Finite-size and Particle-number Effects in an Ultracold Fermi Gas at Unitarity

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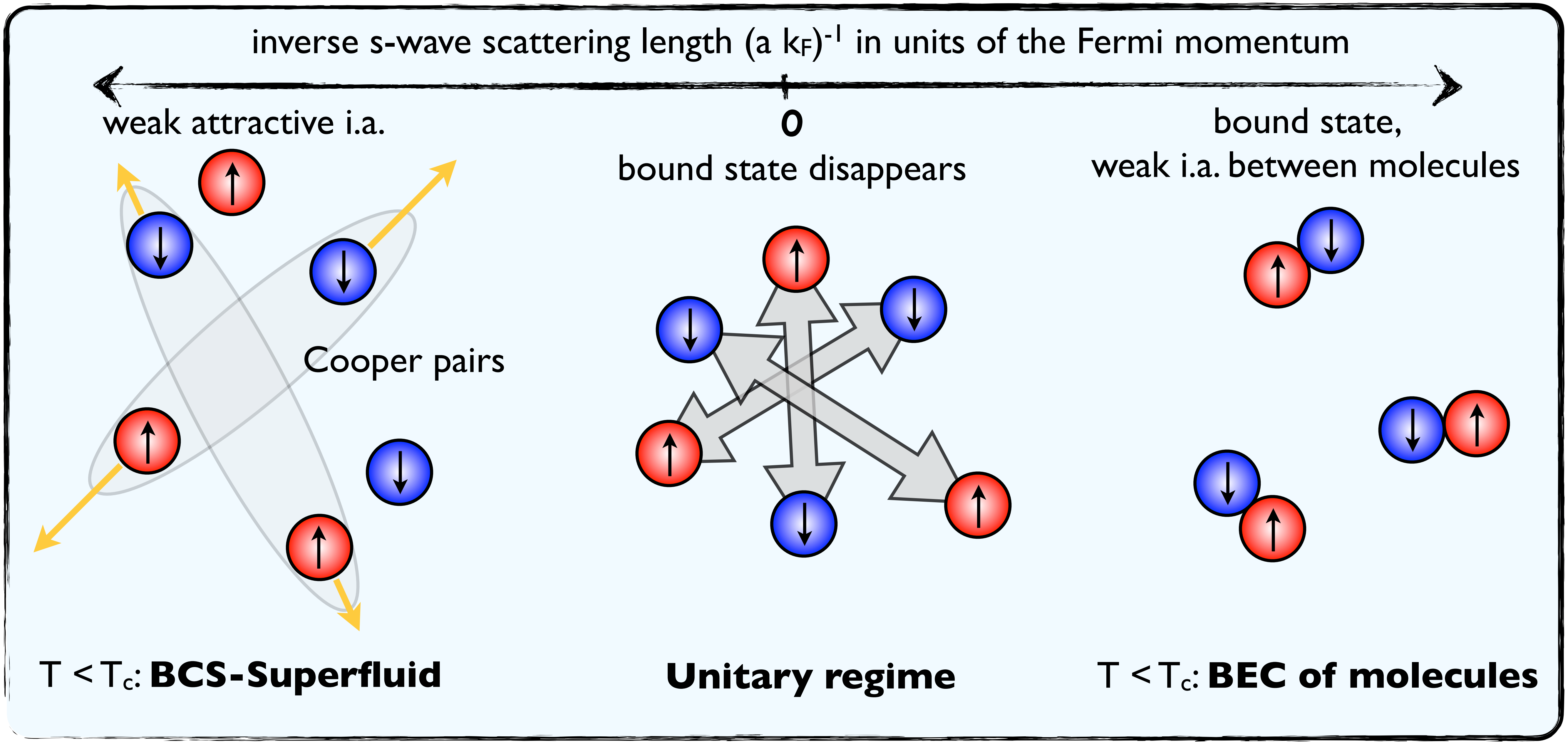
Outline

1. BCS-BEC Crossover: Basics and Phase diagram
2. Overview: FRG Studies of the BCS-BEC Crossover
3. Finite System Size Study
4. Conclusions & Outlook

1. BCS-BEC Crossover: Basics and Phase diagram

BCS-BEC Crossover: Basics

- Ultracold gases of fermionic atoms (^6Li, ^{40}K) → 2 accessible hyperfine spin states
- Spin-balanced case (for strong spin-imbalance, cf. talk by R. Schmidt)

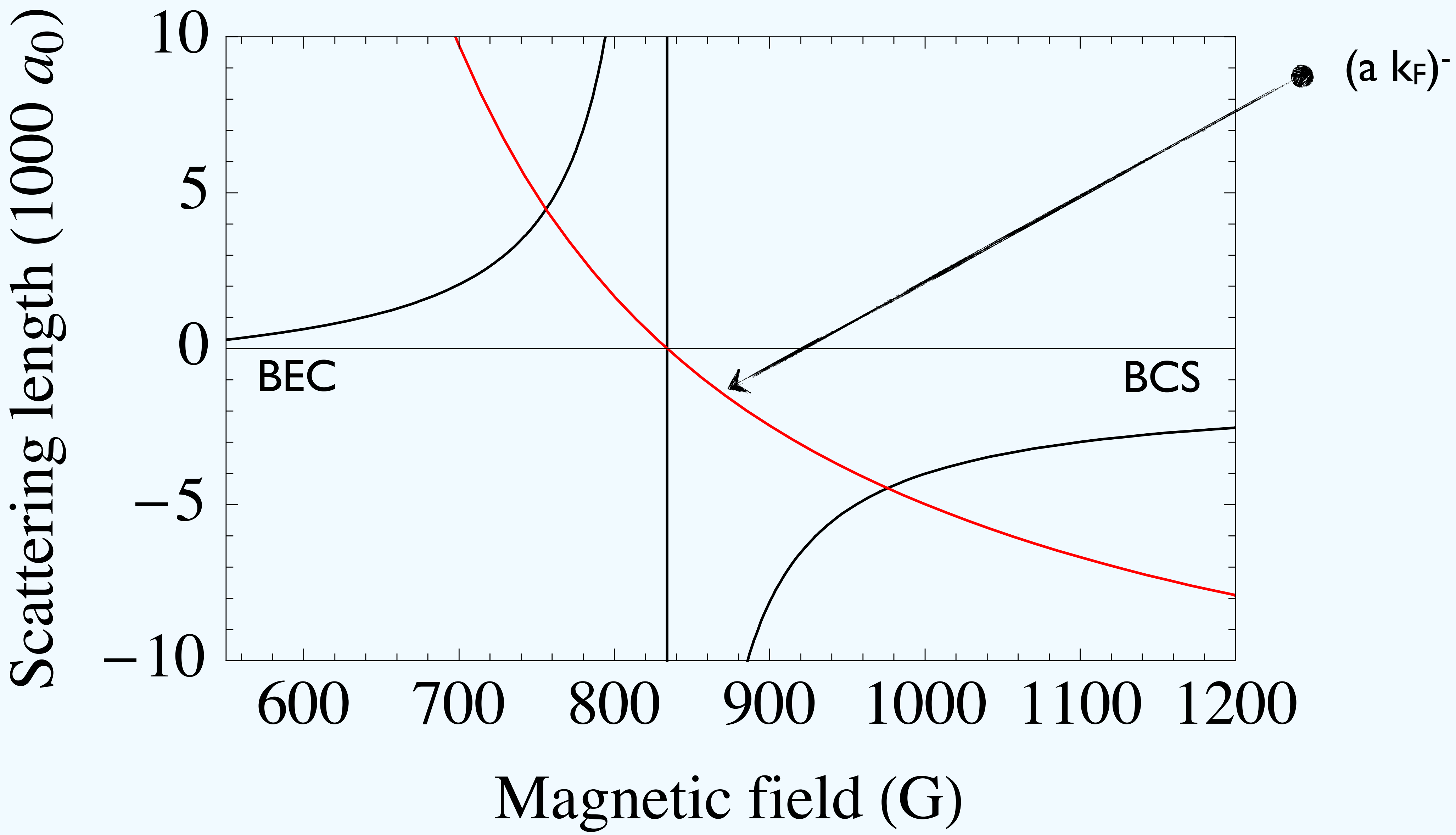


- $(a\,k_F)^{-1} < -1$: weakly attractive, Cooper pairing → below T_c : BCS superfluidity
- $(a\,k_F)^{-1} > \ \ 1$: two-body bound state, formation of molecules → below T_c : interacting BEC
- $|(a\,k_F)^{-1}| < 1$: strongly correlated regime, Unitarity limit at $(a\,k_F)^{-1} \to 0$

BCS-BEC Crossover: Feshbach Resonance

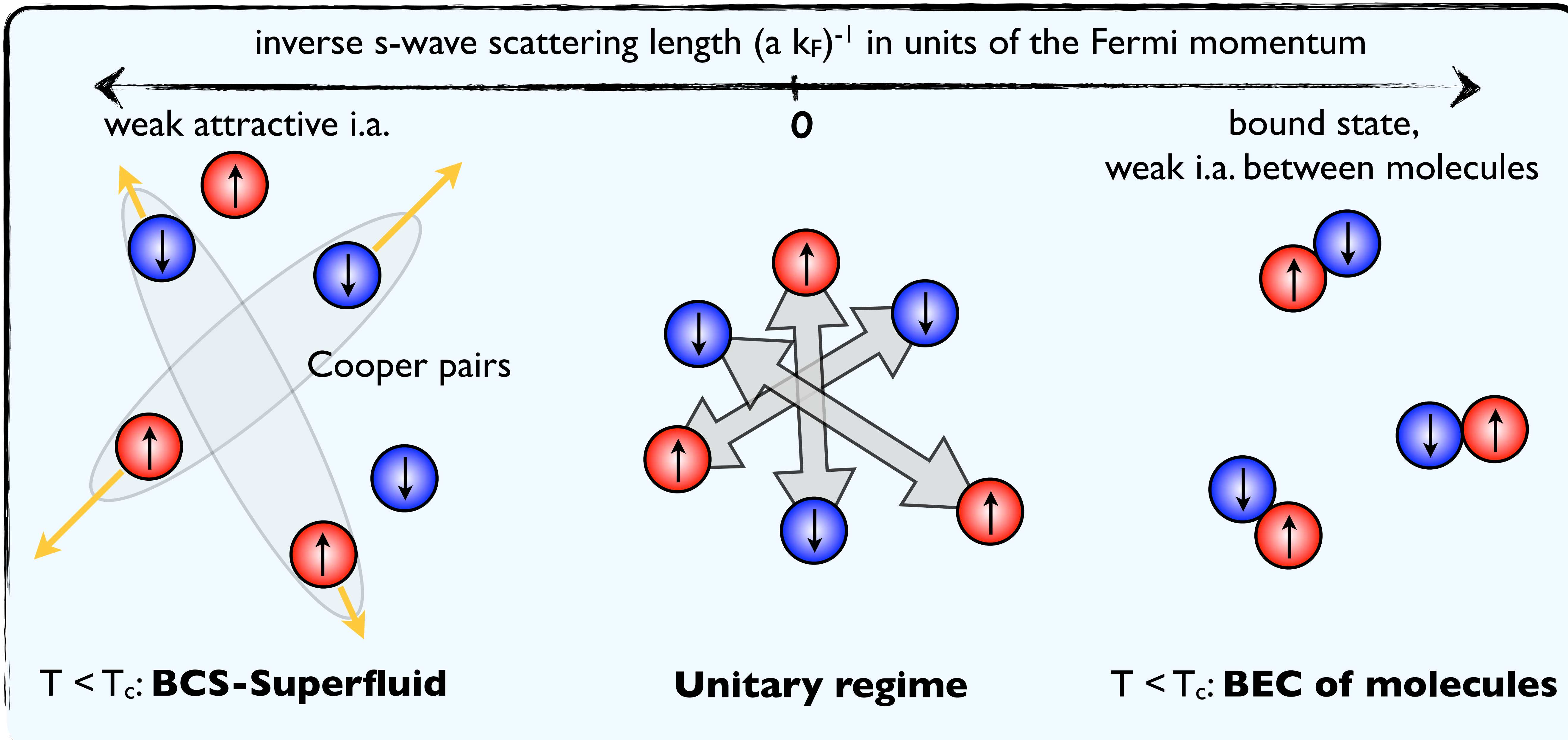
- **Feshbach resonance**: Vary effective i.a. strength or $(a\, k_F)^{-1}$ by external magnetic field

^{6}Li



- Feshbach resonance allows to tune i.a. strength arbitrarily in an experiment
- Challenge and testing ground for non-perturbative approaches to strongly interacting QFTs

BCS-BEC Crossover: Universality



- Limit of broad Feshbach resonances (e.g. experiments with ^{6}Li and ^{40}K)
- TD quantities independent of microscopic details → can be expressed by two parameters:

$$(a\,k_F)^{-1} \quad \& \quad T/T_F$$

- Units set by density $n = (k_F)^3/(3\pi^2)$

BCS-BEC Crossover: Model

- Microscopic model:

$$S[\psi^\dagger,\psi] = \int_0^{1/T} d\tau \int d^3x \{\psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \mu)\psi + \frac{\bar{\lambda}_\psi}{2}(\psi^\dagger\psi)^2\}$$

  - two-component Grassmann field: $\psi = (\psi_1, \psi_2)$
  - chemical potential: μ
  - natural units: $\hbar = k_B = 2m = 1$
  - bare four-fermion coupling: $\bar{\lambda}_\psi = \bar{\lambda}_\psi(B)$

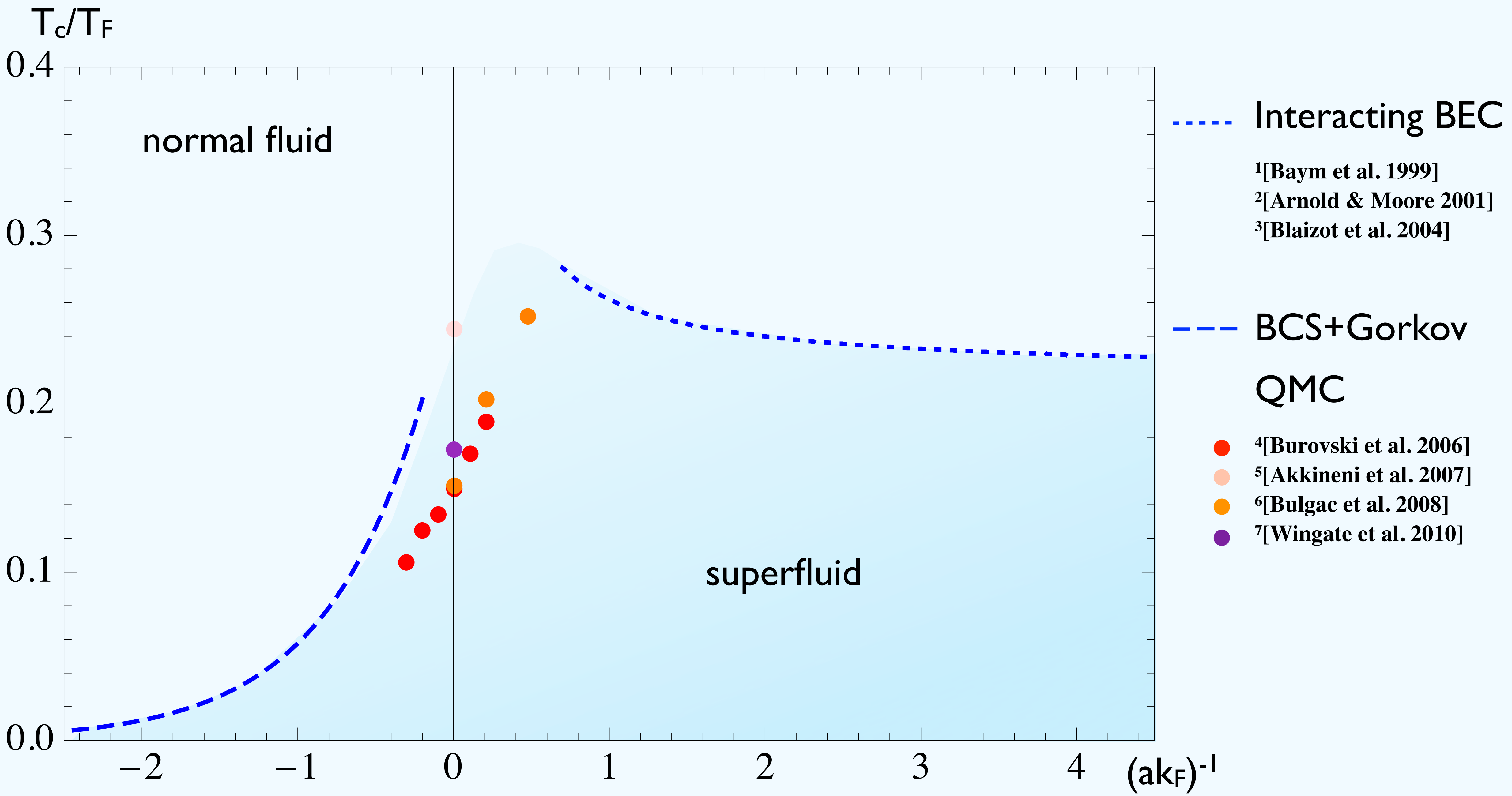
- Observable thermodynamics from grand canonical partition function:

$$Z_G = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger,\psi]}$$

... to be evaluated non-perturbatively!

BCS-BEC Crossover: Phase Diagram

- Critical temperature for the phase transition to superfluidity



2. FRG Studies of the BCS-BEC Crossover

with Stefan Flörchinger, Sebastian Diehl, Holger Gies, Jan Pawlowski
and Christof Wetterich

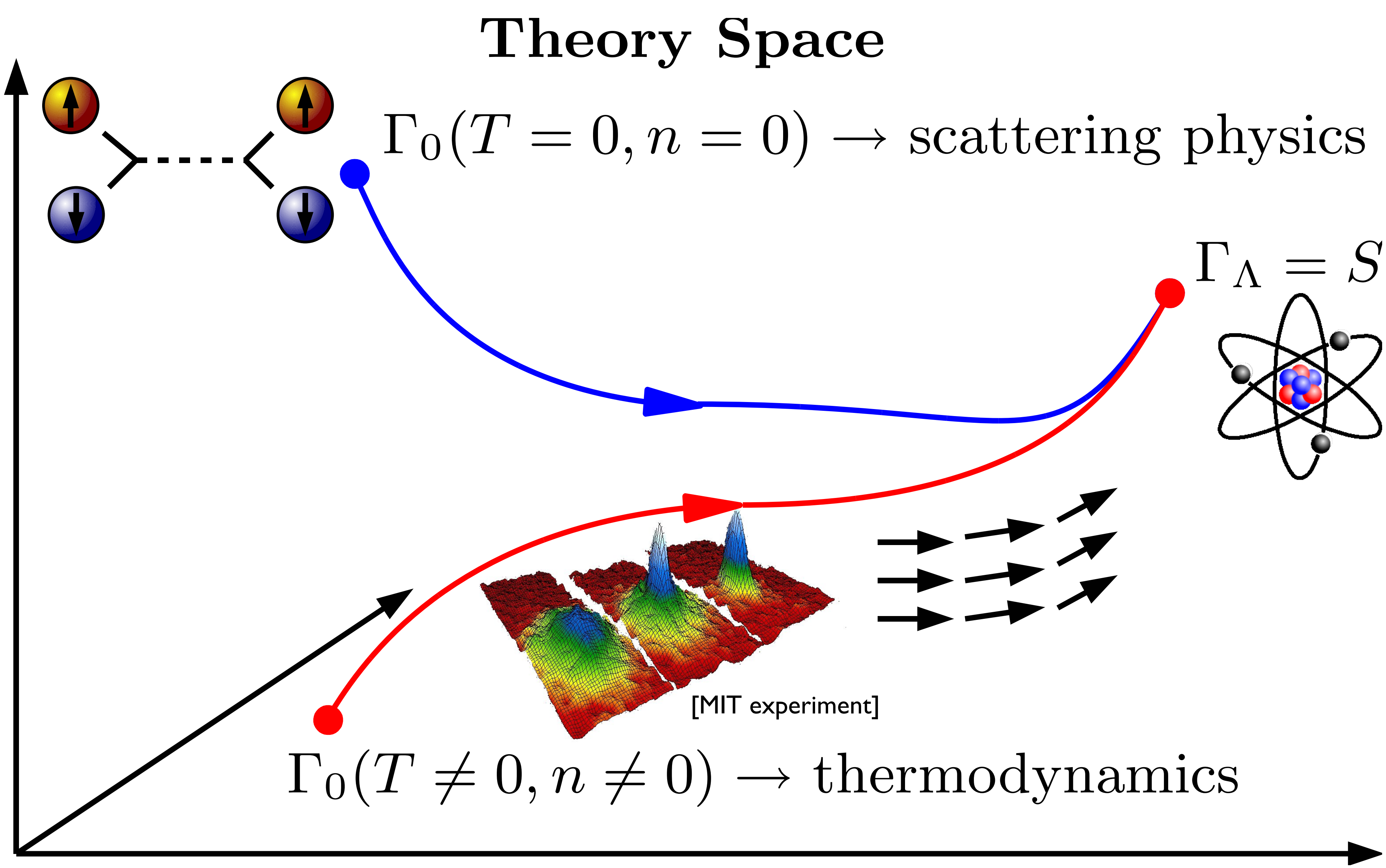
Functional RG and Theory Space

- Continuum formulation in terms of effective action

$$\Gamma[\chi_{\mathrm{eq}}] = \Phi_G/T, \quad \text{where} \quad \Phi_G = -T \ln Z$$

- Wetterich equation:

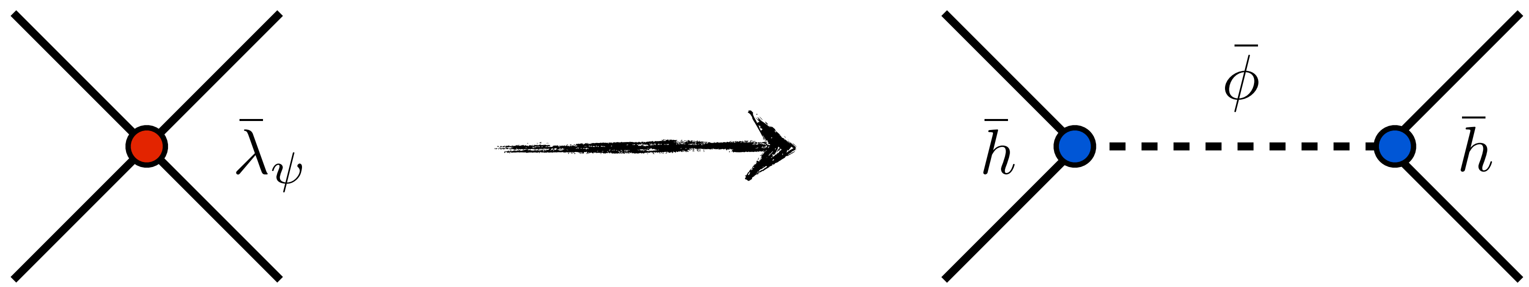
$$\partial_k \Gamma_k[\chi] = \frac{1}{2}\mathrm{STr}\Big[\big(\Gamma_k^{(2)} + R_k\big)^{-1}\partial_k R_k\Big]$$



Hubbard-Stratonovich Field and Yukawa Coupling

$$S[\psi^\dagger, \psi] = \int_0^{1/T} d\tau \int d^3x \{\psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \mu)\psi + \frac{\bar{\lambda}_\psi}{2}(\psi^\dagger\psi)^2\}$$

- Introduce a complex scalar by Hubbard-Stratonovich transformation:



Complex scalar: Molecule field, Cooper pairs,...

- s-wave scattering length:

$$a = -\frac{\bar{h}^2}{8\pi\mu_M(B - B_0)}$$

Truncation and Thermodynamic Phases

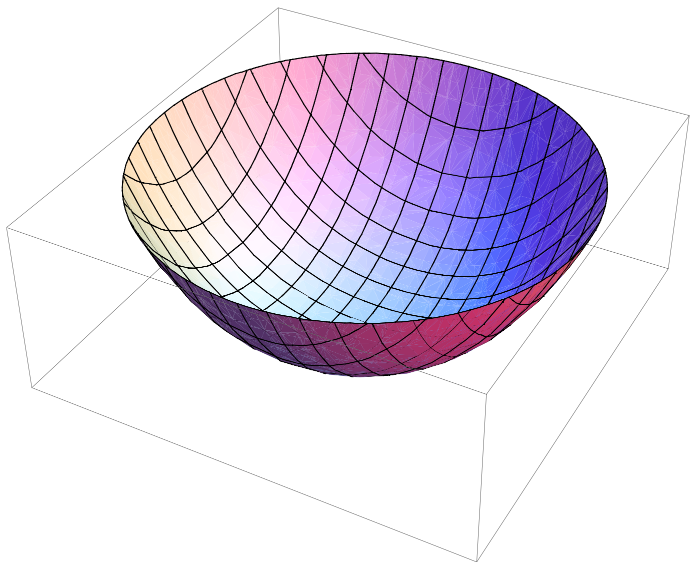
$$\Gamma_k[\Phi] = \int_{\tau,\vec{x}} \left\{ \psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \mu)\psi + \phi^*(Z_\phi\partial_\tau - \frac{\vec{\nabla}^2}{2})\phi + U(\rho,\mu) - h\left(\phi^*\psi_1\psi_2 + \phi\psi_2^*\psi_1^*\right) \right\}$$

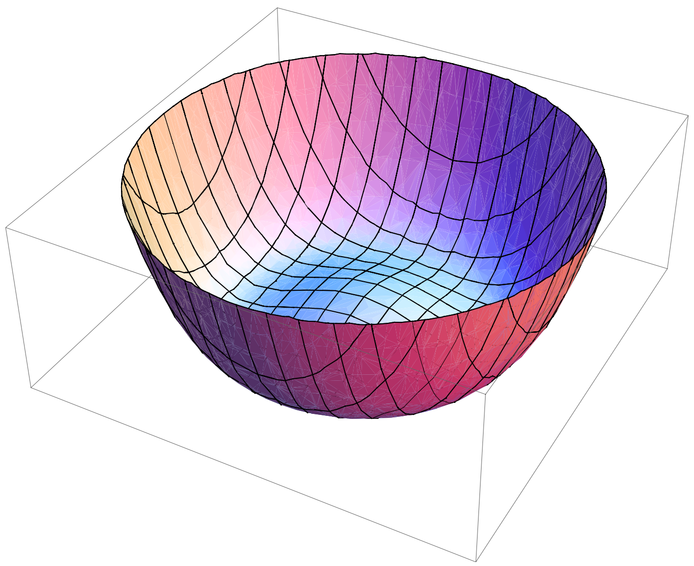
- Effective potential: Expansion around the scale-dependent location of its minimum

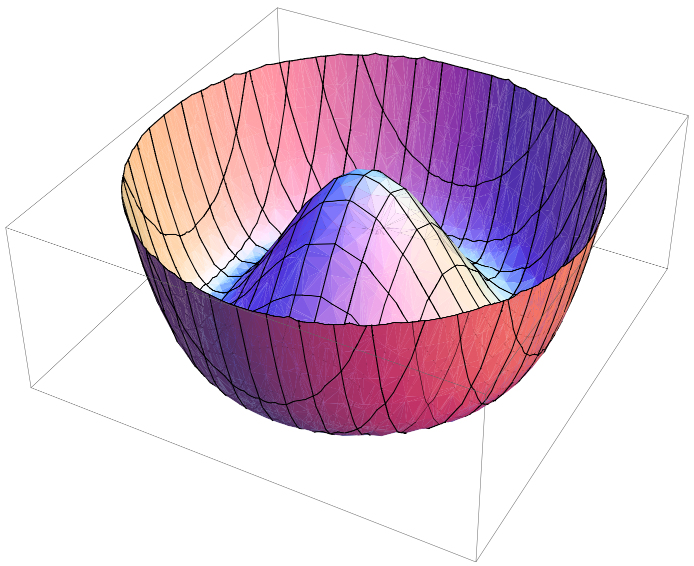
$$U_k(\rho,\mu) = m^2(\rho-\rho_0) + \frac{1}{2}\lambda(\rho-\rho_0)^2 + U(\rho_0,\mu_0) - n(\mu-\mu_0) + \alpha(\mu-\mu_0)(\rho-\rho_0)$$

- Classification of the thermodynamic phases of the system:

$$\begin{aligned} \text{Symmetric regime}: &\quad \rho_0 = 0, \quad m^2 > 0 \\ \text{Symmetry broken regime}: &\quad \rho_0 > 0, \quad m^2 = 0 \\ \text{Phase transition}: &\quad \rho_0 = 0, \quad m^2 = 0 \end{aligned}$$

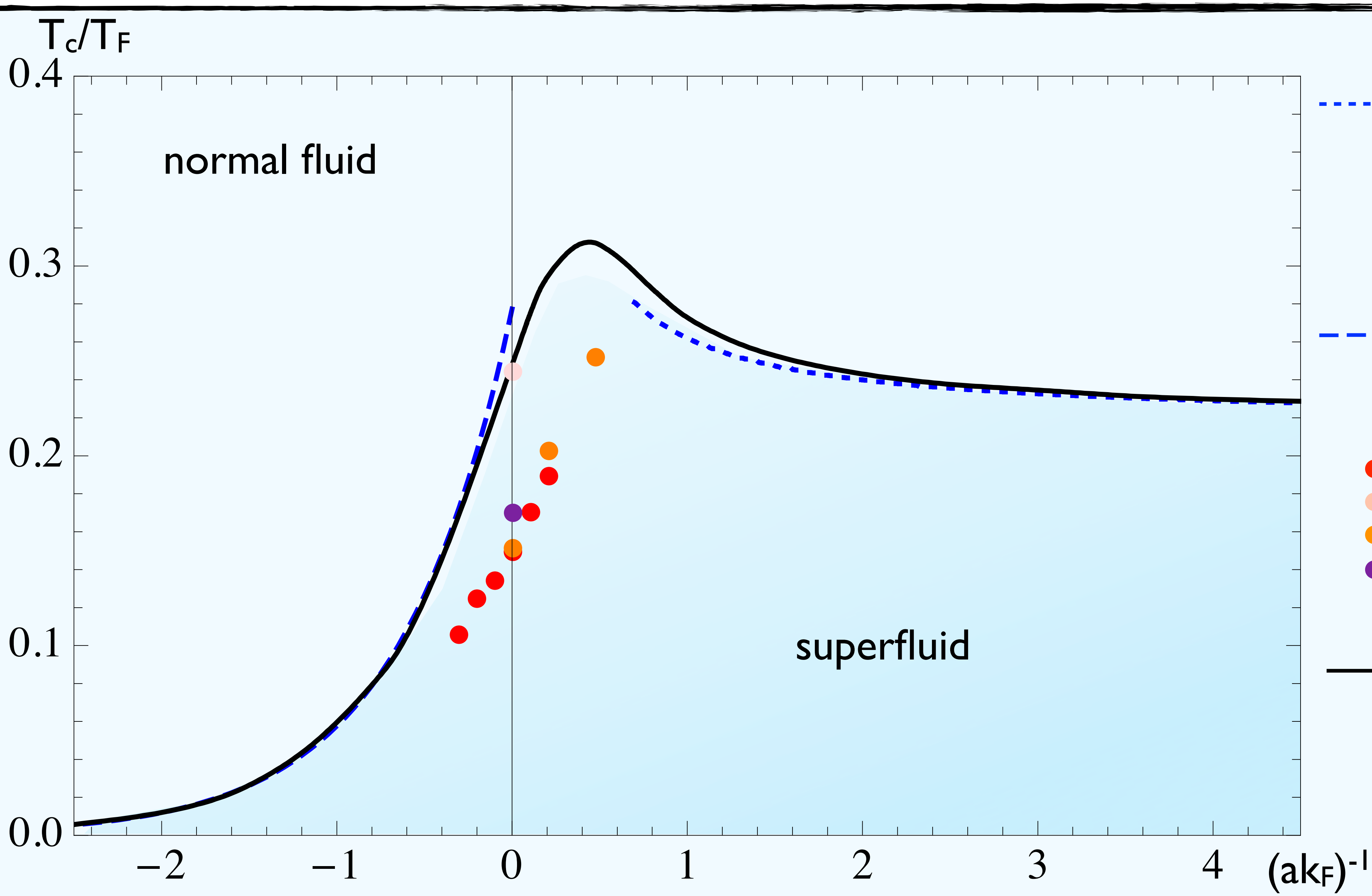






BCS-BEC Crossover: Phase Diagram

- Critical temperature for the phase transition to superfluidity:



- At Unitarity and T=0, n≠0:

	μ/E_F	Δ/E_F
Carlson *et al.* (2003) (QMC)	0.43	0.54
Perali *et al.* (2004) (t-matrix approach)	0.46	0.53
Floerchinger, MS, Wetterich (2010) (FRG)	0.51	0.46*

- Scattering physics in BEC limit: a_M/a = 0.59

exact result: a_M/a = 0.60 [9][Petrov et al. 2004]

* more RG results are available: [10][Krippa 2008] [11][Bartosch et al. 2009]

3. Finite System Size Study

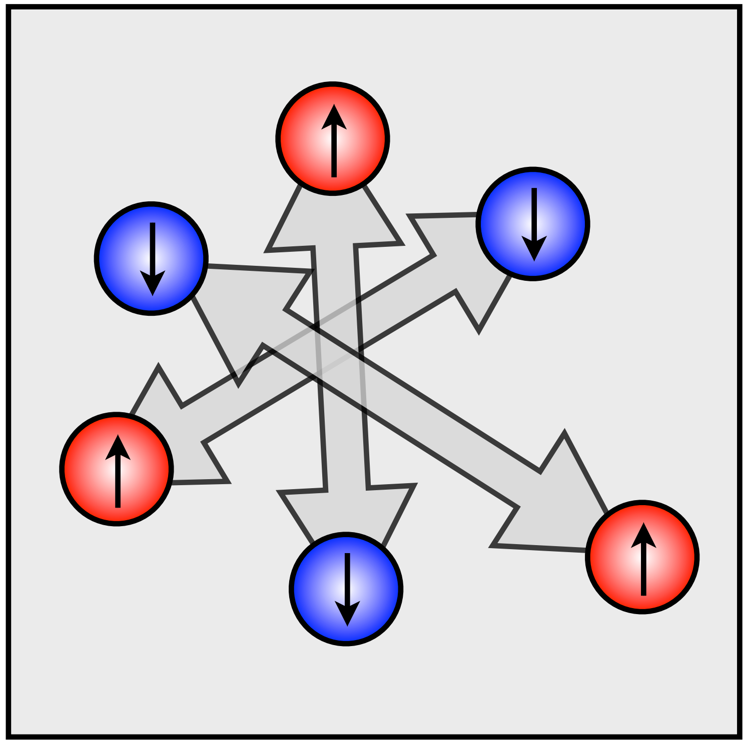
with Jens Braun and Sebastian Diehl

Motivation

- Analysis of data from lattice simulations (performed in a finite volume)
- For unitary Fermi gas: Studies by MC community:

[1][Wingate et al. 2009]
[2][Kaplan et al. 2010]
[3][Forbes et al. 2011]

- Lattice studies:
  - Limited range of system sizes
  - Numerically expensive
  - Cannot investigate transition between finite system and continuum limit
- FRG can! (recall talk by B. Klein)



Unitary regime

Setup for Finite-size Study

- Finite cubic volume V with spatial extent L
- Boundary conditions of fermions in spatial directions are periodic, cf. lattice [1][Bulgac et al. 2006]
- Finite external pairing source J which couples to order-parameter field [2][Kaplan et al. 2003] [3][Wingate et al. 2009]
- Grand canonical ensemble: Average particle number fixed by chemical potential μ

Universal Quantities

- Investigate unitary regime ($a \to \infty$) at T=0 and n≠0
- In continuum limit we have the *universal* quantities:

Bertsch parameter: $$\xi = \frac{\mu}{E_F}$$

Fermion gap: $$\frac{\Delta}{E_F}$$

- In finite volume: Bertsch parameter and fermion gap will depend on L and J
- Study deviation from TD limit as a function of L and J

Truncation with External Source

- Truncation:

$$\Gamma_k[\Phi] = \int_{\tau,\vec{x}} \Big\{ \psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \mu)\psi + \phi^*(Z_\phi\partial_\tau - \frac{\Delta}{2})\phi + U(\rho,\mu) - h\,(\phi^*\psi_1\psi_2 + \phi\psi_2^*\psi_1^*) + \frac{1}{\sqrt{2}}J(\phi+\phi^*) \Big\}$$

- Source J allows to control symmetry breaking in a finite volume, cf. [1][Kaplan et al. 2003] [2][Wingate et al. 2009]

Finite Volume V=L³

- Go to frequency/momentum space by FT: $(\tau,\vec{x}) \to (\omega^{(\phi/\psi)}, \vec{q})$
- In a finite volume, we obtain summation over discrete momenta:

$$\omega^{(\phi)} = 2m\pi T, \quad \omega^{(\psi)} = (2m+1)\pi T, \quad \vec{q} = \vec{n}\frac{2\pi}{L}, \quad \vec{n} = (n_1, n_2, n_3), \quad n_i, m \in \mathbb{Z}$$

- Flow equations can be evaluated for different system sizes L
- In the limit (L → ∞) we recover the well known flow equations for infinite volume

Truncation with External Source

- Truncation:

$$\Gamma_k[\Phi] = \int_{\tau,\vec{x}} \Big\{ \psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \mu)\psi + \phi^*(Z_\phi \partial_\tau - \frac{\Delta}{2})\phi + U(\rho,\mu) - h\left(\phi^*\psi_1\psi_2 + \phi\psi_2^*\psi_1^*\right) + \frac{1}{\sqrt{2}} J(\phi + \phi^*) \Big\}$$

- Study flow of potential at T=0 to extract Bertsch parameter and fermion gap
- In a first step we take into account the fermion fluctuations only

$$\partial_t U(\bar{\rho}, J, L, \mu) = -2k^5 (B_{\rm F}^{>} + B_{\rm F}^{<}) s_{\rm F} \qquad s_{\rm F} = \frac{k^2}{\sqrt{k^4 + \bar{h}_\varphi^2 \bar{\rho}}}$$

$$B_{\rm F}^{>} = \frac{1}{(kL)^3} \sum_{\vec{n}} \theta\left((kL)^2 - (2\pi)^2 \vec{n}^2 + \mu L^2\right) \theta\left((2\pi)^2 \vec{n}^2 - \mu L^2\right) ,$$

$$B_{\rm F}^{<} = \frac{1}{(kL)^3} \sum_{\vec{n}} \theta\left((kL)^2 + (2\pi)^2 \vec{n}^2 - \mu L^2\right) \theta\left(\mu L^2 - (2\pi)^2 \vec{n}^2\right) .$$

- This corresponds to an approximation on a meanfield level
- Effects from boson fluctuations will be included later in the talk

Investigation of the Source J

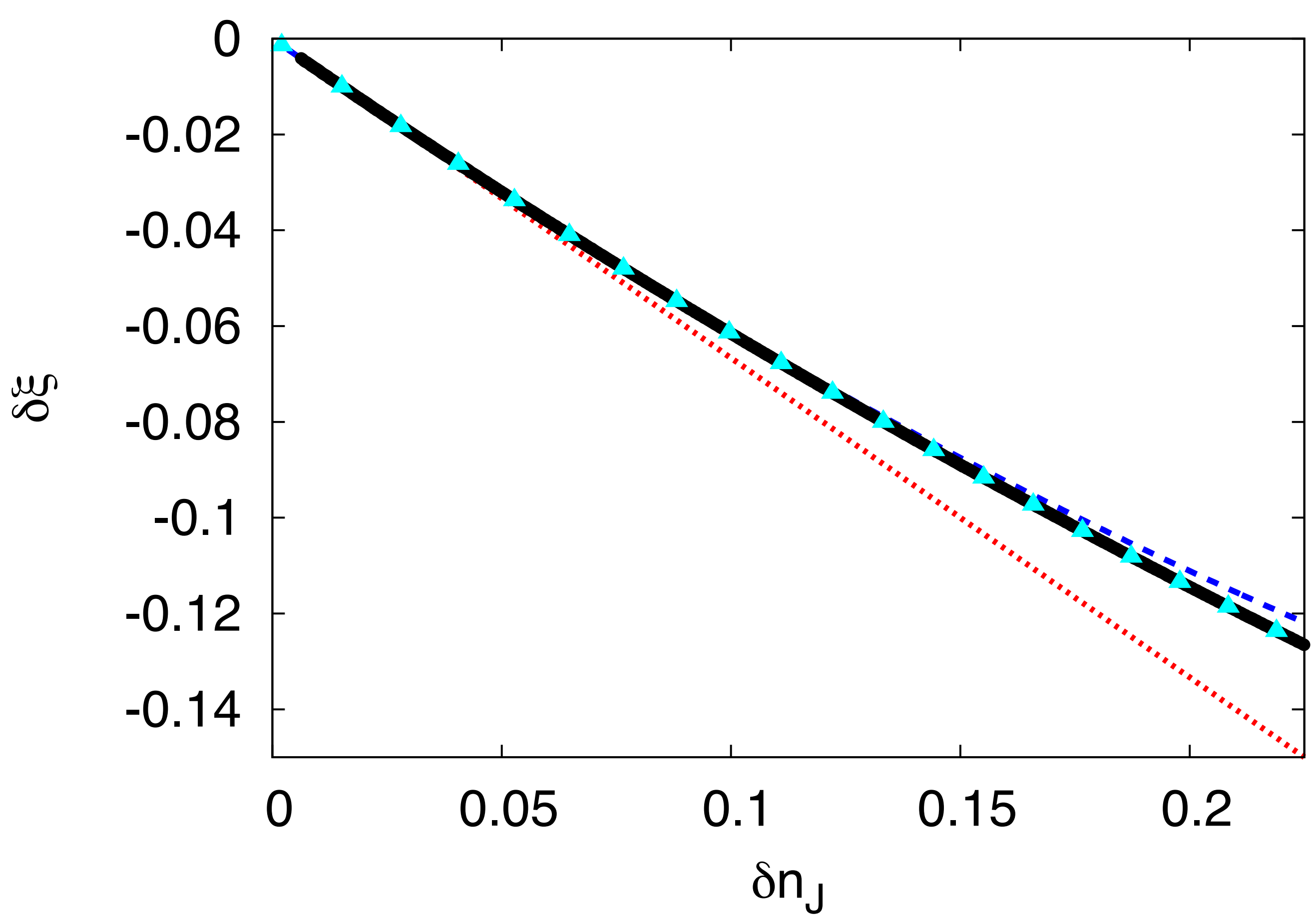
- Truncation:

$$\Gamma_k[\Phi] = \int_{\tau,\vec{x}} \Big\{ \psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \mu)\psi + \phi^*(Z_\phi \partial_\tau - \frac{\Delta}{2})\phi + U(\rho,\mu) - h\,(\phi^*\psi_1\psi_2 + \phi\psi_2^*\psi_1^*) + \frac{1}{\sqrt{2}} J(\phi + \phi^*) \Big\}$$

- Study behaviour of TD observables with source J for infinite L
- Generally, we can expand Bertsch parameter for small but finite J:

$$\delta\xi = \frac{\xi_J - \xi_0}{\xi_0} = -\frac{2}{3}(\delta n_J) + \frac{5}{9}(\delta n_J)^2 + \mathcal{O}\left((\delta n_J)^3\right)$$

$$\delta n_J = \frac{n_J - n_{J=0}}{n_{J=0}}$$



- In lattice simulations only data for finite J is available → J=0 has to be extraced from fit (linear, higher order,...)
- Linear fit justified for $\delta n_J \lesssim 0.05$

Investigation of the Source J

- Truncation:

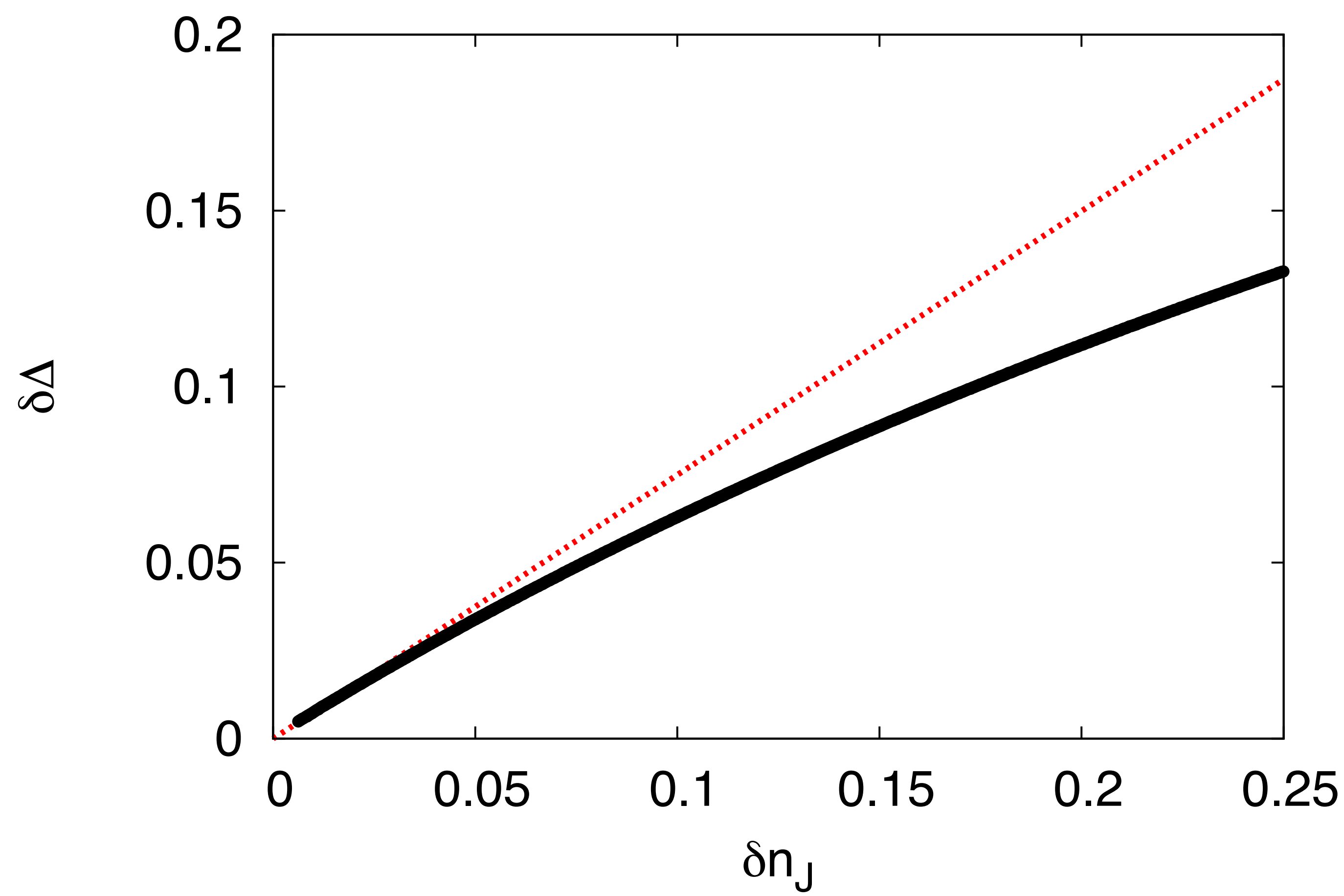
$$\Gamma_k[\Phi] = \int_{\tau,\vec{x}} \Big\{ \psi^\dagger(\partial_\tau - \vec{\nabla}^2 - \mu)\psi + \phi^*(Z_\phi\partial_\tau - \frac{\Delta}{2})\phi + U(\rho,\mu) - h\,(\phi^*\psi_1\psi_2 + \phi\psi_2^*\psi_1^*) + \frac{1}{\sqrt{2}}J(\phi+\phi^*) \Big\}$$

- Study behaviour of TD observables with source J for infinite L
- Similarly, we can expand fermion gap for small but finite J:

$$\delta\Delta = \frac{\Delta_J - \Delta_0}{\Delta_0} = \hat{\Delta}^{(1)}(\delta n_J) + \mathcal{O}((\delta n_J)^2)$$

$$\hat{\Delta}^{(1)} \approx 0.749$$

- fit from MF data

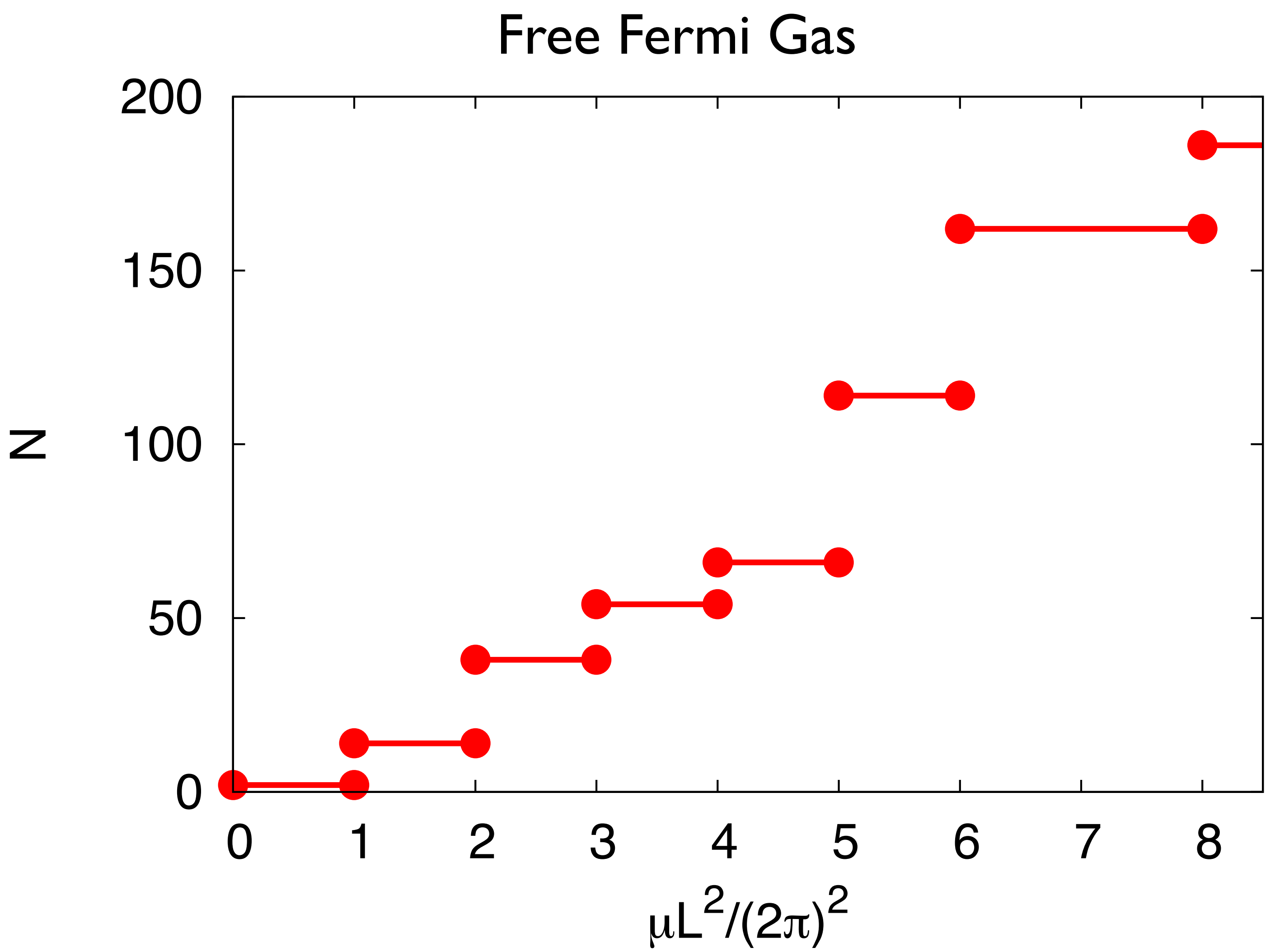


- In lattice simulations only data for finite J is available → J=0 has to be extracted from fit (linear, higher order,...)
- Linear fit justified for $\delta n_J \lesssim 0.05$

Finite Volume V=L^3

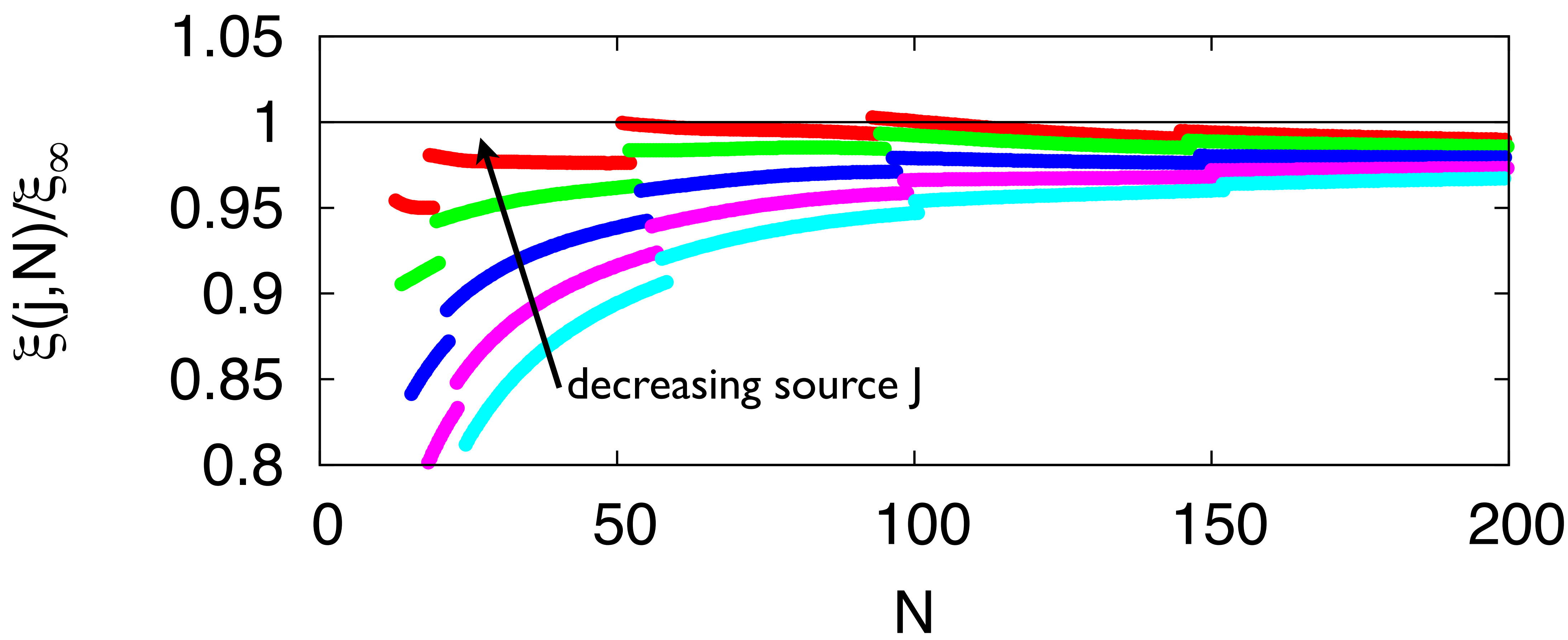
- The (average) particle number N is given by N = n L^3
- Initial condition for RG flow of density is given by free Fermi gas n_{free}
- n_{free} is determined by our choice for the chemical potential.

$$n_{\text{free}} = \frac{s}{L^3} \sum_{\vec{n}, n_i \in \mathbb{Z}} \theta\left(\mu L^2 - (2\pi)^2 \vec{n}^2\right) \overset{(\mu L^2 \to \infty)}{\longrightarrow} \frac{\mu^{\frac{3}{2}}}{3\pi^2}$$



Bertsch parameter at MF Level

- Study Bertsch parameter as function of N (or μ) for various values of J at fixed L (fixes scale)
- For large values of μ at fixed L and J: dimensionless $J\mu^{-7/4} \to 0$, so $\xi \to \xi_\infty$ for large L
- For small N we observe shell effects (discontinuities)

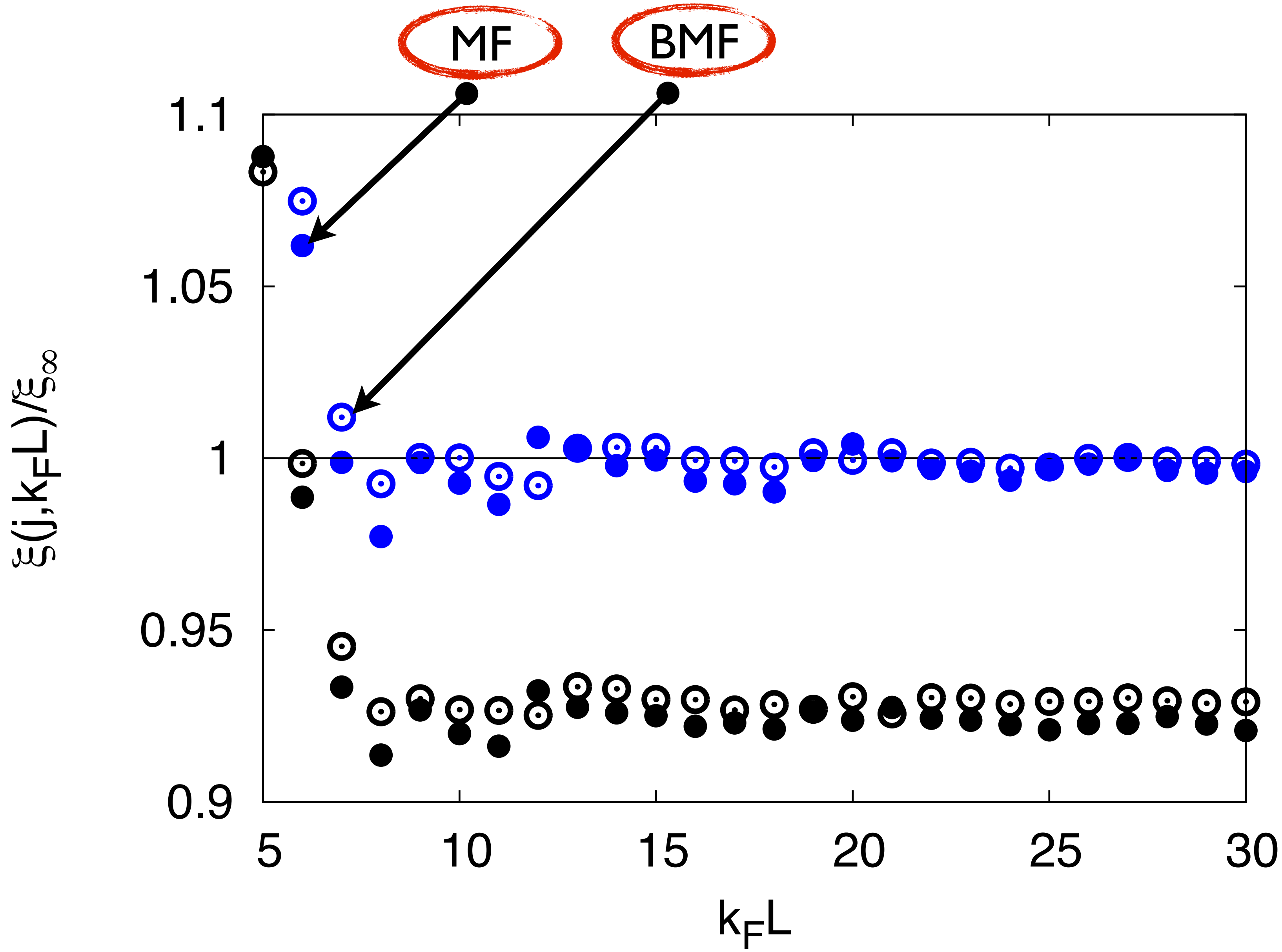


$$N > 50 : \delta\xi \sim c_{\mathrm{N}} N^{-\frac{2}{3}} \sim c_\mu \left(\mu L_0^2\right)^{-1}$$

- Large-N behaviour follows from definition of Bertsch parameter
- Constants c only depend on $JL^{7/2}$
- For N>200 (and our choice of L) Bertsch parameter is already close to cont. limit (>98%)
- Convergence behaviour depends on J (very clearly for N<200)

Bertsch parameter at fixed density

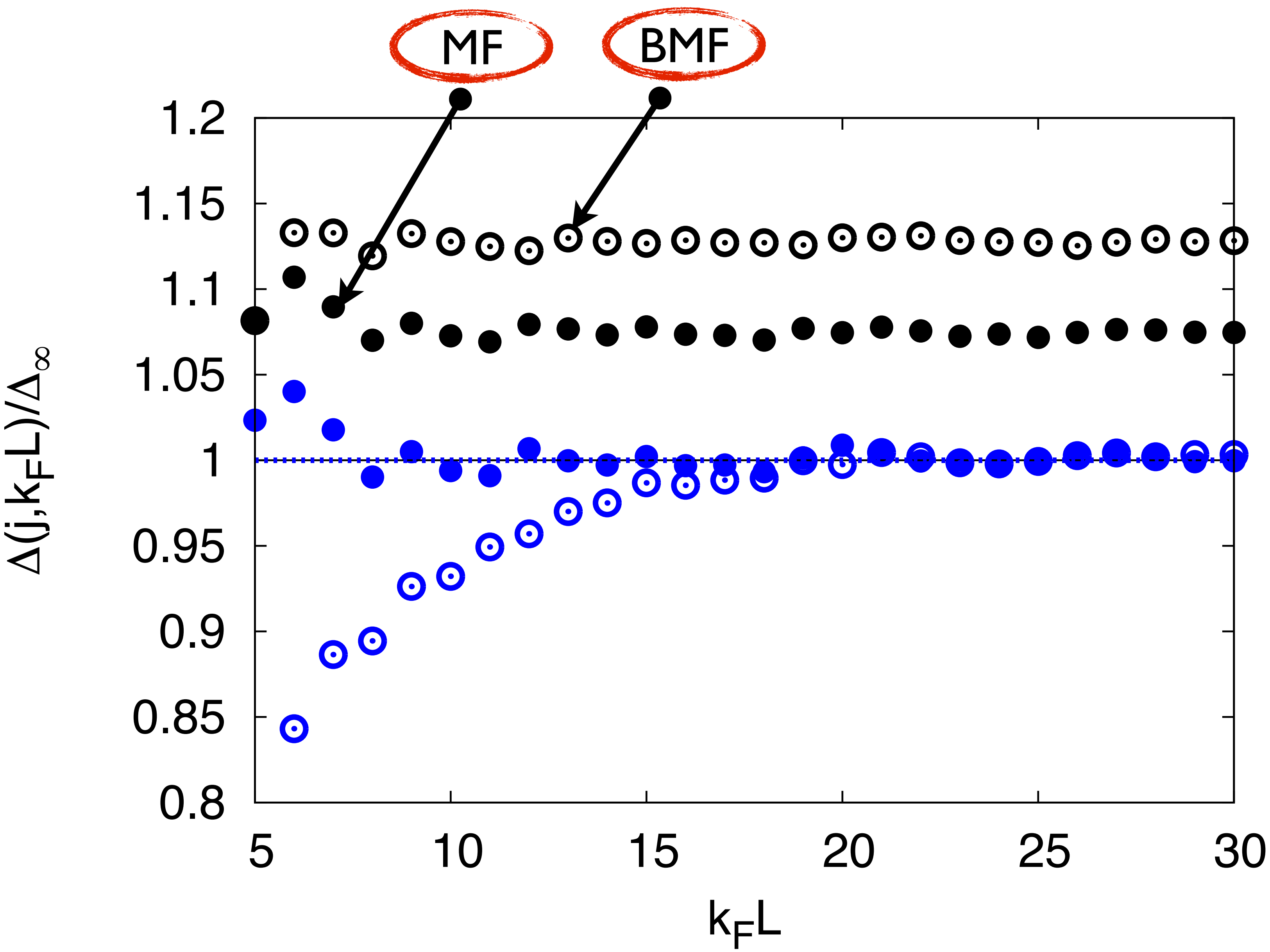
- Behavior of Bertsch parameter as a function of dimensionless quantity $k_F L$ for fixed density:
  - Small $k_F L$: shell effects (washed out for larger source)
  - Large $k_F L$: TD limit is approached (as it should for fixed density)
  - Finite source J: Does not approach J $\rightarrow$0 limit (due to constant fraction of n_J)



- BMF: Include boson loops in flow of effective potential, running wave-function renormalization

Fermion Gap beyond MF

- Fermion gap is more sensitive to the inclusion of order- parameter fluctuations



- Large $k_F L$: TD limit is approached
- Different values for different densities and sources J
- For large source J: Gap almost independent from $k_F L$ (wavelength of Goldstone smaller than spatial extent L)

  →

  Order parameter fluctuations are not affected by boundary
- Small source J: large deviations

$$m_{\mathrm{G}}^2 = \frac{J}{\sqrt{2\rho_0}}\,, \qquad m_{\mathrm{R}}^2 = m_{\mathrm{G}}^2 + \lambda_\varphi \rho_0$$

Conclusions

- FRG connects BCS-/BEC-limits continuously with unitary regime and gives results with a reasonable accuracy throughout the whole crossover
- Using the FRG we have access to the shape of the volume and the particle number dependence of observables over a wide range of system sizes
- Volume-effects depend strongly on observable
- Improves understanding of convergence of finite volume systems, useful for MC simulations

& Outlook

- Finite size study of $T_c(J,L)$