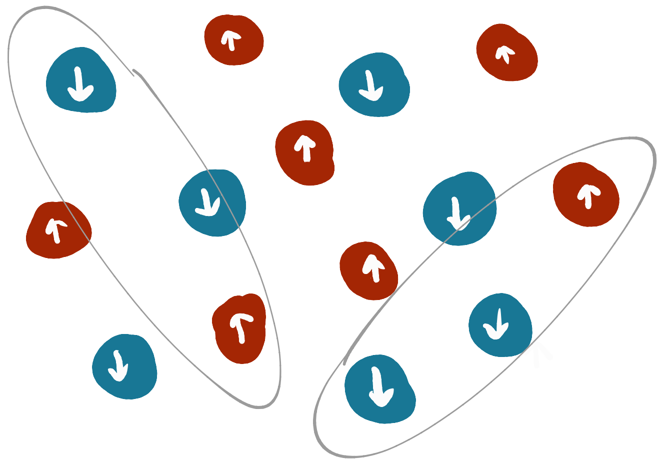
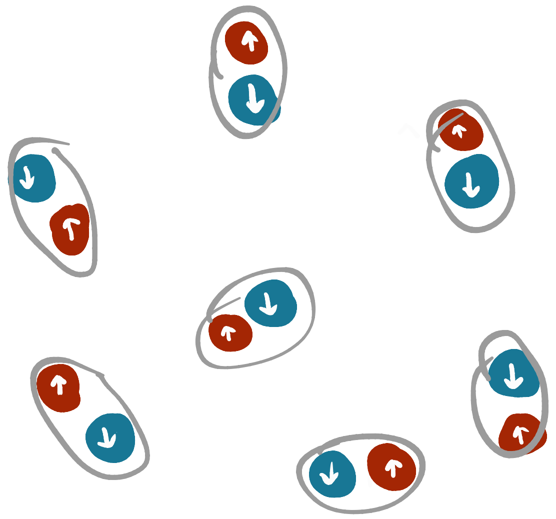
the BCS-BEC crossover

[reviews: Giorgini,Pitaevskii,Stringari '08; Zwerger '12]



scattering length small and negative



scattering length small and positive

weak attractive interaction, mean-field solution (BCS theory)

weakly repulsive (composite) bosons, BEC regime

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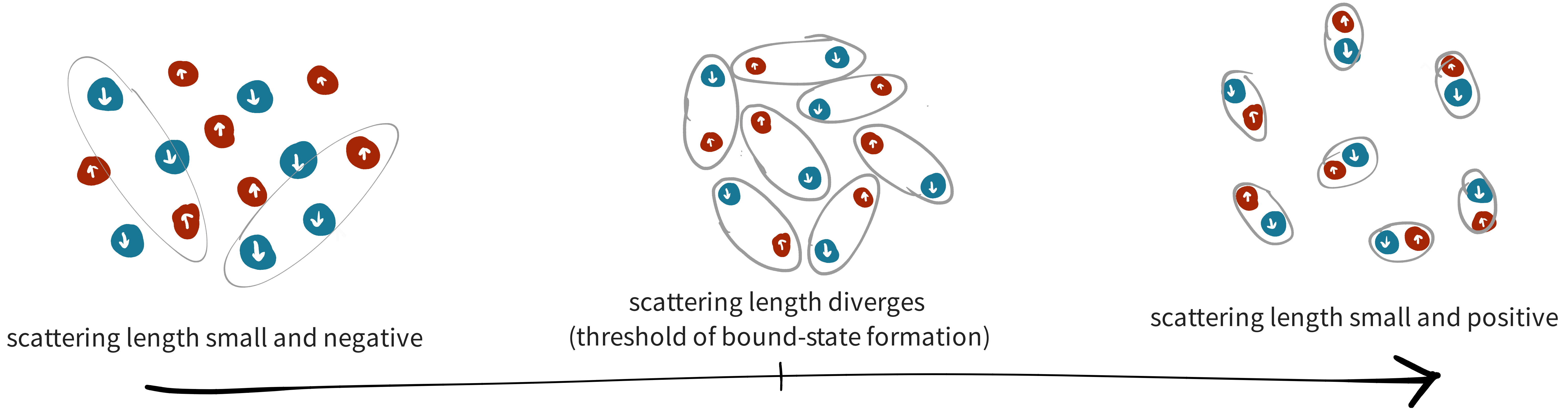

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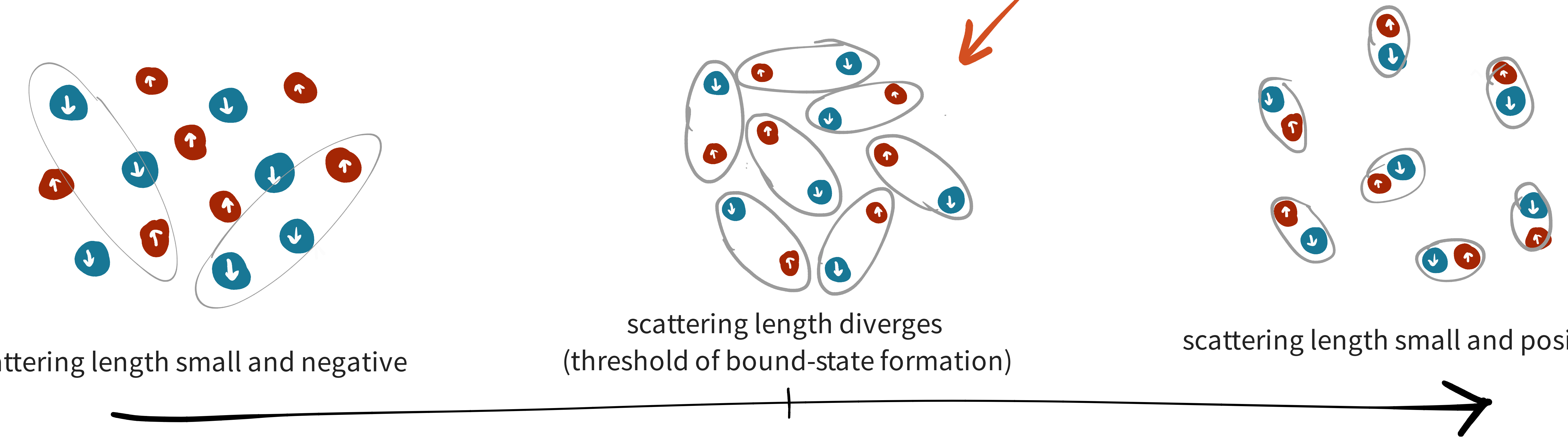
unitary Fermi gas (UFG)

strongly correlated,
non-perturbative many-body
problem



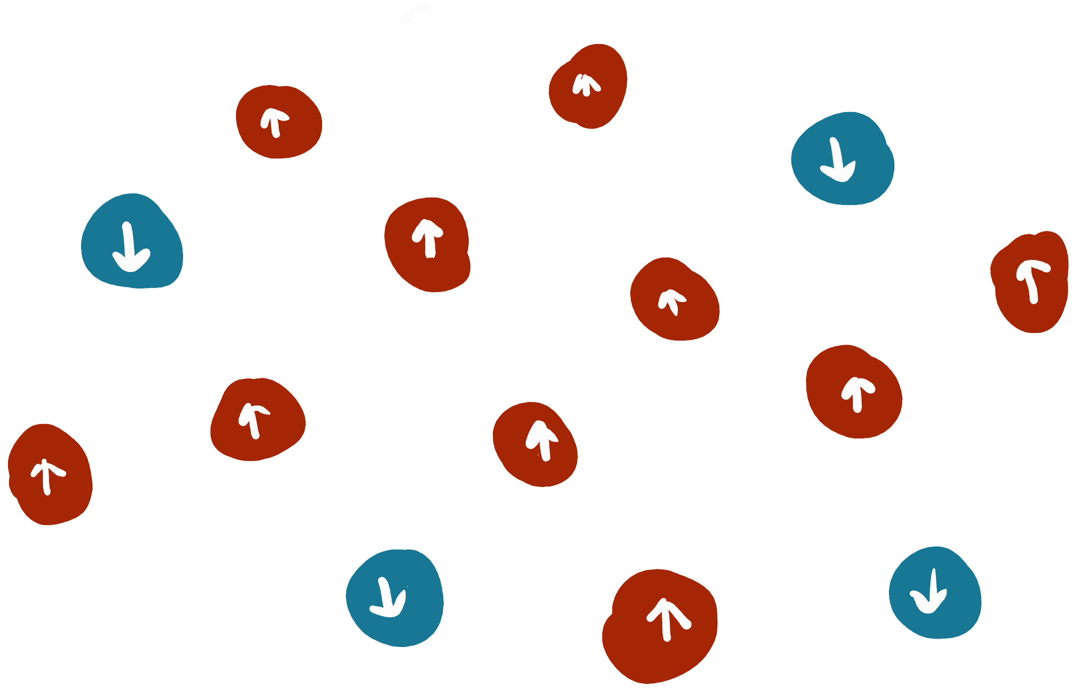
weak attractive interaction, mean-field solution (BCS theory)

weakly repulsive (composite) bosons, BEC regime

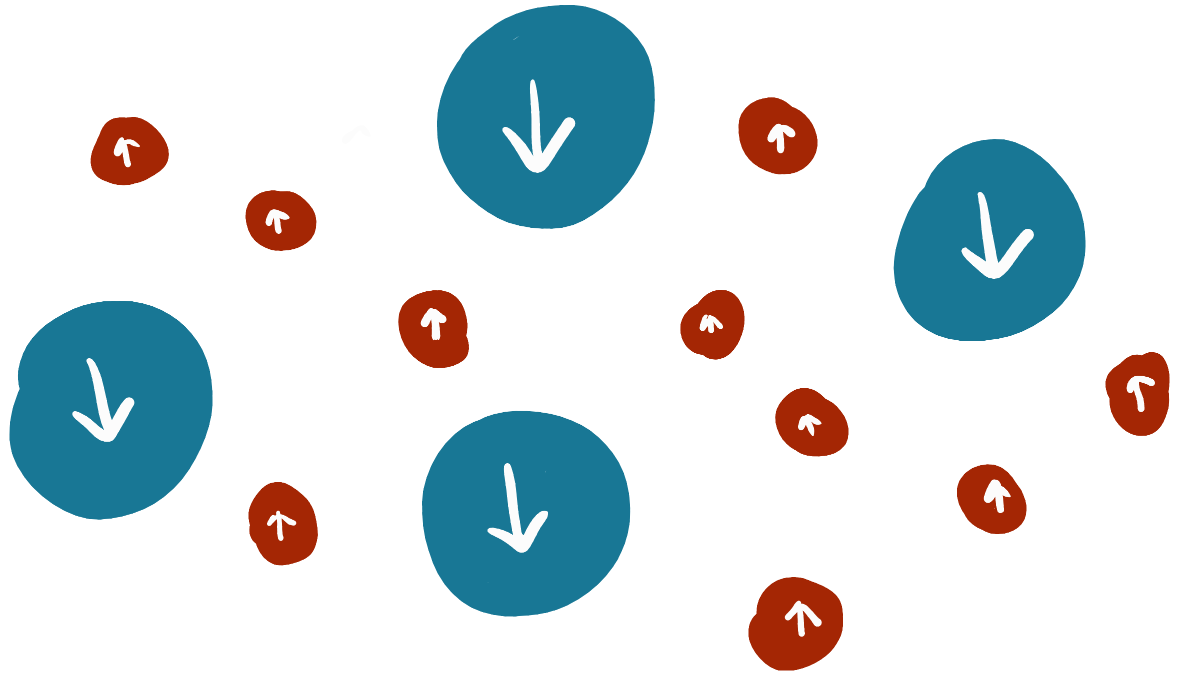
imbalanced Fermi gases

[Chevy,Mora '10; Radzihovsky,Sheehy '10; Gubbels,Stoof '13]

spin polarization



mass imbalance



key questions:

thermodynamics? critical imbalance for superfluidity?

structure of pairing? inhomogeneous phases?

model & computational challenge

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

model & computational challenge

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

what we need to compute:

$$\mathcal{Z} = \mathrm{Tr}[\mathrm{e}^{-\beta \hat{H}}] = \int \mathcal{D}\phi \, \mathrm{e}^{-S[\phi]}$$

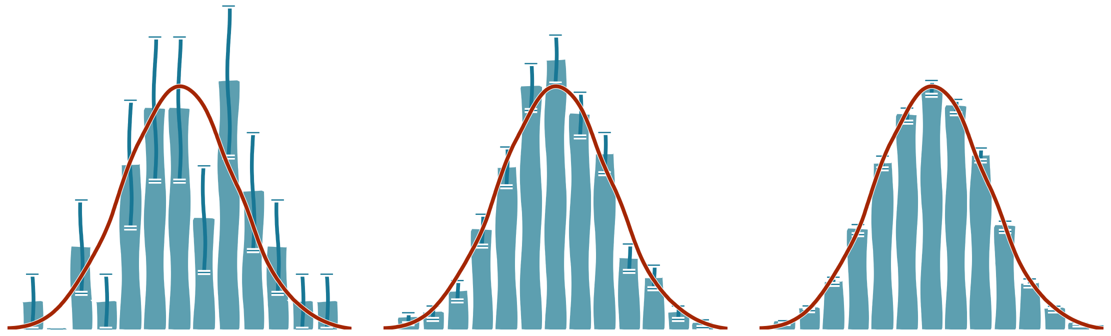
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}[\hat{\mathcal{O}} \, \mathrm{e}^{-\beta \hat{H}}] = \int \mathcal{D}\phi \, P[\phi] \mathcal{O}[\phi]$$

Monte Carlo integration in a nutshell

$$\langle\hat{\mathcal{O}}\rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi\, \mathcal{O}[\phi]\, \mathrm{e}^{-S[\phi]} \equiv \underbrace{\int \mathcal{D}\phi\, \mathcal{O}[\phi]\, P[\phi]}$$

stochastic evaluation:

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



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

Monte Carlo integration in a nutshell

$$\langle\hat{\mathcal{O}}\rangle = \frac{1}{\mathcal{Z}}\int\mathcal{D}\phi\,\mathcal{O}[\phi]\,\mathrm{e}^{-S[\phi]} \equiv \int\mathcal{D}\phi\,\mathcal{O}[\phi]\,P[\phi]$$

efficiency of MC relies on **positive semidefinite probability measure**,
otherwise we encounter a **sign problem**!

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otherwise we encounter a **sign problem**!

$$\langle\hat{\mathcal{O}}\rangle = \frac{\int\mathcal{D}\phi\ \mathcal{O}[\phi]\ P[\phi]}{\int\mathcal{D}\phi\ \ P[\phi]} = \frac{\int\mathcal{D}\phi\ \mathcal{O}[\phi]\ s\ |P[\phi]|}{\int\mathcal{D}\phi\ |P[\phi]|}\,\frac{\int\mathcal{D}\phi\ |P[\phi]|}{\int\mathcal{D}\phi\ s\ |P[\phi]|} = \frac{\langle s\hat{\mathcal{O}}\rangle_{pq}}{\langle s\rangle_{pq}}$$

reweighting is **no (efficient) solution:** relative uncertainty $\propto e^{\#V\beta}$

why?

why?

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

why?

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

probability measure **not positive (semi-)definite**

if any of these conditions applies:

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

stochastic quantization

[Parisi,Wu '81; Damgaard,Hüffel '87]

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \, \mathcal{O}[\phi] \, \mathrm{e}^{-S[\phi]} \equiv \underbrace{\int \mathcal{D}\phi \, \mathcal{O}[\phi] \, P[\phi]}$$

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KEY IDEA:

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

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

fictitious Langevin time
(not physical)

noise term

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

stochastic quantization

[Parisi,Wu '81; Damgaard,Hüffel '87]

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \, \mathcal{O}[\phi] \, \mathrm{e}^{-S[\phi]} \equiv \int \mathcal{D}\phi \, \mathcal{O}[\phi] \, P[\phi]$$

KEY IDEA:

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

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

stochastic quantization

[Parisi,Wu '81; Damgaard,Hüffel '87]

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \, \mathcal{O}[\phi] \, \mathrm{e}^{-S[\phi]} \equiv \int \mathcal{D}\phi \, \mathcal{O}[\phi] \, P[\phi]$$

complex action $\longrightarrow$ complex Langevin equation

[Parisi '83; Klauder '84; Koonin,Adami '01; Berges,Stamatescu '05; Aarts '08; LR,Porter,Drut,Braun '17; LR,Loheac,Drut,Braun '18; Berger et al. '19]

$$\phi_R^{(n+1)} = \phi_R^{(n)} - \mathrm{Re}\left[\frac{\delta S[\phi]}{\delta \phi}\right] \Delta t_L + \sqrt{2 \Delta t_L}\,\eta$$

$$\phi_I^{(n+1)} = \phi_I^{(n)} - \mathrm{Im}\left[\frac{\delta S[\phi]}{\delta \phi}\right] \Delta t_L$$

however...

complex probabilities

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

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

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

complex probabilities & possible issues

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

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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; '20]

take home: the sign problem & CL

the sign problem is hard to solve,
most likely there is no generic solution

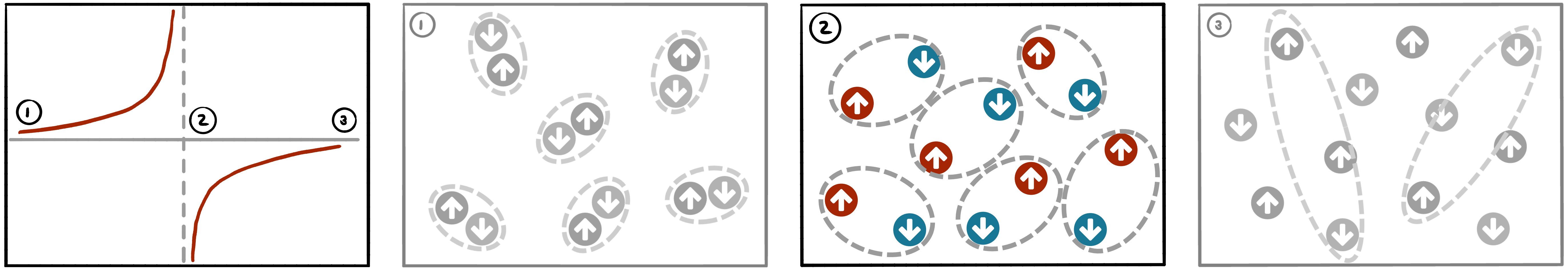
complex Langevin is a versatile approach
that works for some theories (but fails for others)

the unitary Fermi gas (UFG)

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

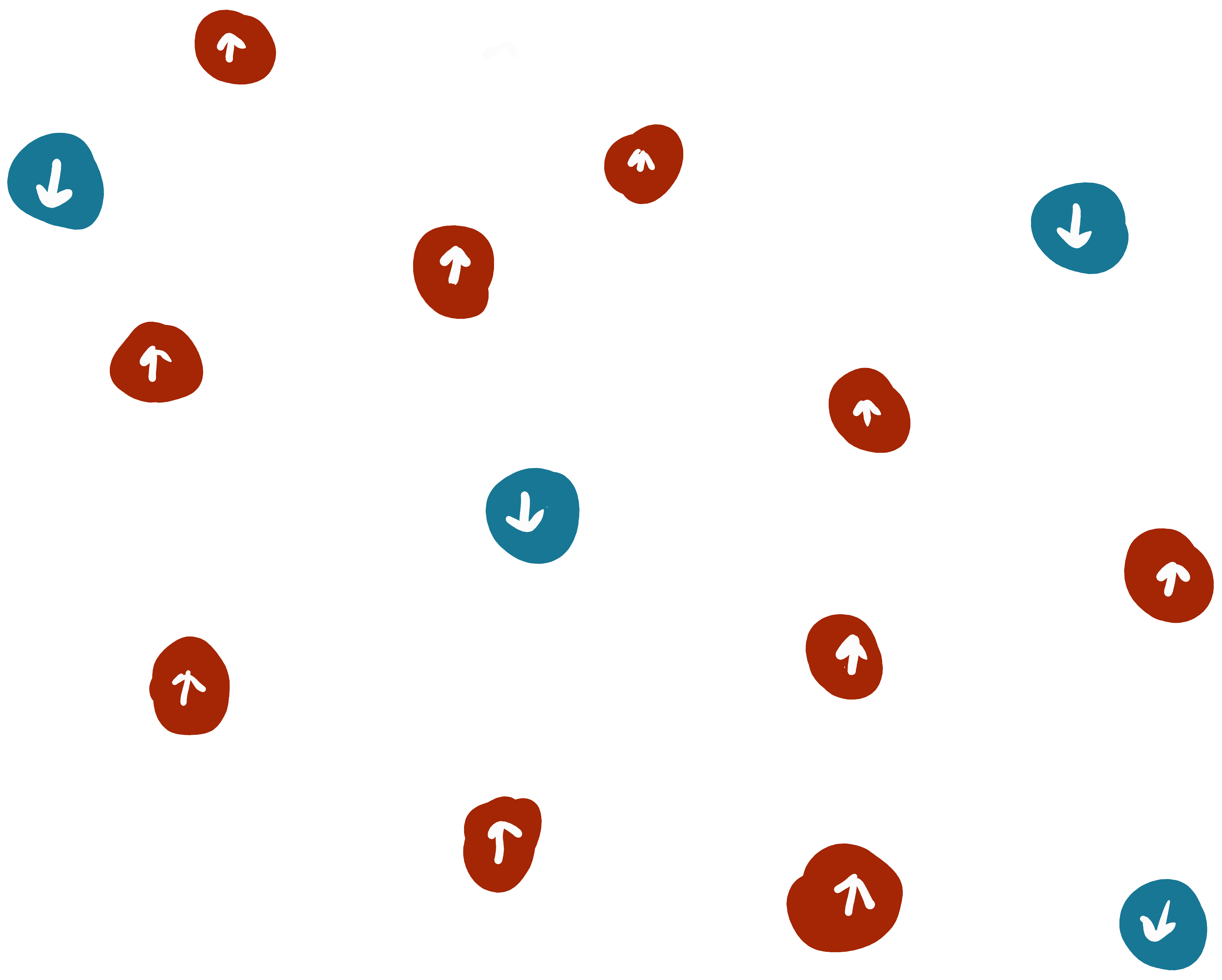
$$a_S \gg n^{-1/3} \gg r_0$$

- **universal behavior:** physical properties insensitive to microscopic details of the interaction
- experimentally realized with Feshbach resonances
  [Regal,Greiner,Jin '04; Zwierlein et al. '04; Kinast et al. '04; Shin,Schunck,Schirotzek,Ketterle '08; Chin,Grimm,Julienne,Tiesinga '10; Nascimbène et al. '10; van Houcke et al. '12; Ku,Sommer,Cheuck,Zwierlein '12; Carcy et al. '19; Mukherjee et al. '19; ...]



the spin-polarized UFG

[Chevy,Mora '10; Radzihovsky,Sheehy '10; Gubbels,Stoof '13]



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temperature

polarization

the spin-polarized UFG

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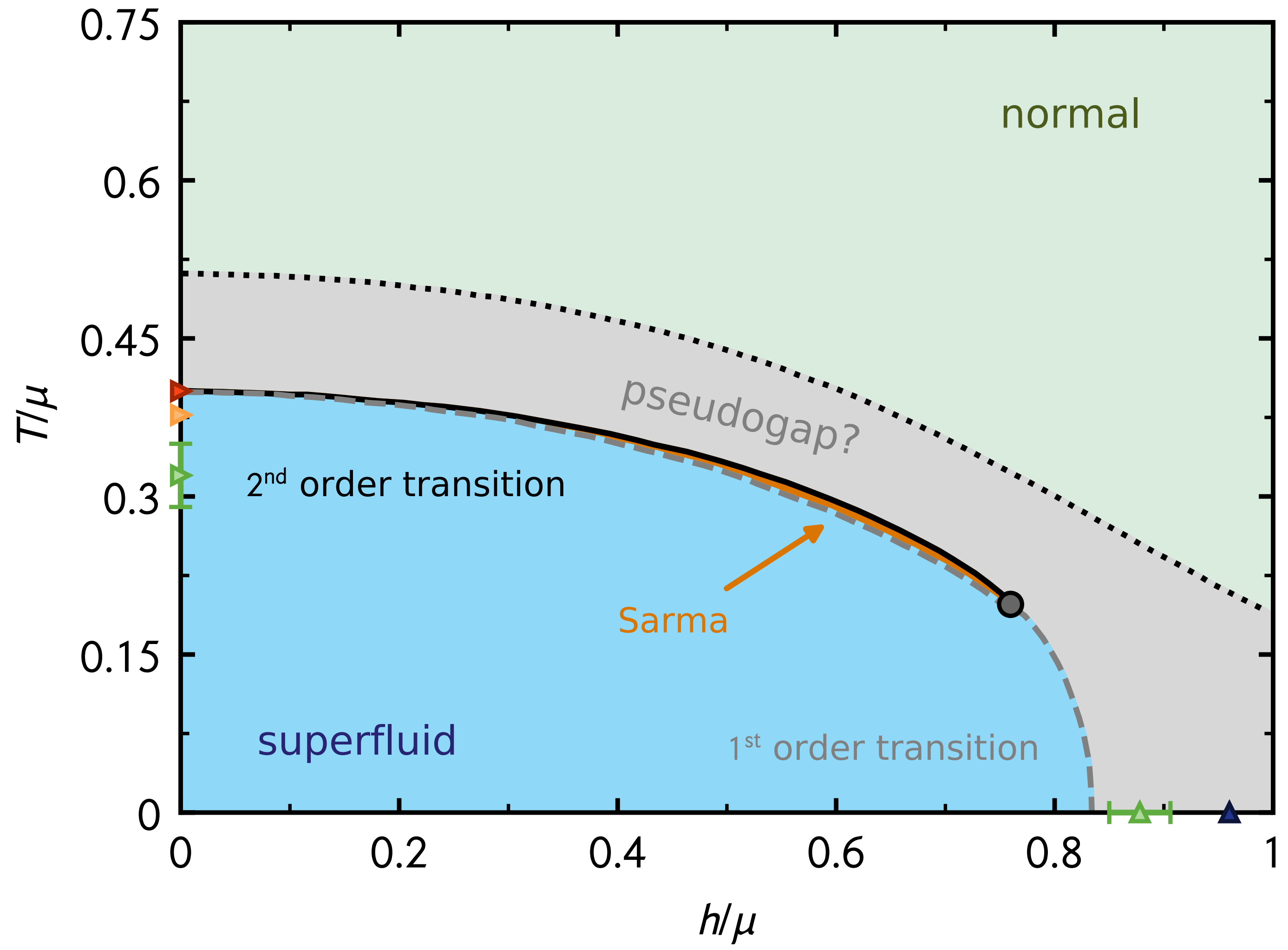
[Fulde,Ferell '64; Larkin,Ovchinnikov '65;
Sarma '63; Liu,Wilczek '03; Bulgac,Forbes,Schwenk '06]

[Combescot,Recati,Lobo,Chevy '07;
Schirotzek,Wu,Sommer,Zwierlein '09;
Nascimbène et al. '10; Yan et al. '19]

temperature

polarization

the grand canonical description



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

$$= \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N}-h\hat{M})}\right]$$

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

[fRG: Boettcher et al. '15]
[balanced T_c: Ku,Sommer,Cheuck,Zwierlein '12;
Nascimbene et al. '10; Nascimbene et al. '11]

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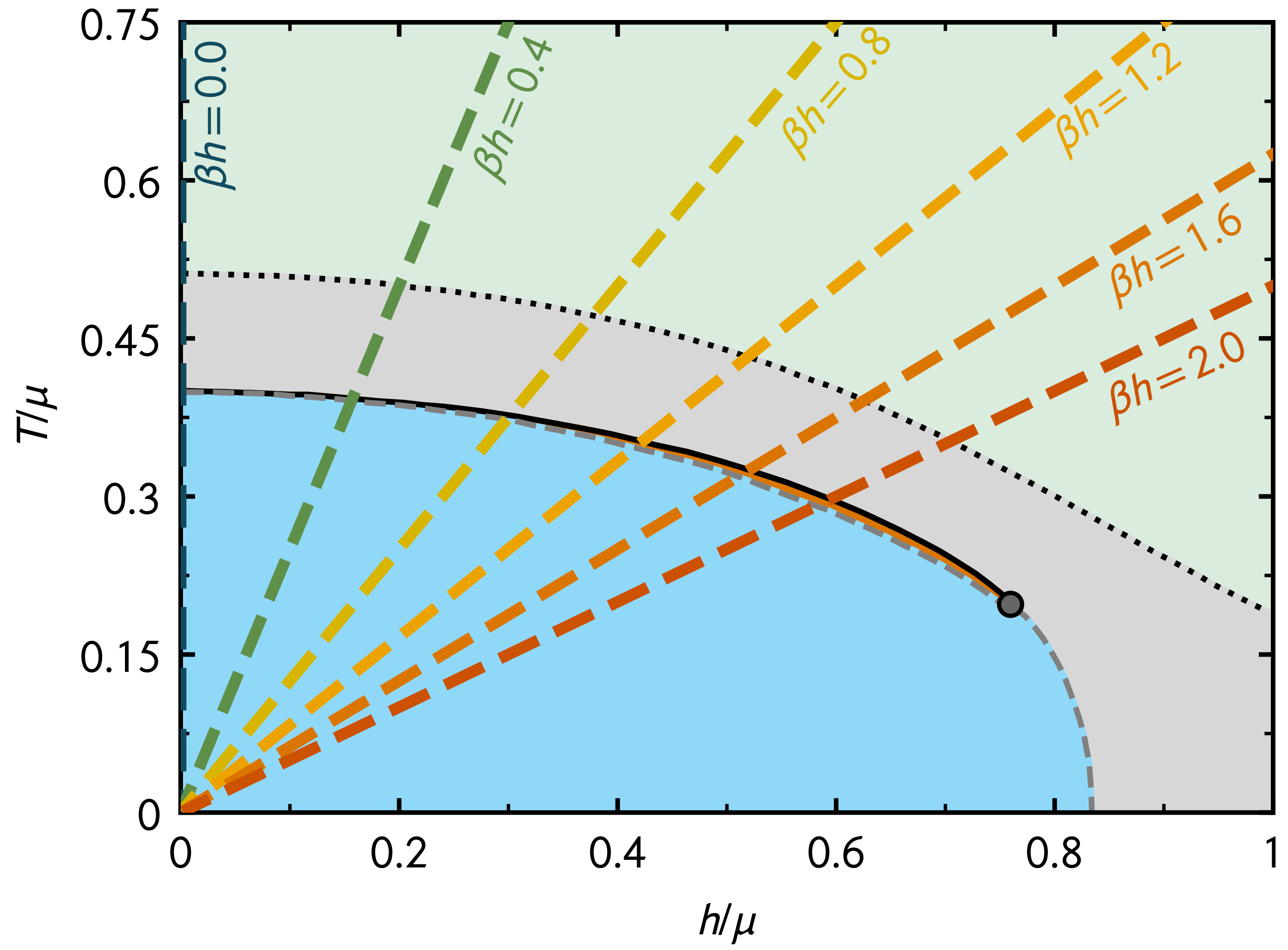

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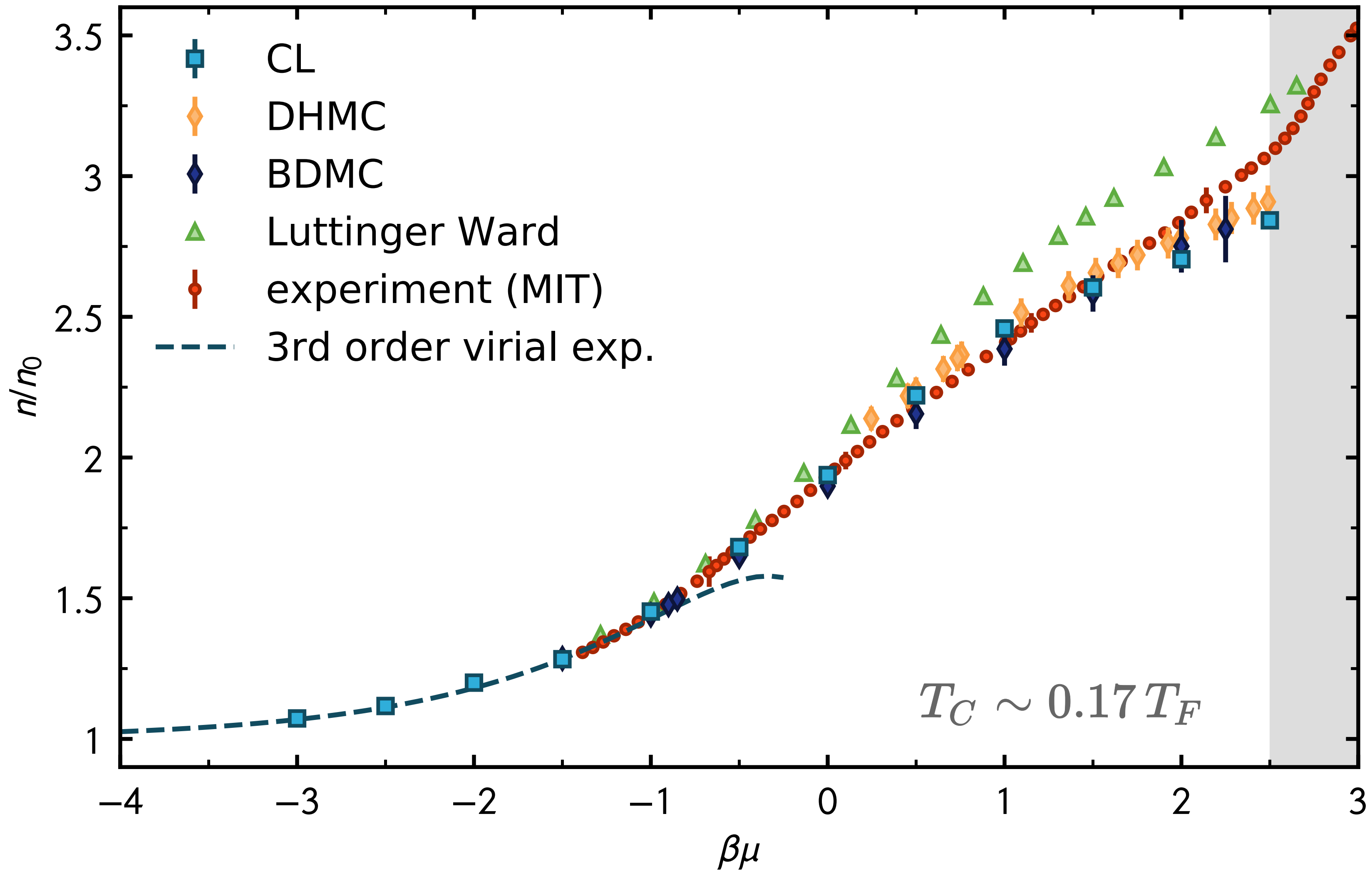
density equation of state

[LR,Loheac,Drut,Braun '18]

[experiment/BDMC: van Houcke et al. '12]
[DHMC: Drut,Lähde,Wlazlowski,Magierski '12]
[Luttinger-Ward: Frank,Lang,Zwerger '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

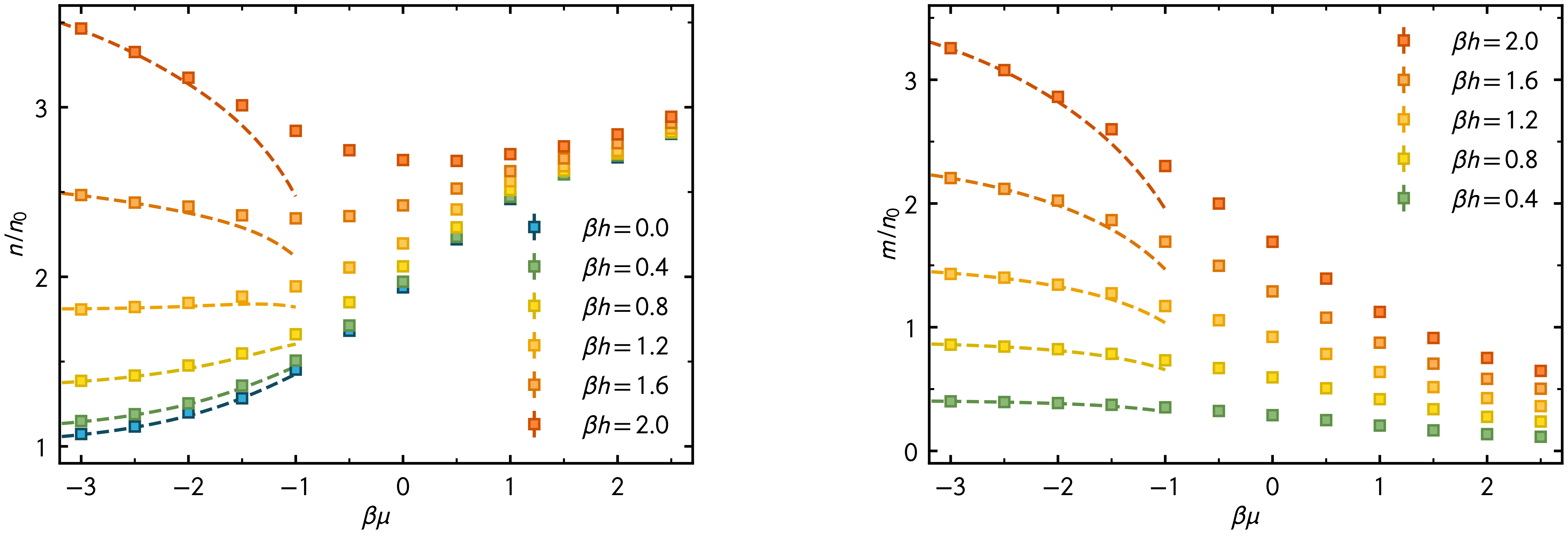
E_F dominates

density & magnetization EOS (polarized)

[LR,Loheac,Drut,Braun '18]

$$n = n_\uparrow + n_\downarrow = \frac{\partial \ln \mathcal{Z}}{\partial(\beta\mu)}$$

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



experimentally testable predictions!

more thermodynamics

[Ho '04; Pathria,Beale '12]

density & magnetization equations of state

$$n(\beta\mu, \beta h) = \frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial(\beta\mu)}$$

$$m(\beta\mu, \beta h) = \frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial(\beta h)}$$

pressure & energy

$$P(\beta\mu) = \frac{1}{\beta} \int_{-\infty}^{\beta\mu} n(x)\, dx \qquad E = \frac{3}{2} PV$$

compressibility & specific heat

$$\kappa_{\mathrm{T}} = \frac{1}{n} \left[\frac{\partial n}{\partial P}\right]_{\beta h, T, V} \qquad C_{\mathrm{V}}/N = \left[\frac{\partial E}{\partial T}\right]_{N,V}$$

spin susceptibility

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

more thermodynamics

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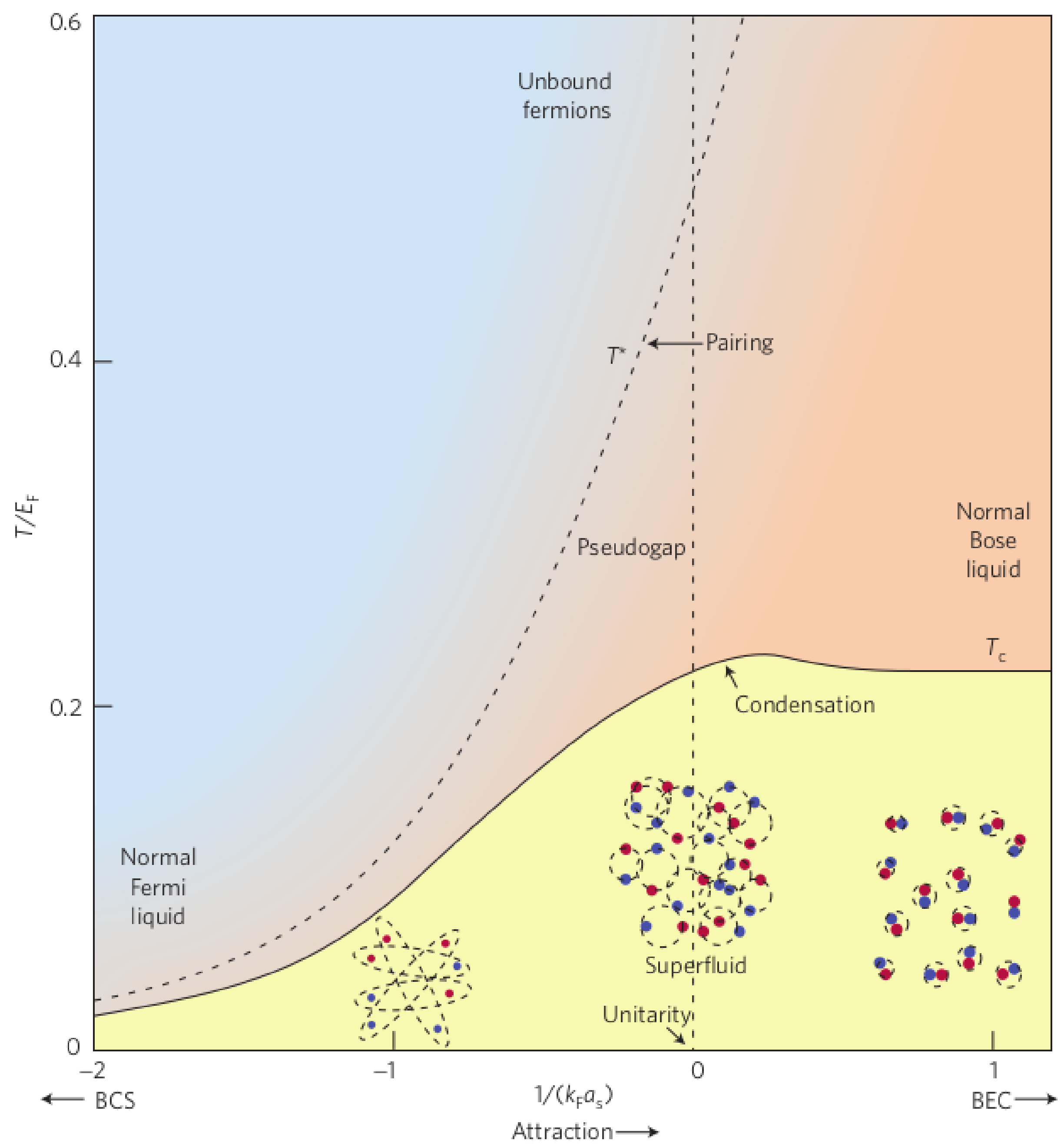
pairing above the critical temperature

[pseudogap reviews: Chen,Wang '14; Mueller '17; Jensen,Gilbreth,Alhassid '19]



[BCS-BEC phase diagram (sketch): Randeria '10]

- a pseudogap regime predicts pre-formed pairs already above the superfluid phase at $T^* > T_C$
- theoretical and experimental studies predict varying scenarios

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

- pseudogap: would cause a suppression of χ for $T > T_C$

[Randeria,Trivedi,Moreo,Scalettar '92; Trivedi,Randeria '95]

spin susceptibility (unpolarized)

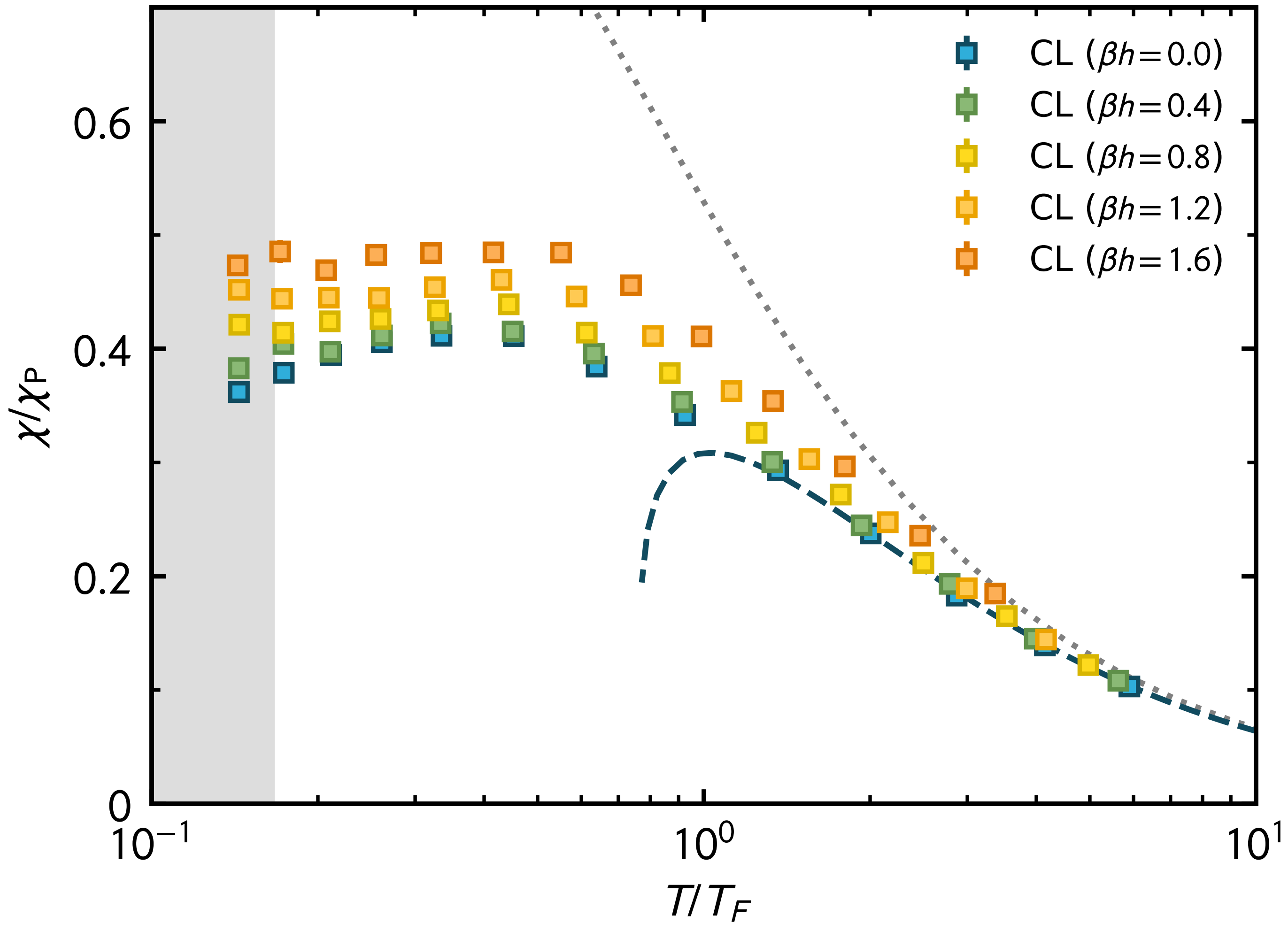
[LR,Loheac,Drut,Braun *in preparation*]

- high temperature: Curie's law $\chi \propto T^{-1}$
- theory & experiment agree at high temperature
- **low temperature: discrepancy between experiment and theory**
- no clear suppression of χ above critical temperature
- **CL results suggest that T^* and T_C appear to be very close, if not identical**

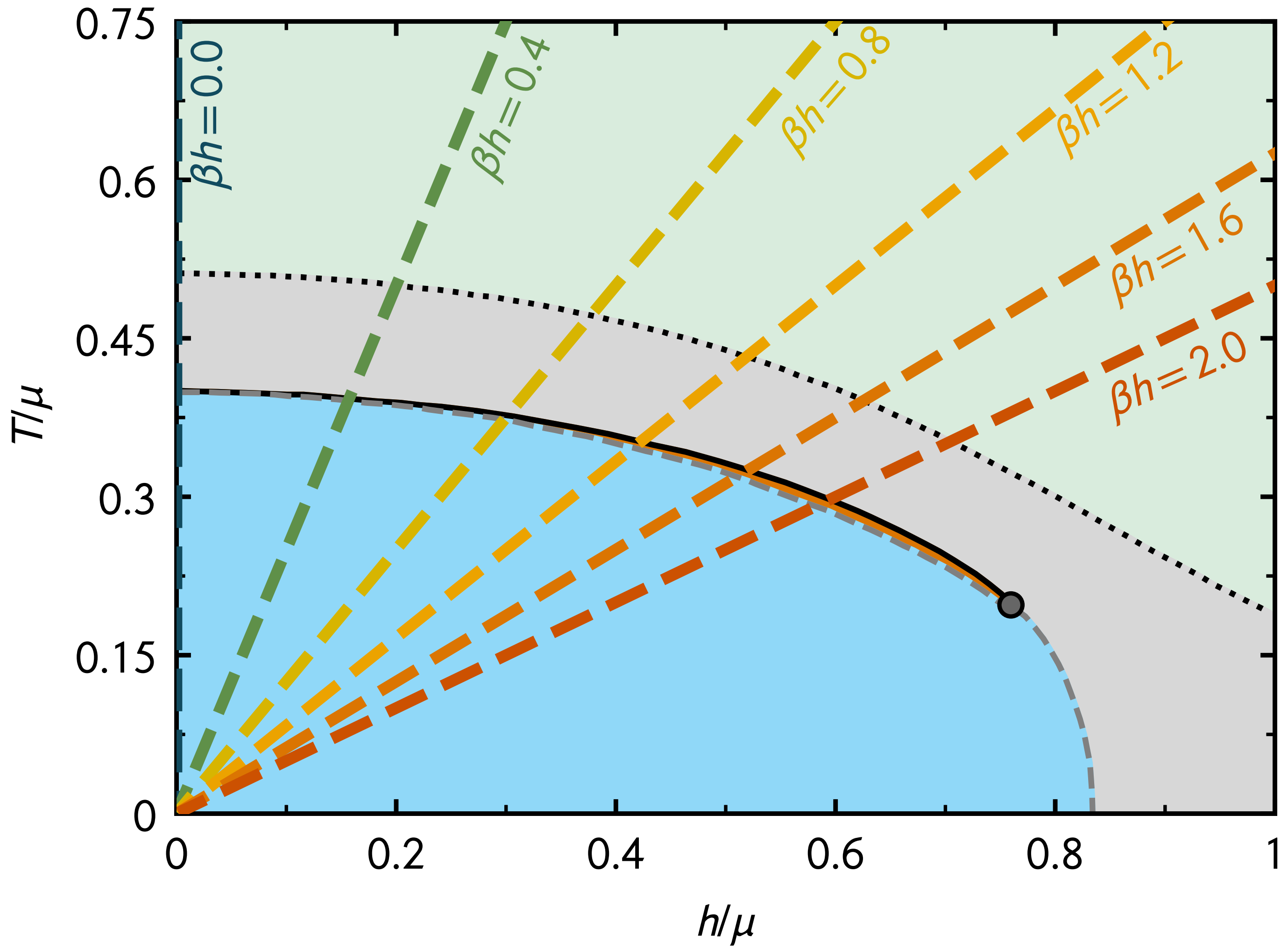
[recent review: Jensen,Gilbreth,Alhassid '19]

spin susceptibility (polarized)

[LR,Drut,Braun *in preparation*]



[fRG: Boettcher et al. '15]



CL suggests a small difference in T_C and T^* for all polarizations studied

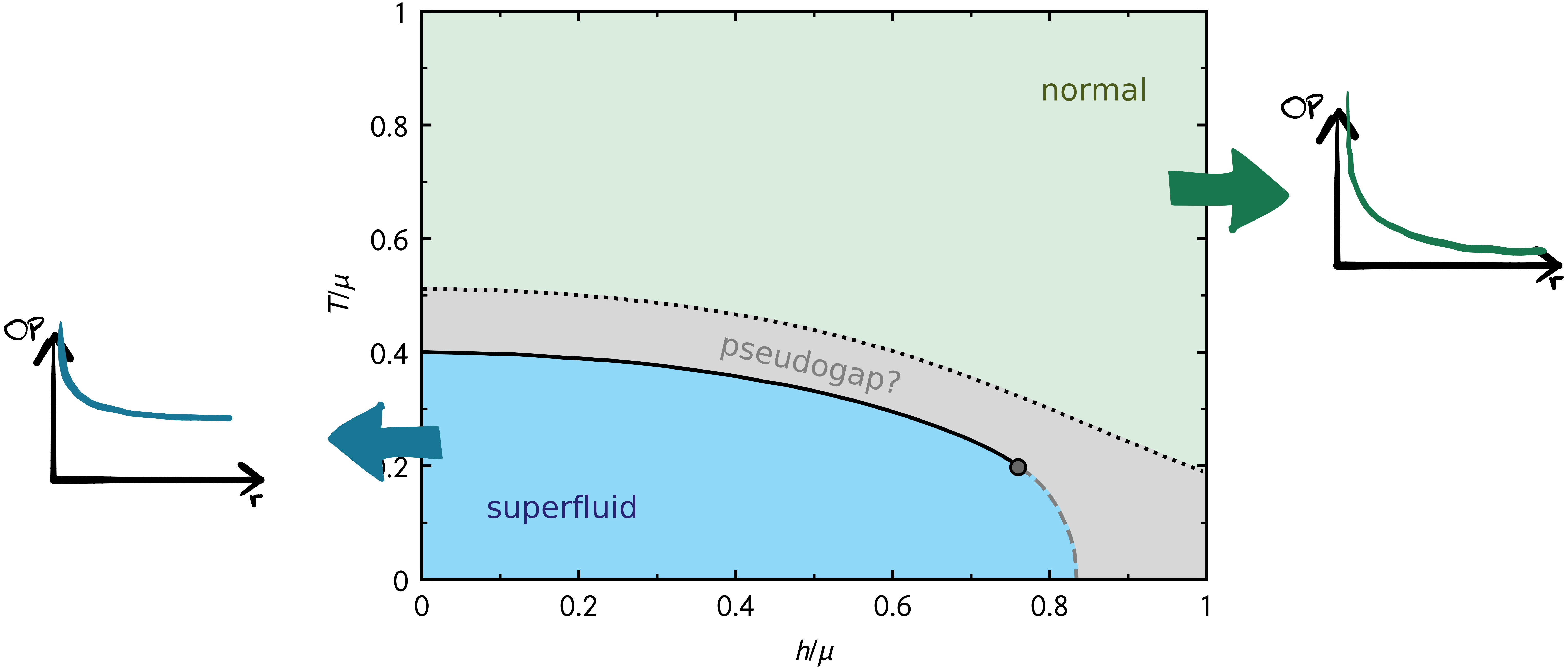
recap: 3D unitary fermions

CL delivers accurate thermodyamic quantities for the
unitary Fermi gas at finite temperature and polarization

provides experimentally testable predictions
for previously inaccessible quantities

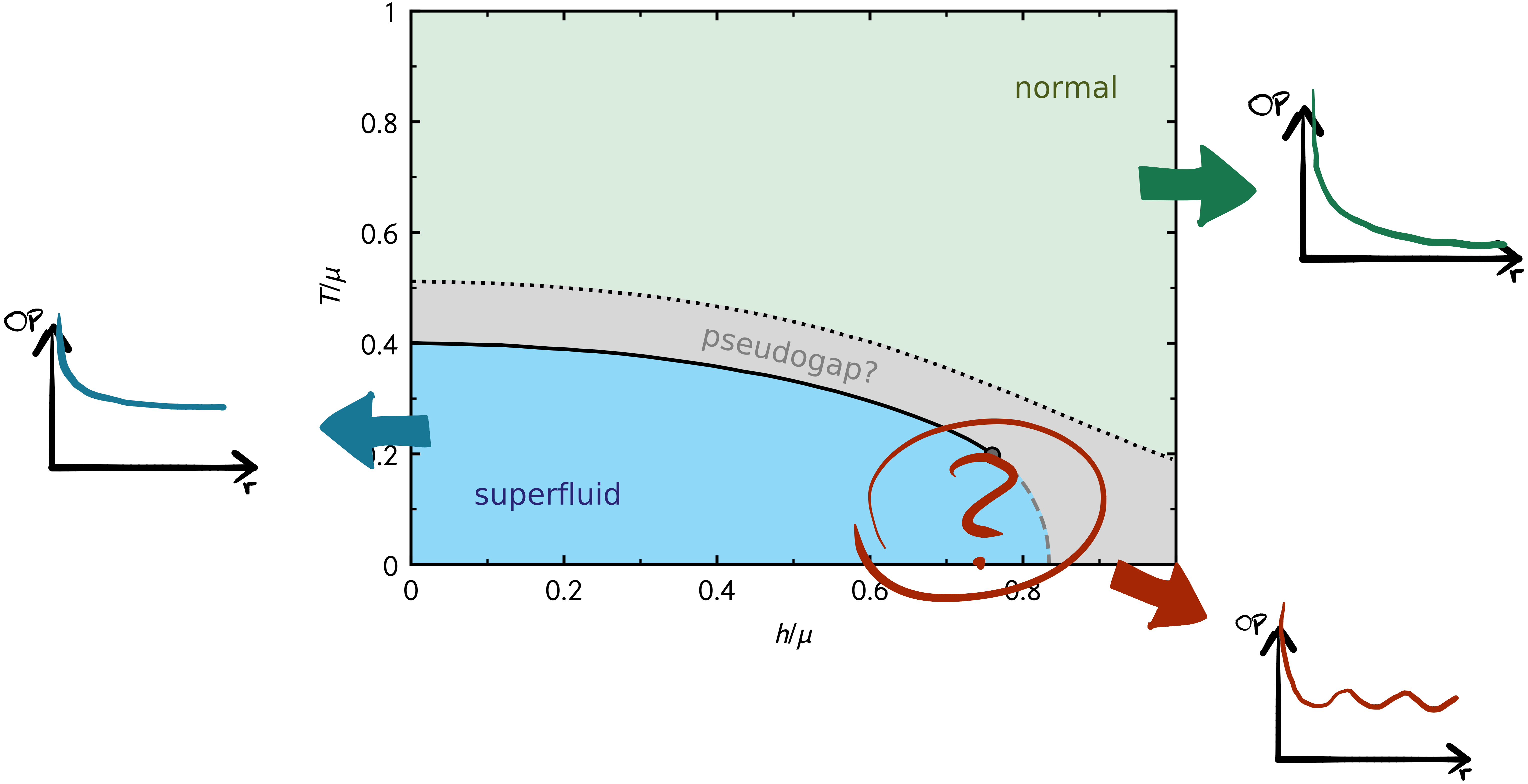
UFG phase diagram

[fRG PD: Boettcher et al. '15]



UFG phase diagram

[fRG PD: Boettcher et al. '15]



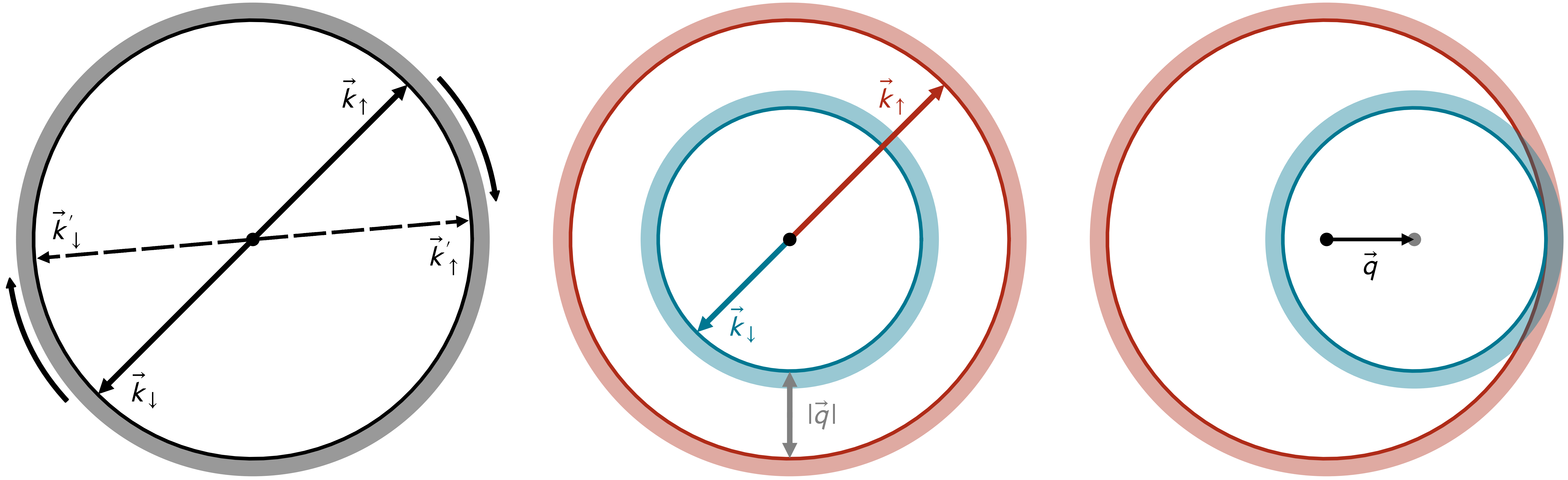
spin-polarized 1D fermions

[Feiguin,Heidrich-Meisner,Orso,Zerger '12]

- (some) exact solutions available via **Bethe ansatz**
  [Guan,Batchelor,Lee '13]
- **FFLO type pairing** stable in a wide parameter range
  [Lüscher,Noack,Läuchli '08]
- no true long-range order in 1D, **polynomial decay of correlation functions:**

$$|C(r)| \propto r^{-\Delta}$$

pairing (schematically in 2D)

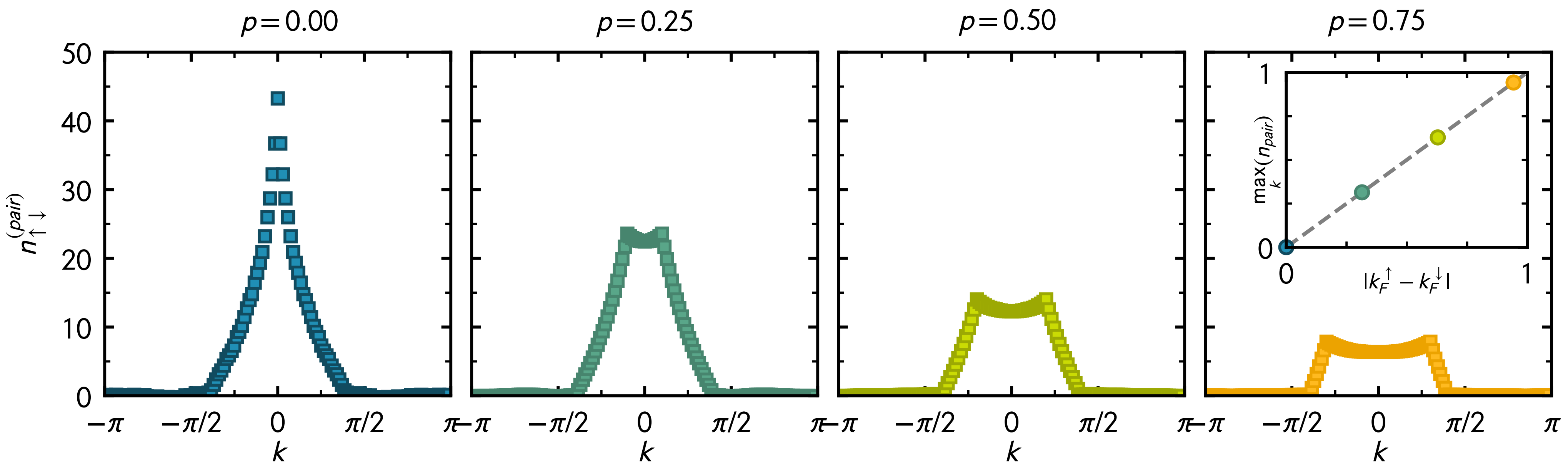


pair correlations

[LR, Drut, Braun in preparation]

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

~ likelihood to find a pair with momentum $\boldsymbol{k}$



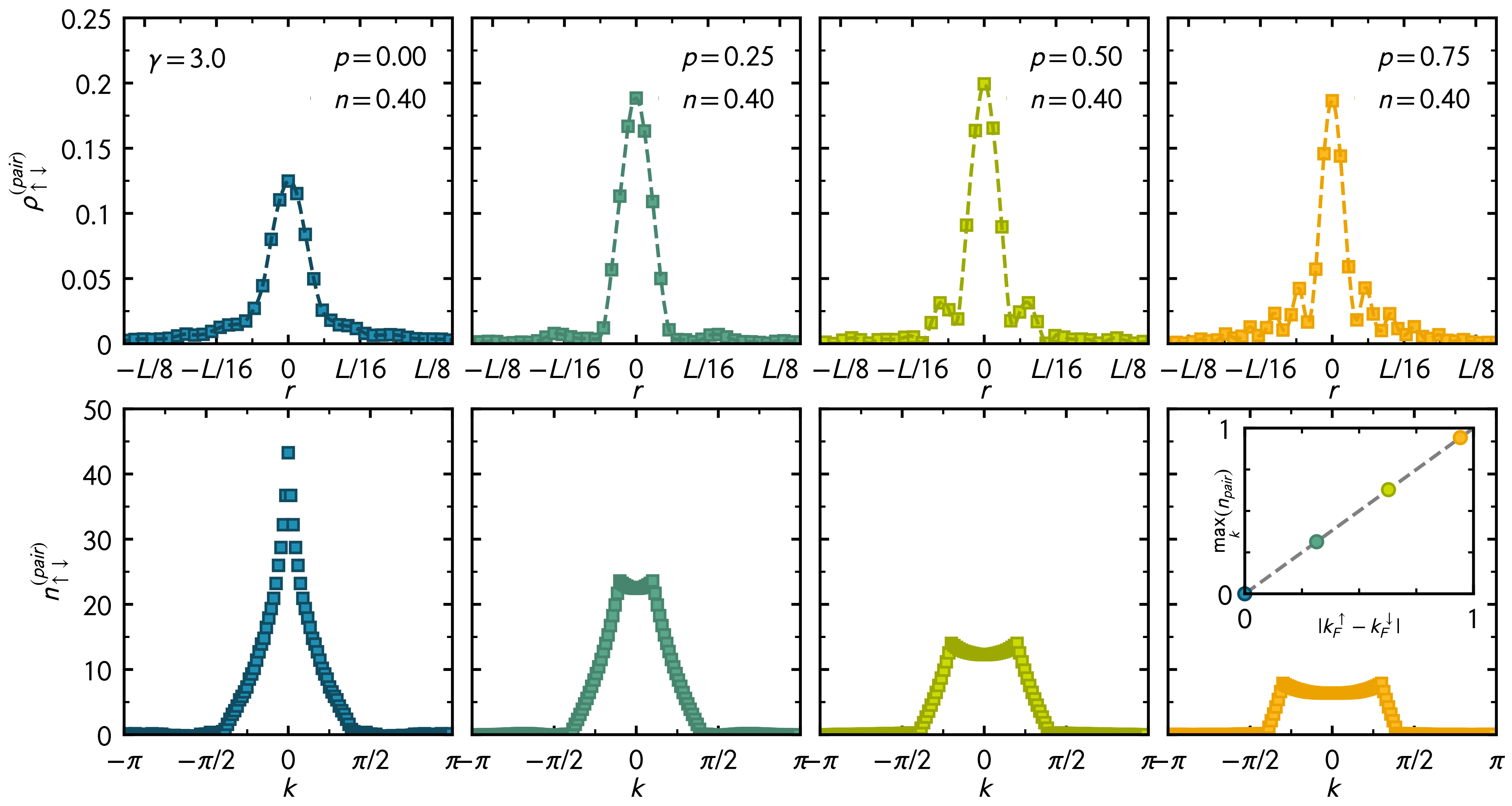
$$p = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

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

pair correlations

[LR, Drut, Braun in preparation]

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



spatially fluctuating "order parameter"

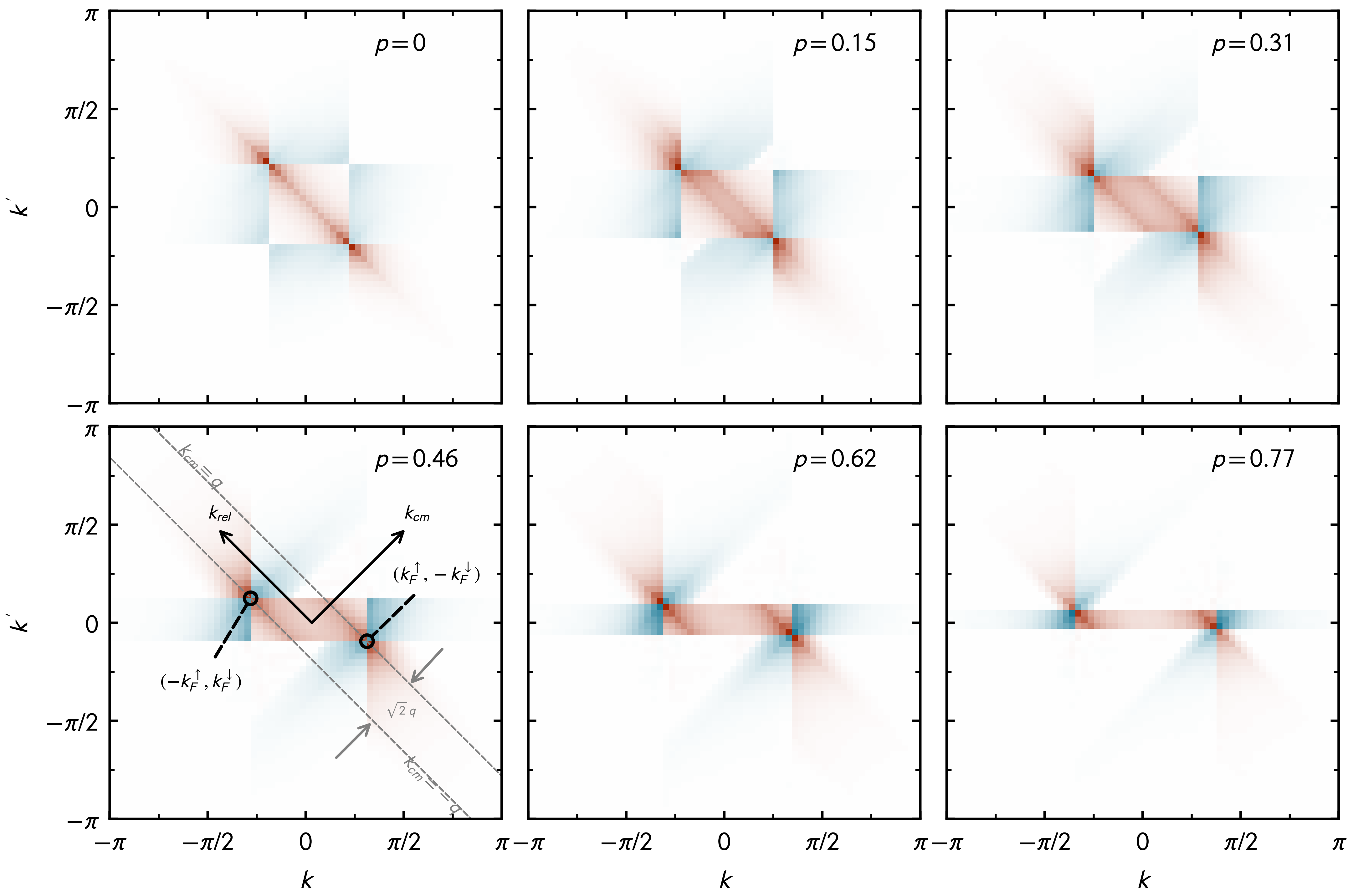
~ likelihood to find a pair with momentum $\boldsymbol{k}$

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

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

density-density correlation (shot noise)

[LR, Drut, Braun in preparation]



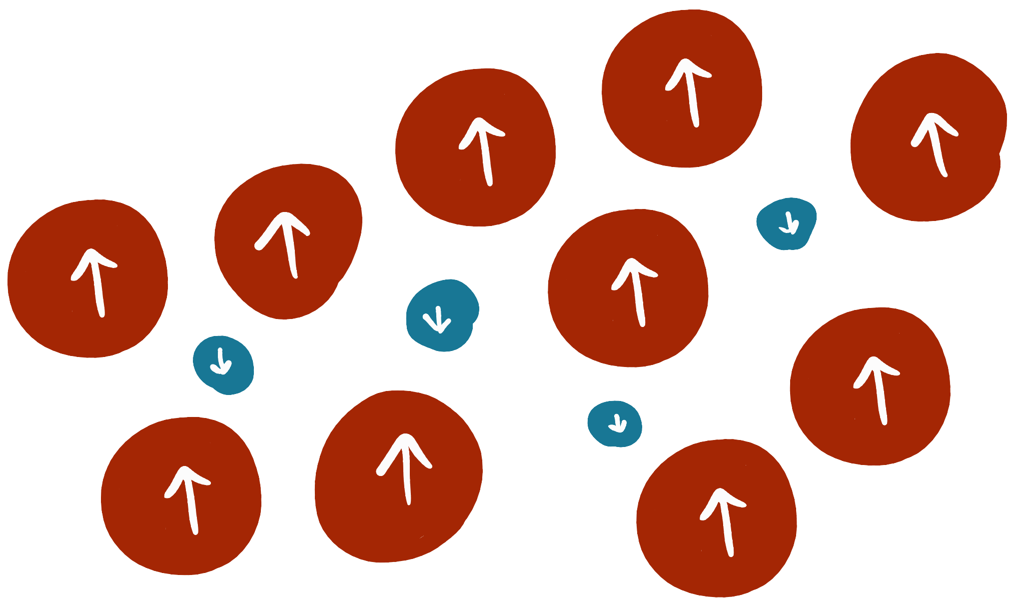
$$n_{\uparrow\downarrow}(k,k') = \langle \hat{\psi}^\dagger_{k\uparrow}\,\hat{\psi}_{k\uparrow}\hat{\psi}^\dagger_{k'\downarrow}\,\hat{\psi}_{k'\downarrow}\rangle - \langle \hat{\psi}^\dagger_{k\uparrow}\,\hat{\psi}_{k\uparrow}\rangle\langle \hat{\psi}^\dagger_{k'\downarrow}\,\hat{\psi}_{k'\downarrow}\rangle$$

resolution of **momentum structure** of fermion pairs

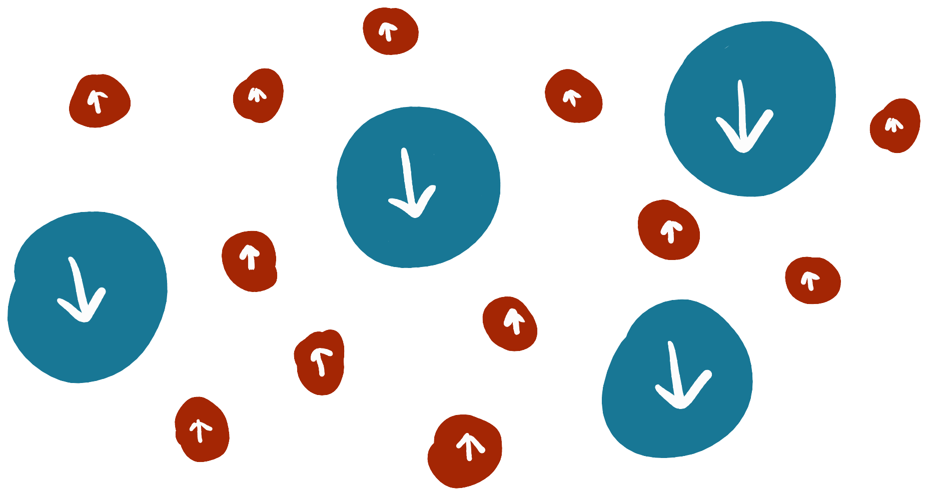
positive correlations: particle-particle
negative correlations: particle-hole

the effect of mass-imbalance

- **not** integrable via Bethe ansatz
- mass-imbalance parameter: $\boldsymbol{\kappa} = \frac{m_\uparrow}{m_\downarrow}$



heavy majority

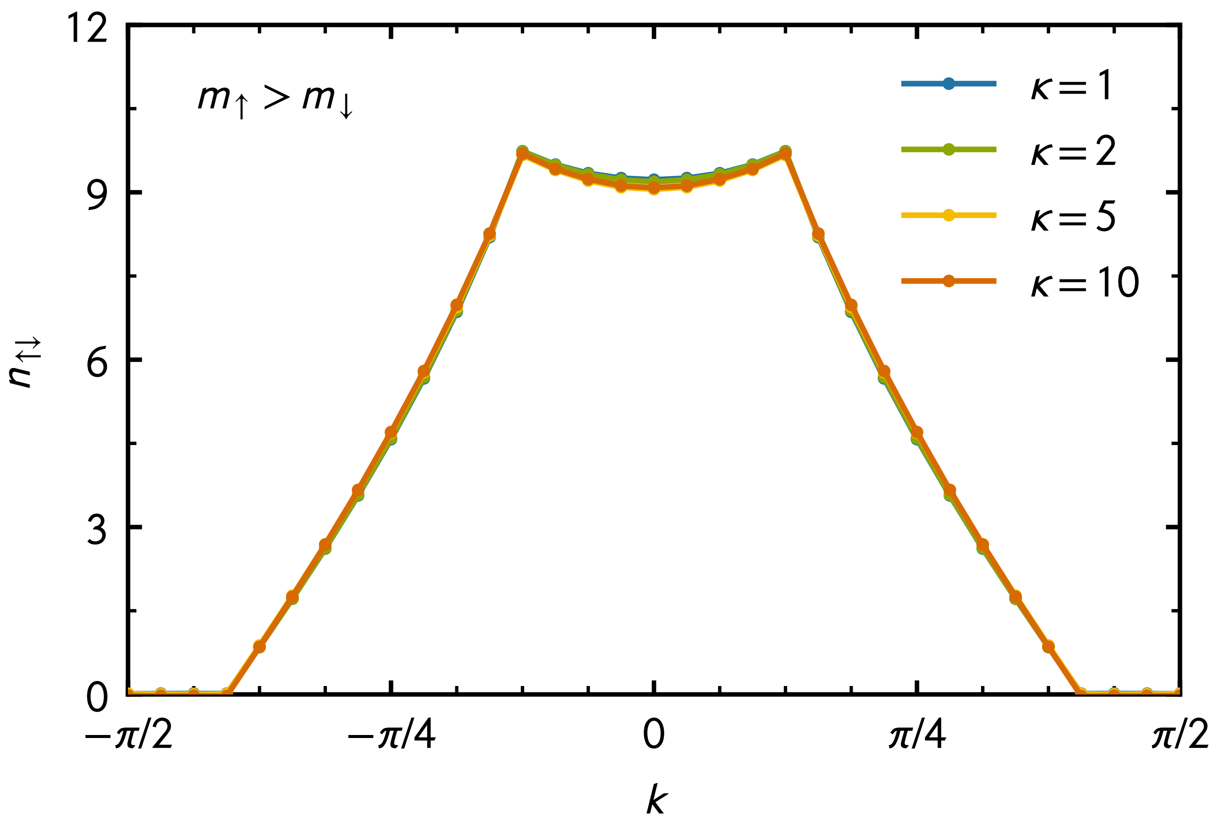


heavy minority

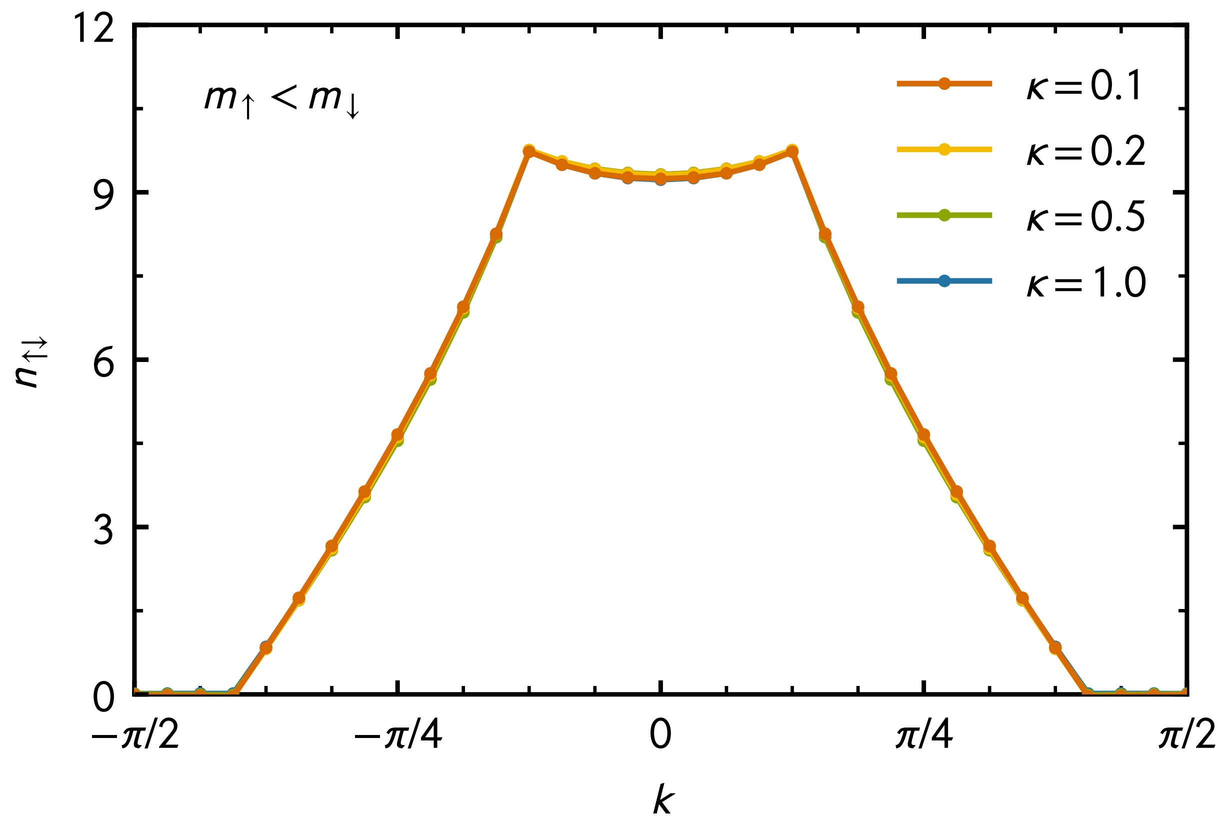
the effect of mass-imbalance

[LR,Drut,Braun in preparation]

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



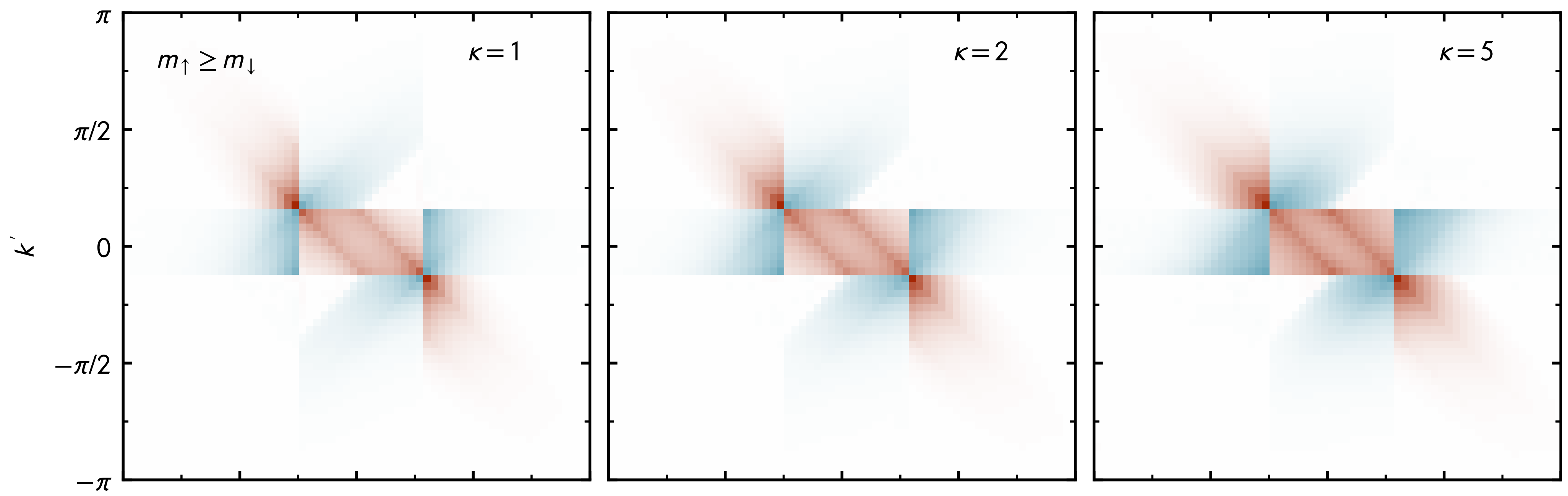
heavy majority



heavy minority

shot noise for mass-imbalanced systems

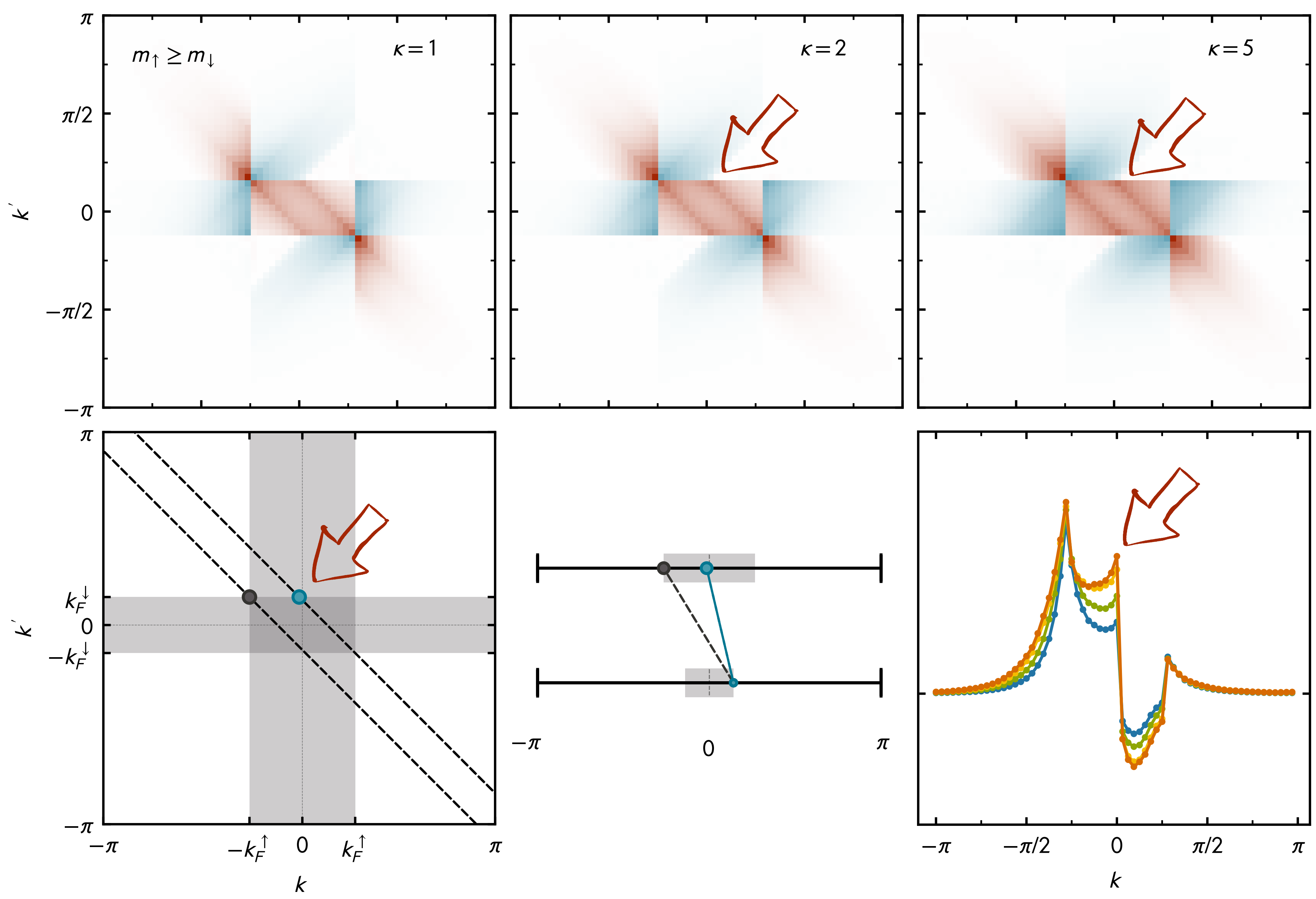
[LR,Drut,Braun in preparation]



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

shot noise for mass-imbalanced systems

[LR,Drut,Braun in preparation]



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

mass-imbalance **does not destroy FFLO ordering**

occurrence of **additional peaks** with $|k_{cm}| = |q|$

recap

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

stay tuned!

extension of shot-noise anlalysis to 2D/3D Fermi gases
(observable in experiment?)

thermodynamics of mass-imbalanced unitary Fermions
(possible FFLO stabilization?)

attack FFLO type pairing with continuous-space methods
(diagrammatic MC?)

team CL

Jens Braun | Florian Ehmann | Joaquin Drut | Andrew Loheac







Juliane Helbich | LR (now LMU) | Josh McKenney | Casey Berger

TU Darmstadt

UNC Chapel Hill

appendix

interlude: the virial expansion

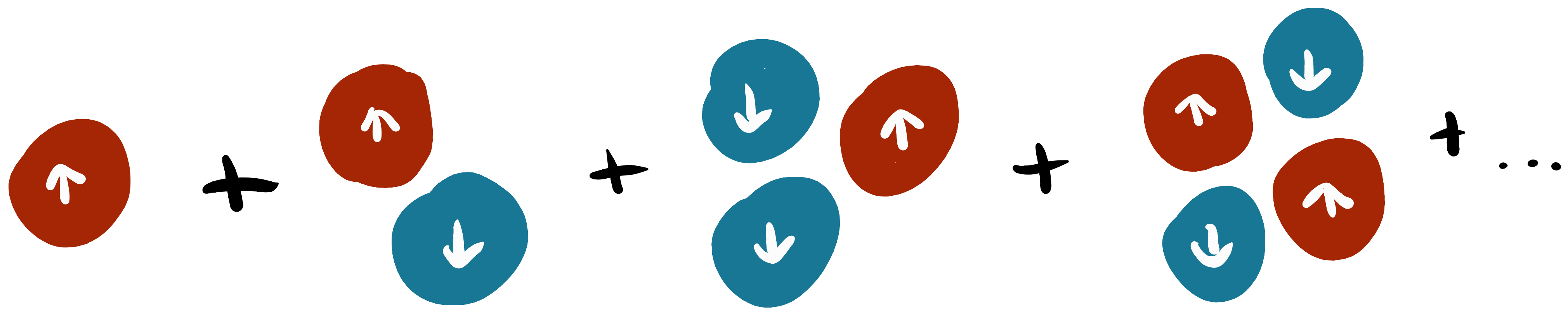
[Liu '13]

dilute gases: few-body correlations dominate

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

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

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

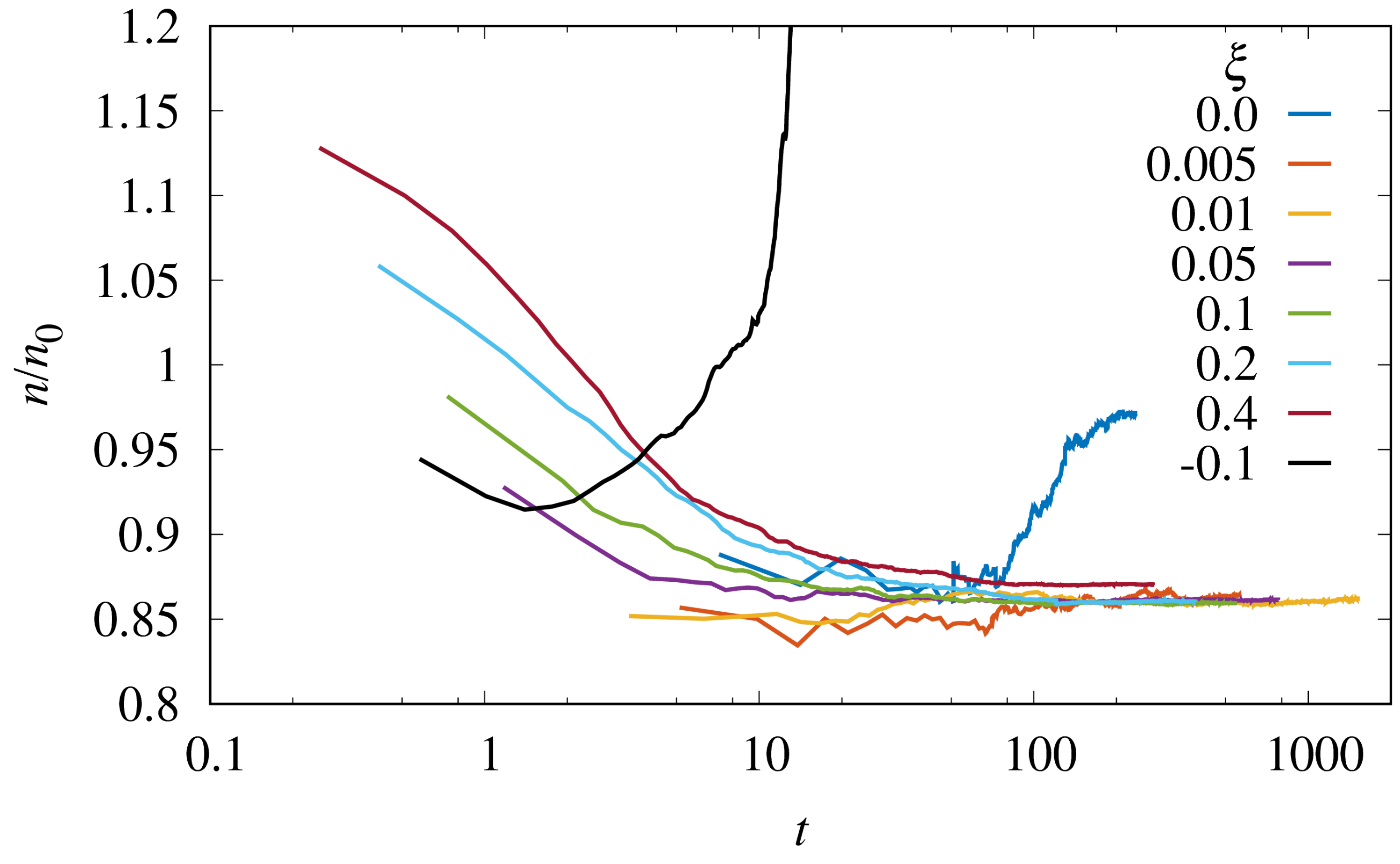


mass-term as "regulator"

[Loheac,Drut '17]

$$\phi_R^{(n+1)} = \phi_R^{(n)} - \mathrm{Re}\left[\frac{\delta S[\phi]}{\delta\phi}\right]\Delta t_L + \sqrt{2\Delta t_L}\,\eta \;+\; 2\xi\Delta t\phi_R^{(n)}$$

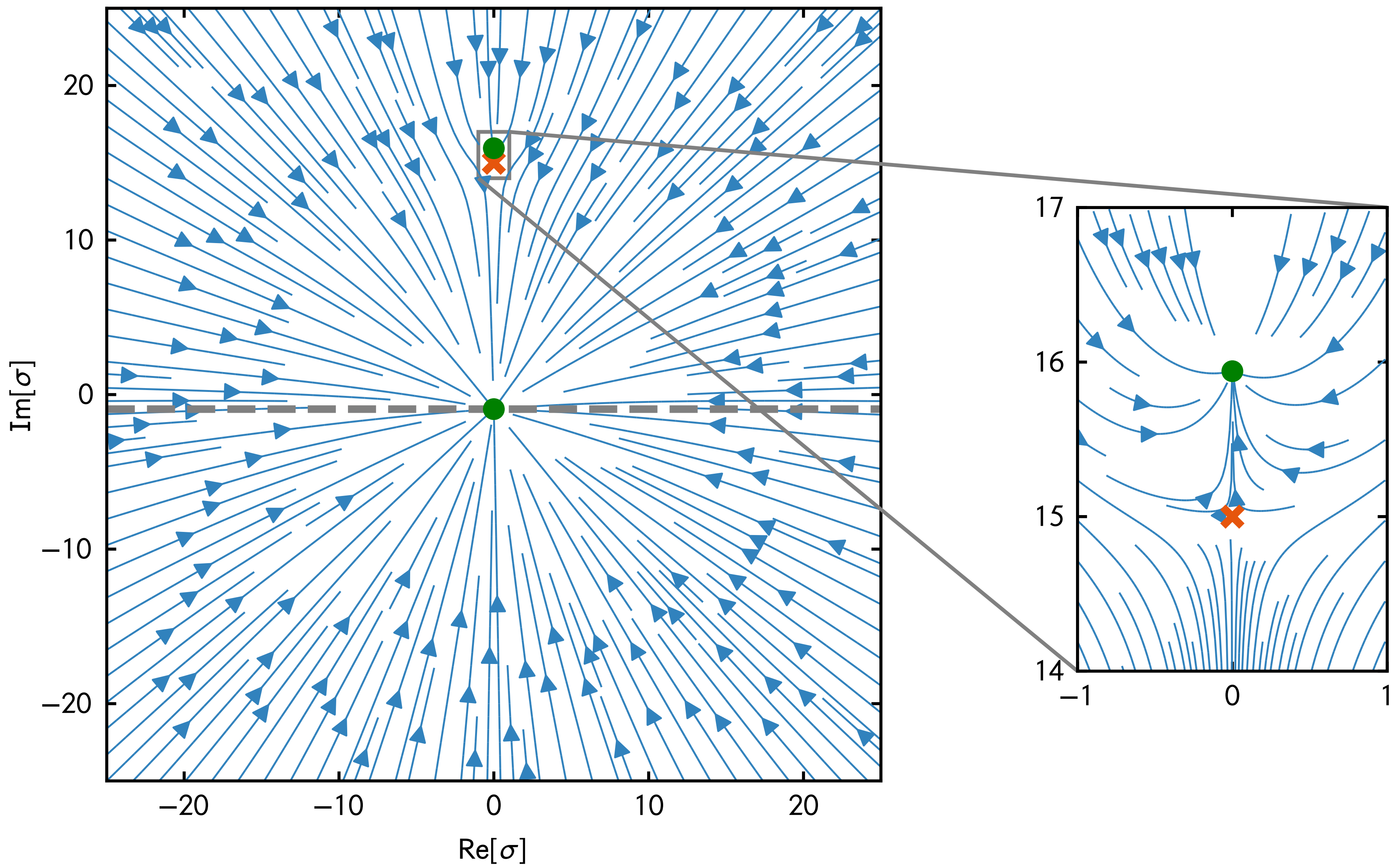
$$\phi_I^{(n+1)} = \phi_I^{(n)} - \mathrm{Im}\left[\frac{\delta S[\phi]}{\delta\phi}\right]\Delta t_L \;+\; 2\xi\Delta t\phi_I^{(n)}$$



- unregulated runs tend to fail: ξ **stabilizes CL trajectories**
- similar approach in QCD: "dynamic stabilization" [Attanasio,Jäger '18]

"classical" flow pattern

[Berger et al. '19]



$$\mathcal{Z} = \int \mathrm{d}\sigma\, \mathrm{e}^{-S(\sigma)} = \int \mathrm{d}\sigma\, \mathrm{e}^{-\left[\frac{\lambda}{24}\sigma^2 - \frac{1}{2}\log \frac{\lambda}{12\mu + 2\mathrm{i}\lambda\sigma}\right]}$$