Equation of state & pair-correlations in mass-imbalanced one-dimensional Fermi systems

Lukas Rammelmüller

Institut für Kernphysik, TU Darmstadt

with William J. Porter[3], Joaquín E. Drut[3], and Jens Braun[1,2]

[1] Institut für Kernphysik, Technische Universität Darmstadt,
[2] ExtreMe Mater Institute EMMI, GSI,
[3] Department of Physics and Astronomy, University of North Carolina at Chapel Hill

Arbeitstreffen Kernphysik

Schleching, March 7, 2017.

HIC for FAIR
Helmholtz International Center

HGS-HIRe for FAIR
Helmholtz Graduate School for Hadron and Ion Research

Outline

- Motivation: strongly interacting quantum gases
- Method: Hybrid Monte Carlo
- Results: discussion of EOS & pair-correlations
  - connection to RG method
- Summary, conclusions & future work

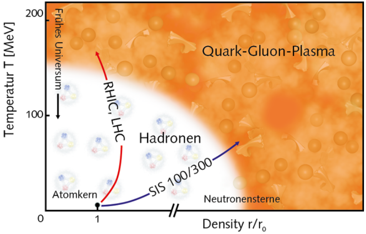
Strong interactions in ultracold gases

Phases of strongly interacting theories

TECHNISCHE UNIVERSITÄT DARMSTADT

- explore & understand phases of strongly-interacting theories
- universal behavior: *unitary fermi gas* (UFG)
- ultracold quantum gases are a versatile tool to probe strongly-interacting systems (in experiment and theory)
  A.N. Wenz *et al.*, *Science* **25**, 2013.
- many available methods, exchange with lattice QCD
- 1D often a benchmark for new methods

FAIR @ GSI

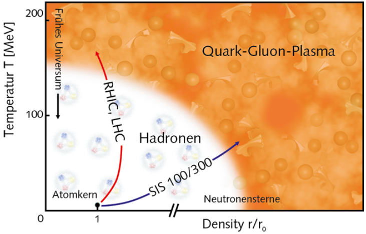


Strong interactions in ultracold gases

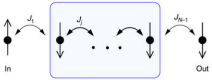
Phases of strongly interacting theories

TECHNISCHE UNIVERSITÄT DARMSTADT

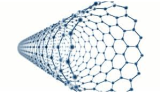
FAIR @ GSI



- explore & understand phases of strongly-interacting theories
- universal behavior: *unitary fermi gas* (UFG)
- ultracold quantum gases are a versatile tool to probe strongly-interacting systems (in experiment and theory)
  A.N. Wenz *et al.*, *Science* **25**, 2013.
- many available methods, exchange with lattice QCD
- 1D often a benchmark for new methods, *but also interesting physics!*



O.V. Marchukov *et al.*, *Nature Comm.* **7**, 2016.



S. Iijima, *Nature* **354**, 1991.

Model:
Fermions on the lattice

TECHNISCHE UNIVERSITÄT DARMSTADT

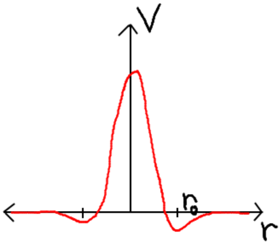
- Gaudin-Yang model for fermions in 1D

$$\hat{H} = -\sum_{s=\uparrow,\downarrow} \sum_{x} \hat{\psi}_s^\dagger(x) \frac{\hbar^2 \nabla^2}{2m_s} \hat{\psi}_s(x) + g \sum_{x} \hat{\psi}_\uparrow^\dagger(x) \hat{\psi}_\uparrow(x) \hat{\psi}_\downarrow^\dagger(x) \hat{\psi}_\downarrow(x)$$

Model:
Fermions on the lattice

- Gaudin-Yang model for fermions in 1D

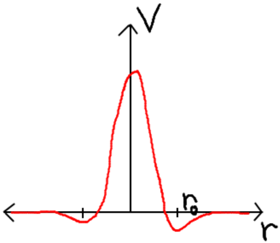
$$\hat{H} = -\sum_{s=\uparrow,\downarrow} \sum_{x} \hat{\psi}_s^\dagger(x) \frac{\hbar^2 \nabla^2}{2m_s} \hat{\psi}_s(x) + g \sum_{x} \hat{\psi}_\uparrow^\dagger(x) \hat{\psi}_\uparrow(x) \hat{\psi}_\downarrow^\dagger(x) \hat{\psi}_\downarrow(x)$$



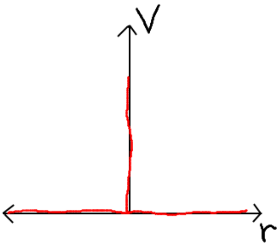
Model: Fermions on the lattice

- Gaudin-Yang model for fermions in 1D

$$\hat{H} = -\sum_{s=\uparrow,\downarrow} \sum_{x} \hat{\psi}_s^\dagger(x) \frac{\hbar^2 \nabla^2}{2 m_s} \hat{\psi}_s(x) + g \sum_{x} \hat{\psi}_\uparrow^\dagger(x) \hat{\psi}_\uparrow(x) \hat{\psi}_\downarrow^\dagger(x) \hat{\psi}_\downarrow(x)$$



$$k_F^{-1} \gg r_0 \longrightarrow$$



Model:
Fermions on the lattice

TECHNISCHE
UNIVERSITÄT
DARMSTADT

- Gaudin-Yang model for fermions in 1D

$$\hat{H} = -\sum_{s=\uparrow,\downarrow} \sum_{x} \hat{\psi}_s^\dagger(x) \frac{\hbar^2 \nabla^2}{2m_s} \hat{\psi}_s(x) + g \sum_{x} \hat{\psi}_\uparrow^\dagger(x) \hat{\psi}_\uparrow(x) \hat{\psi}_\downarrow^\dagger(x) \hat{\psi}_\downarrow(x)$$

- problem: $\hat{H} = \hat{T} + \hat{V}$ not generally diagonalizable simultaneously
- in some cases exactly solvable with Bethe ansatz

M. Gaudin, *Phys. Lett. A* **24**, 1967.
C.N. Yang, *Phys. Rev. Lett.* **19**, 1967.

Method:
Hybrid Monte Carlo (HMC) in a nutshell

TECHNISCHE UNIVERSITÄT DARMSTADT

- ground-state partition function as a function of imaginary time

$$\mathcal{Z}(\beta) = \langle \psi_0(\beta) \,|\, \psi_0(\beta) \rangle = \langle \psi_0(0) |\, \mathrm{e}^{-\beta \hat{H}} \,| \psi_0(0) \rangle$$

- rewrite with time-discretization & Hubbard-Stratonovich transform: path-integral over *auxiliary field* σ

$$\mathcal{Z}(\beta) = \int \mathcal{D}\sigma \;\det U_\sigma^{(\uparrow)}(\beta) \det U_\sigma^{(\downarrow)}(\beta) = \int \mathcal{D}\sigma \; P[\sigma, \beta]$$

- instead of one very complicated many-body problem: many single-particle problems in an external field
- high-dimensional: integration with Monte Carlo
- "hybrid": smarter choice of new field-configurations (molecular dynamics)

S. Duane, A.D. Kennedy, B.J. Pendleton, D. Roweth, *Phys. Lett. B* **195**, 1987.
A. Bulgac, J.E. Drut, P. Magierski, *Phys. Rev. Lett.* **96**, 2006.

Method:
Hybrid Monte Carlo (HMC) in a nutshell

When is it useful?

- transfer matrices $U_\sigma^{(s)}$ are equal for homogeneous case, otherwise: sign-problem

$$\mathcal{Z} = \int \mathcal{D}\sigma \; \det U_\sigma^{(\uparrow)} \det U_\sigma^{(\downarrow)} \equiv \int \mathcal{D}\sigma \; P[\sigma]$$

$$\downarrow$$

$$\mathcal{Z} = \int \mathcal{D}\sigma \; \det^2 U_\sigma$$

- probability-measure positive-semidefinite

Results: Equation of state

ground-state energy vs. coupling strength

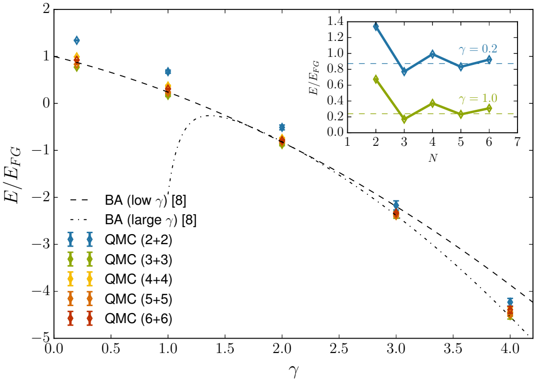
- ground-state energy experimentally accessible
- computed via

$$\langle \hat{H} \rangle = -\frac{\partial}{\partial \beta} \log \mathcal{Z}(\beta)$$

- excellent agreement with Bethe ansatz

  M. Wadati, T. Iida, *Phys. Lett. A* **360**, 2007.

- limit of large γ: bosonic behavior



$$\gamma = g/n$$

LR, W.J. Porter, A.C. Loheac, and J.E. Drut, *Phys. Rev. A* **92**, 2015.

Method II:
Density functional theory + RG (DFT-RG)

TECHNISCHE UNIVERSITÄT DARMSTADT

- Hohenberg-Kohn theorem: energy can be written as functional of the density
- ground-state energy via minimization

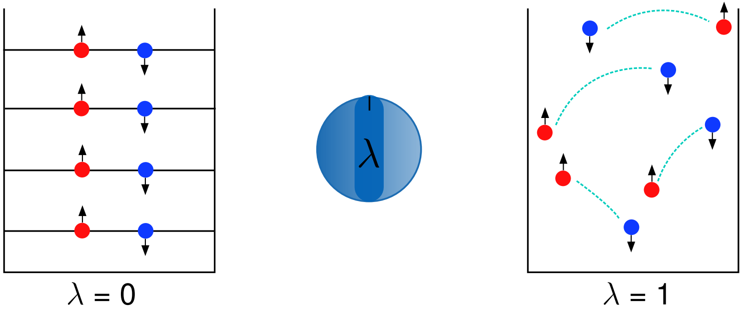
$$E_{\mathrm{gs}} = \inf_{\rho} E[\rho]$$

- problem: no recipe for the energy functional

- typically: minimization of global ansatz for energy density functional
- DFT-RG: method to incorporate microscopic interactions

  S. Kemler, J. Braun, *Journ. Phys. G* **40**, 2013.
  S. Kemler, M. Pospiech and J. Braun, *Journ. Phys G* **44**, 2017.

Method II: Density functional theory + RG (DFT-RG)



$$\partial_\lambda \Gamma_\lambda = \frac{1}{2}\rho_\sigma U_{\sigma\sigma'}\rho_{\sigma'} + \frac{1}{2}\mathrm{Tr}\left\{ U_{\sigma\sigma'} \left[\left(\Gamma^{(2)}_{\lambda,\sigma'\sigma} \right)^{-1} + \rho_{\sigma'} \cdot \mathbb{1}_{(\sigma,x)} \right] \right\}$$

Results: Equation of state

ground-state energy for few-body systems

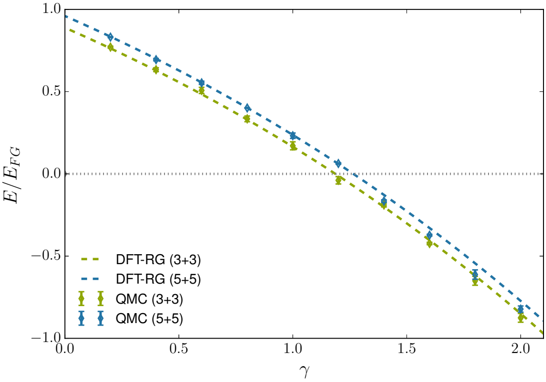
- ground-state energy experimentally accessible
- computed via

$$\langle \hat{H} \rangle = -\frac{\partial}{\partial \beta} \log \mathcal{Z}$$

- excellent agreement with Bethe ansatz

  M. Wadati, T. Iida, *Phys. Lett. A* **360**, 2007.
- limit of large γ: bosonic behavior
- perfect agreement with few-body DFT-RG

  S. Kemler, M. Pospiech and J. Braun, *in preparation*



$$\gamma = g/n$$

Method revisited: Mass-imbalance and the sign problem

- typically subject to a sign-problem:
  unequal masses $\rightarrow$ unequal transfer matrices

$$\mathcal{Z} = \int \mathcal{D}\sigma \ \det U_\sigma^{(\uparrow)} \det U_\sigma^{(\downarrow)} = \int \mathcal{D}\sigma \ P[\sigma]$$

$$\not\Downarrow$$

$$\mathcal{Z} = \int \mathcal{D}\sigma \ \det^2 U_\sigma$$

- exponentially increasing numerical effort with larger systems

Method revisited: Imaginary mass-imbalance to the rescue!

TECHNISCHE UNIVERSITÄT DARMSTADT

- sign-problem surmounted by rewriting
  $m_\uparrow = m_0(1 + i\delta m)$ and $m_\downarrow = m_0(1 - i\delta m)$
  J. Braun, J.E. Drut, D. Roscher., *Phys. Rev. Lett.* **114**, 2014.

$$\mathcal{Z} = \int \mathcal{D}\sigma \; \det U_\sigma^{(\uparrow)} \det U_\sigma^{(\downarrow)} \equiv \int \mathcal{D}\sigma \; P[\sigma]$$

$$\downarrow$$

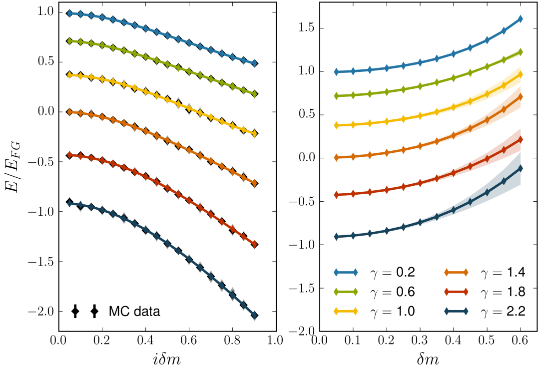
$$\mathcal{Z} = \int \mathcal{D}\sigma \left| \det U_\sigma \right|^2$$

- probability-measure again positive-semidefinite

Results: Equation of state

Mass-imbalanced systems

- experimental realization of ^{6}Li and ^{40}Ka mixture ($\delta m \sim 0.74$)
- real mass-imbalance via analytic continuation (Padé approximation)



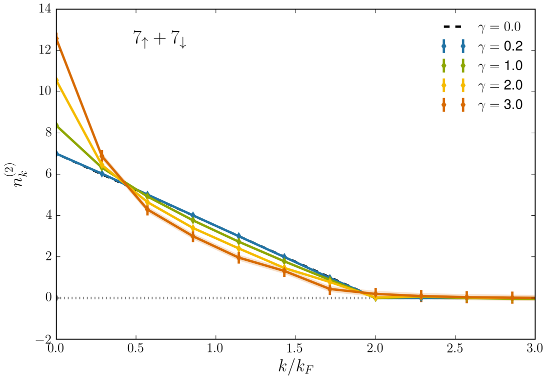
$\gamma = g/n$

LR, W.J. Porter, J. Braun, J.E. Drut, *in preparation.*

Results: Pair-correlation

Mass-balanced systems

- pairing properties through pair-correlation function
  $$\rho_{(2)}(|x - x'|) = \langle \hat{\psi}^\dagger_\uparrow(x)\, \hat{\psi}^\dagger_\downarrow(x)\, \hat{\psi}_\downarrow(x')\, \hat{\psi}_\uparrow(x') \rangle$$
- smooth increase of peak at $k = 0$ with interaction strength
- formation of tightly-bound pairs
- crossover from BCS-pairing *Bose-Einstein condensate*



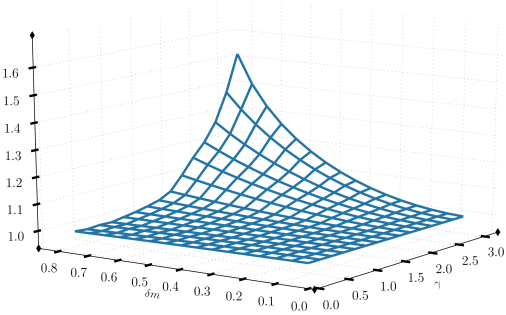
$$\gamma = g/n$$

LR, W.J. Porter, J. Braun, J.E. Drut, *in preparation.*

Results: Pair-correlation

Mass-imbalanced systems

- peak still at $k = 0$: no FFLO-phase observed
- normalized peak height to mass-balanced system: influence of imbalance larger at strong coupling



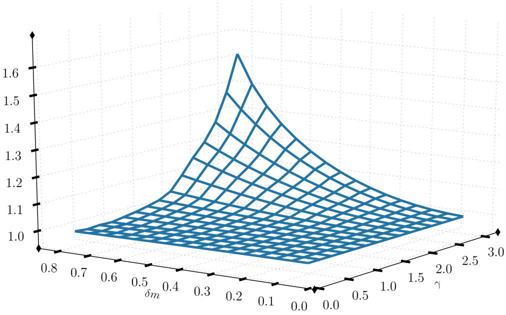
$\gamma = g/n$

LR, W.J. Porter, J. Braun, J.E. Drut, *in preparation.*

Results: Pair-correlation

Mass-imbalanced systems

- peak still at $k = 0$: no FFLO-phase observed
- normalized peak height to mass-balanced system: influence of imbalance larger at strong coupling



PRELIMINARY

$\gamma = g/n$

LR, W.J. Porter, J. Braun, J.E. Drut, *in preparation.*

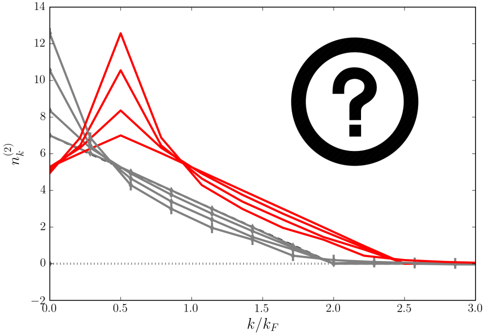
Outlook: Pair-correlation

Spin-imbalanced systems

- hallmark of Fulde-Ferell-Larkin-Ovchinnikov phase: peak at nonzero momentum $k = \left|k_F^{(\uparrow)} - k_F^{(\downarrow)}\right|$

P. Fulde, R.A. Ferrell, *Phys. Rev.* **135**, 1964.

A.I. Larkin, Y.N. Ovchinnikov, *Sov. Phys. JETP* **20**, 1965.



Summary, conclusion & outlook

TECHNISCHE UNIVERSITÄT DARMSTADT

Summary

- precise calculation of energies and correlations
  agreement for few-body systems, convergence to thermodynamic limit
- stable results for high mass-imbalances
- observed formation of bosonic pairs in the ground state
- no FFLO behavior in purely mass-imbalanced systems

Summary, conclusion & outlook

TECHNISCHE
UNIVERSITÄT
DARMSTADT

Summary

- precise calculation of energies and correlations
  agreement for few-body systems, convergence to thermodynamic limit
- stable results for high mass-imbalances
- observed formation of bosonic pairs in the ground state
- no FFLO behavior in purely mass-imbalanced systems

Future work

- spin-imbalance (FFLO behavior expected)
- long-term goal: nonperturbative phase-diagrams of 3D unitary Fermi gas