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

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Motivation

In recent years tremendous effort was put forward to investigate the physics of ultracold atomic gases which has led to the observation of a rich variety of phenomena ranging from BCS superfluidity to Bose-Einstein condensation. Experimentally, this is made possible in particular by the use of *Feshbach-resonances*. Moreover it became possible to realize experimental setups for low-dimensional quantum gases [1] such that observables for two- and even one-dimensional (1D) configurations are accessible these days. These advances necessitate theoretical exploration of fundamental observables such as the ground-state energy as well as one- and two-body correlations, especially in the theoretically challenging strongly-coupled regime.

Model, Method & Scales

a) Model

We consider two equally populated species of fermions on a 1D lattice in the ground state with an attractive contact-interaction between spin-up and -down particles which is described by the *Gaudin-Yang* model

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

b) Quantum Monte Carlo method

Despite the possibility to extract observables for this model analytically via the highly nontrivial Bethe ansatz [2], we employ a *Quantum Monte Carlo (QMC)* approach to obtain nonperturbative numerical results. The latter approach is readily extended to e.g harmonically trapped systems whereas the analytic method is restricted to the ground state.

As typical for QMC algorithms in the ground state, we work in imaginary time. We utilize a *Suzuki-Trotter decomposition* to discretize the temporal axis, followed by a *Hubbard-Stratonovich transformation* to write the two-body interaction as a sum of coupled one-body operators. Collecting all the resulting parts into a single path integral, we can write for the partition function

$$\mathscr{Z} = \int \mathscr{D}\sigma\;\det U_{\sigma}^{(\uparrow)}\;\det U_{\sigma}^{(\downarrow)}$$

where $U_{\sigma}^{(s)}$ denotes the *transfer matrix* for the spin-species s. Already for 1D systems, where we typically use a spacetime-lattice of $N_x \times N_\tau = 80 \times (500-1000)$, these integrals are high dimensional and we therefore employ the *Hybrid Monte Carlo (HMC)* algorithm [3] to estimate observables.

For mass-imbalanced systems, which are typically subject to a sign problem, we can rewrite the mass in terms of an *imaginary mass imbalance*

$$m_\uparrow = m_0(1 + i\delta m)$$
$$m_\downarrow = m_0(1 - i\delta m),$$

where and m_0 is the average mass and δm the mass imbalance between up- and down-fermions. This renders the transfer matrices of the two spin-species complex-conjugate to each other and therefore yields a non-negative probability measure in the path integral [4]. Results for real mass-imbalances can then be obtained by *Padé-approximation* followed by an *analytic continuation* to the real axis.

c) Scales

We work in units where $k_B = \hbar = m_0 = 1$. The only scale remaining in this convention is the particle density n, which we use to define the dimensionless coupling $\gamma = g/n$ with g being the bare interaction strength.

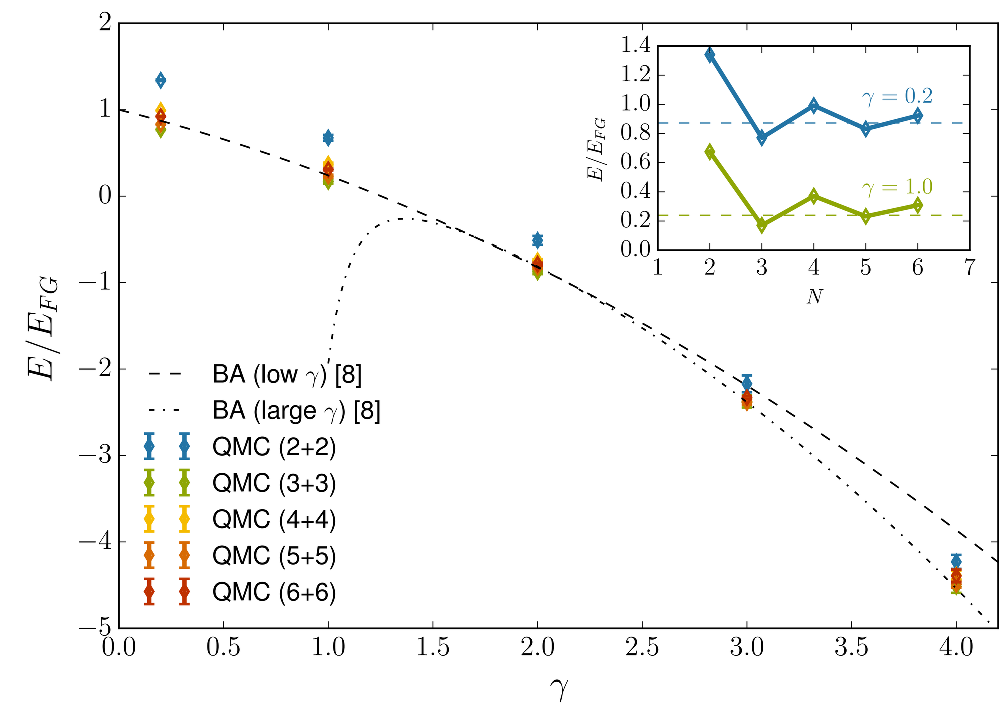
Results & Discussion

a) Equation of state

The ground-state energy is calculated by a log-derivative of the partition function $\mathscr{Z}$ with respect to β:

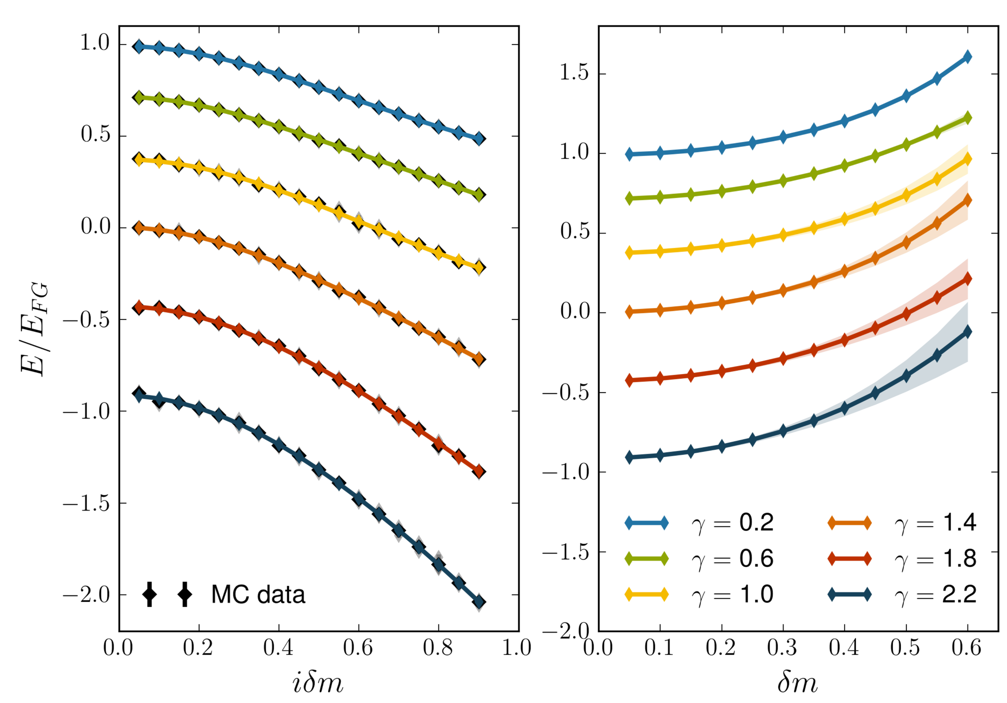
$$\langle \hat{H} \rangle = -\frac{\partial}{\partial\beta}\log\mathscr{Z}$$

Energy vs. coupling



- perfect agreement with few-body results from DFT-RG calculations [5]
- convergence to thermodynamic limit with increasing particle number for mass-balanced systems [6]

EOS for mass-imbalanced systems



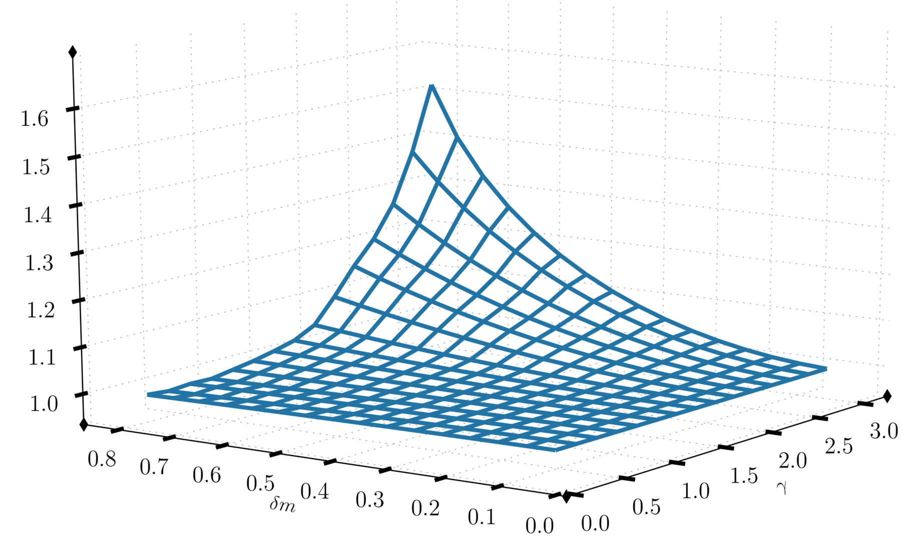
- results stable for mass-imbalances up to $\delta m \sim 0.6$, in the order of ^{6}Li and ^{40}Ka mixtures

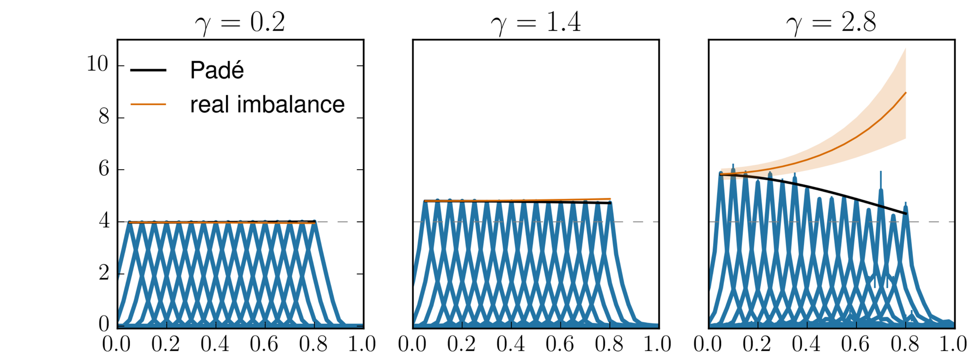
b) Pair correlations

By inserting a source term we can extract the on-site pair-correlation $\rho^{(2)}(r)$:

$$\rho_{(2)}(|x-x'|) = \langle \hat{\psi}^{\dagger}_{\uparrow}(x)\;\hat{\psi}^{\dagger}_{\downarrow}(x)\;\hat{\psi}_{\downarrow}(x')\;\hat{\psi}_{\uparrow}(x')\rangle$$

- growing peak in momentum space at $k = 0$ for increasing interaction strength
- formation of tightly-bound *bosonic pairs*
- effect of mass imbalance dominant at strong coupling
- no indication for the formation of a *Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)* phase in contrast to the 1D spin-imbalanced Fermi gas [7]





The figure shows the height of the pairing-peak at momentum $k = 0$. To underline the effect of mass-imbalance, the peak is normalized with the mass-balanced peak-height at the corresponding interaction strength.

Conclusion & Outlook

We presented precise numerical results for the ground-state energy of 1D Fermi gases in excellent agreement with previous studies. Further, we observed that the formation of bosonic pairs with zero momentum is energetically most favorable - a precursor of the formation of a superfluid ground state, at least in higher dimensions.

Our future work will aim at calculating inhomogeneous phases in Fermi gases such as the FFLO phase. Further steps towards this goal will include

- spin-imbalanced systems
- extension to the 3D unitary Fermi gas
- long-term goal: nonperturbative phase-diagrams of spin- and mass-imbalanced Fermi gases

References

[1] M.G. Ries, A.N. Wenz, G. Zürn, L. Bayha, I. Boettcher, D. Kedar, P.A. Murthy, M. Neidig, T. Lompe, and S. Jochim. *Phys. Rev. Lett.* **114**(23):230401, 2015.

[2] M. Gaudin. *Phys. Lett. A* **24**(1):55-56, 1967; C.N. Yang. *Phys. Rev. Lett.* **19**(23):1312-1315, 1967.

[3] S. Duane, A.D. Kennedy, B.J. Pendleton, and D. Roweth. *Phys. Lett. B* **195**(2):216-222, 1987.

[4] J. Braun, J.E. Drut, D. Roscher. *Phys. Rev. Lett.* **115**(5):050404, 2015.

[5] S. Kemler, M. Pospiech and J. Braun. *Journ. Phys G* **44**(1):015101, 2017.

[6] L. Rammelmüller, W.J. Porter, A.C. Loheac, and J.E. Drut. *Phys. Rev. A* **92**(1):013631, 2015.

[7] Y. Liao, A.S.C. Rittner, T. Paprotta, W. Li, G.B. Partridge, R.G. Hulet, S.K. Baur, and E.J. Mueller. *Nature* **467**:567-569, 2010.

[8] M. Wadati, T. Iida. *Phys. Lett. A* **360**(3):423-428, 2007.

[9] L. Rammelmüller, W.J. Porter, J.E. Drut, and J. Braun. *in preparation*.

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