computational studies of Fermi mixtures

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Theoretical treatment of imbalanced Fermi systems is challenging. Exact analytic methods, if available, are limited to 1D setups and thus numerical treatment is often the only viable option. Among the most successful methods for balanced Fermi gases, in particular for systems beyond the few-body regime, are Quantum Monte Carlo (QMC) approaches. For imbalanced Fermi systems, however, these approaches suffer from an exponential scaling with system size: the infamous sign-problem. A way to circumvent this issue is provided by the complex Langevin method which we employ to 1D imbalanced fermions as well as the 3D unitary Fermi gas with finite spin asymmetry. [recent review: Berger, LR, Loheac, Ehmann, Braun, Drut (*Phys. Rep.* '20)]

complex Langevin in a nutshell

- after discretizing space and (imaginary) time and performing a Hubbard-Stratonovich transformation, we can write the partition sum $\mathcal{Z}$ as a path integral over the auxiliary field ϕ:

$$\mathcal{Z} \equiv \mathrm{Tr}[e^{-\beta\hat{H}}] = \cdots = \int \mathcal{D}\phi \, \det M_\phi^\uparrow \, \det M_\phi^\downarrow \equiv \int \mathcal{D}\phi \, e^{-S[\phi]}$$

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

- similarly, we can compute observables:

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

- key idea of stochastic quantization: a $(d+1)$-dimensional random process is used to sample the measure of a d-dimensional euclidean path integral

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

- with a discrete Langevin equation we can generate a Markov chain of complexified auxiliary fields ϕ that can be used to compute observables stochastically
- the hope is to avoid the sign-problem by sampling a real (and positive) distribution in the complex plane instead of a complex distribution on the real line

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

1D fermions: polarization & mass imbalance

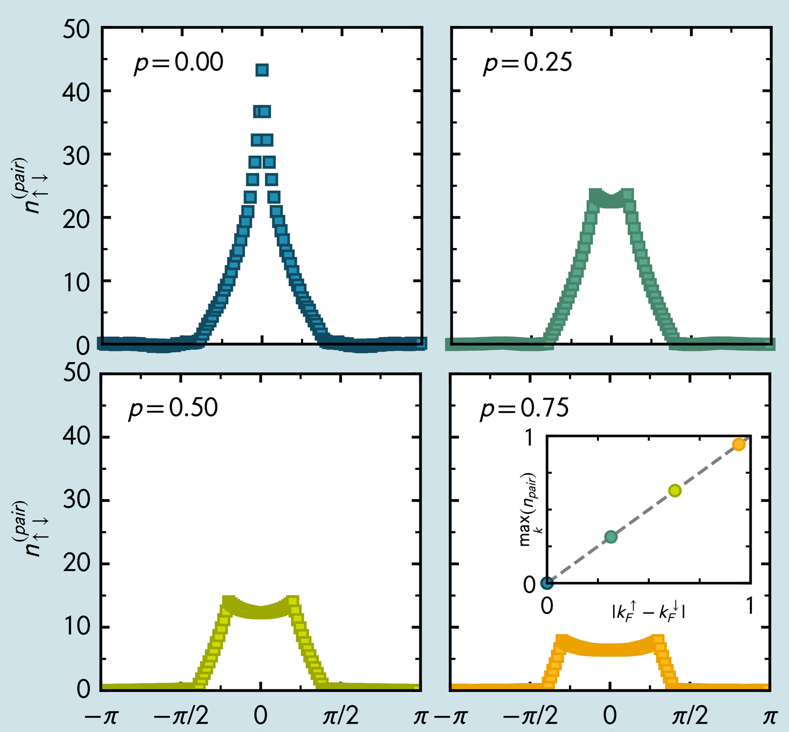
[LR, Drut, Braun (*Scipost* '20)]

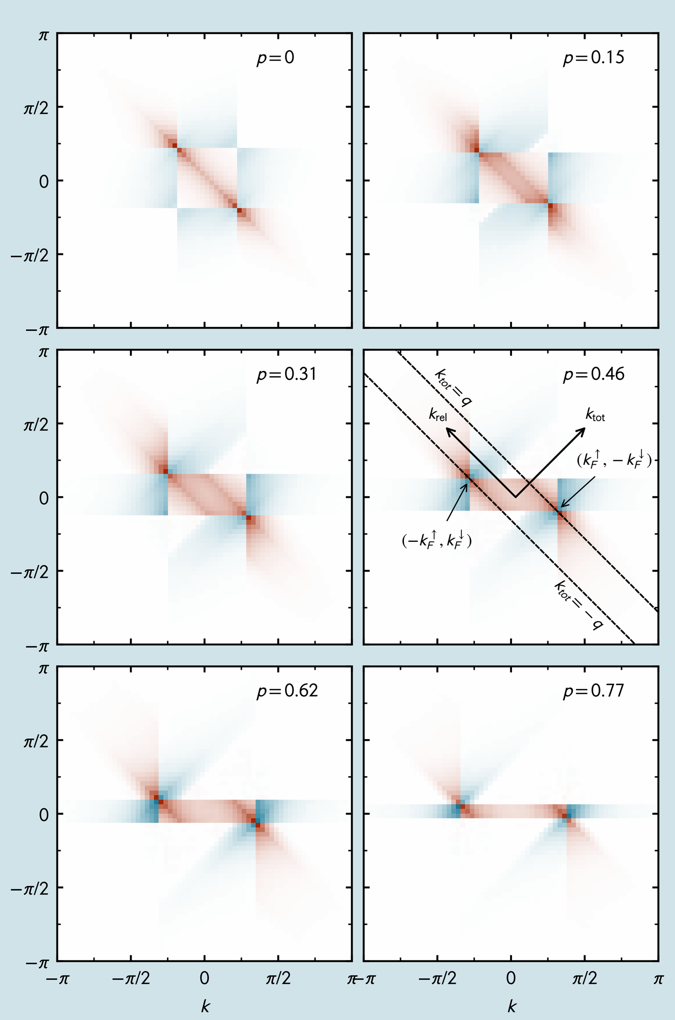
$$\hat{H} = -\sum_{s=\uparrow,\downarrow} \int \mathrm{d}^d x \, \hat{\psi}_s^\dagger(\vec{x}) \left(\frac{\hbar^2\vec{\nabla}^2}{2m_s}\right) \hat{\psi}_s(\vec{x}) + g \int \mathrm{d}^d x \, \hat{\psi}_\uparrow^\dagger(\vec{x}) \hat{\psi}_\uparrow(\vec{x}) \hat{\psi}_\downarrow^\dagger(\vec{x}) \hat{\psi}_\downarrow(\vec{x})$$

on-site pair-correlation function:

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

- off-center peak in pair-momentum distribution at $q = |k_F^\uparrow - k_F^\downarrow|$
- spatially oscillating "order parameter" (inhomogeneous pairing)

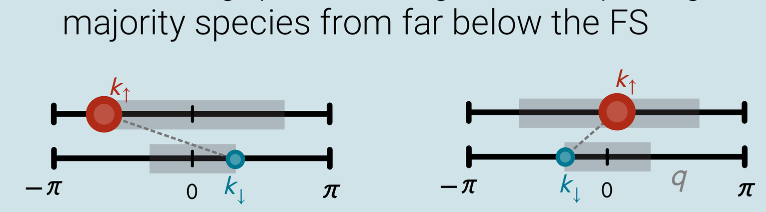


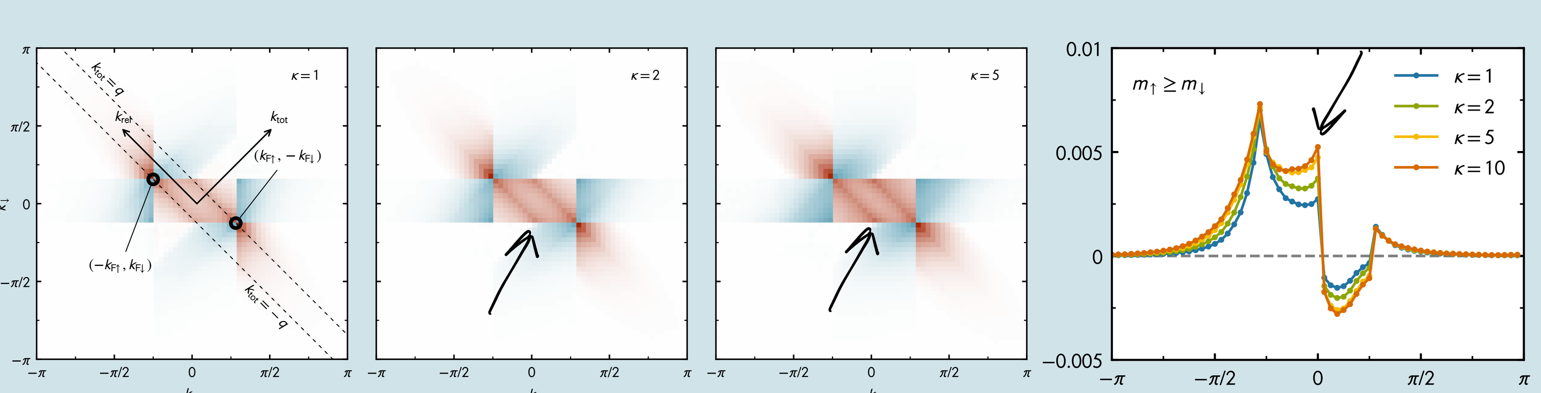


density-density correlations (k-space):

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

- clean signal of FFLO-type pairing
- peak position in pair-momentum distribution remains constant despite increasing mass imbalance, density-density correlator shows difference in structure
- sub-leading peak emerges, with pairing of majority species from far below the FS

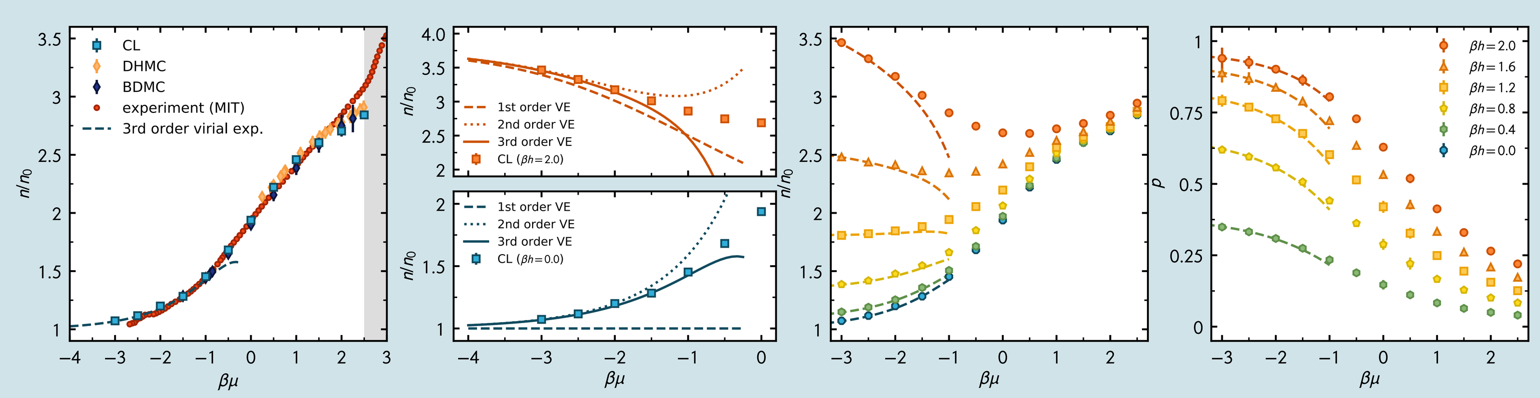




3D spin-polarized unitary Fermi gas

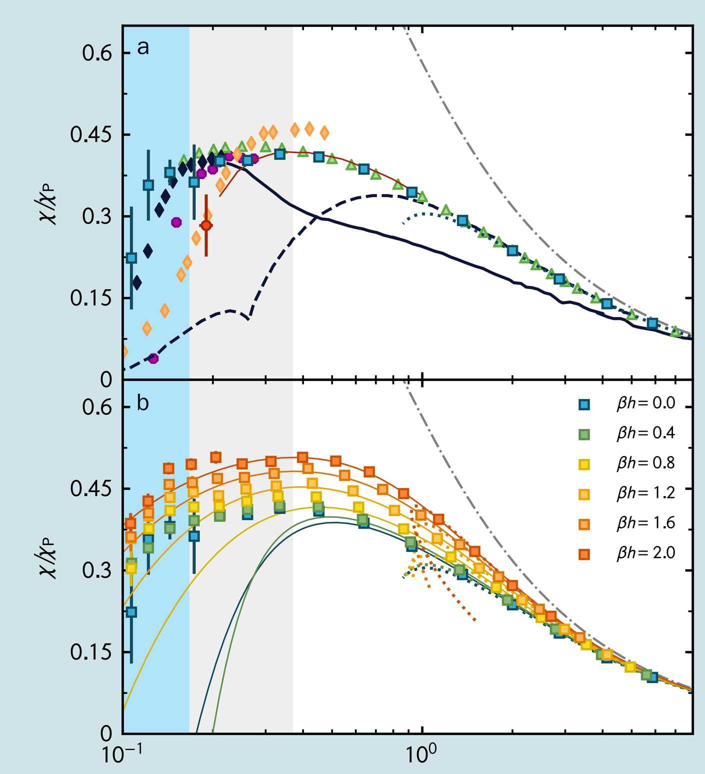
[LR, Loheac, Drut, Braun (*PRL* '18); LR, Hou, Drut, Braun (*to appear in PRA* '21)]

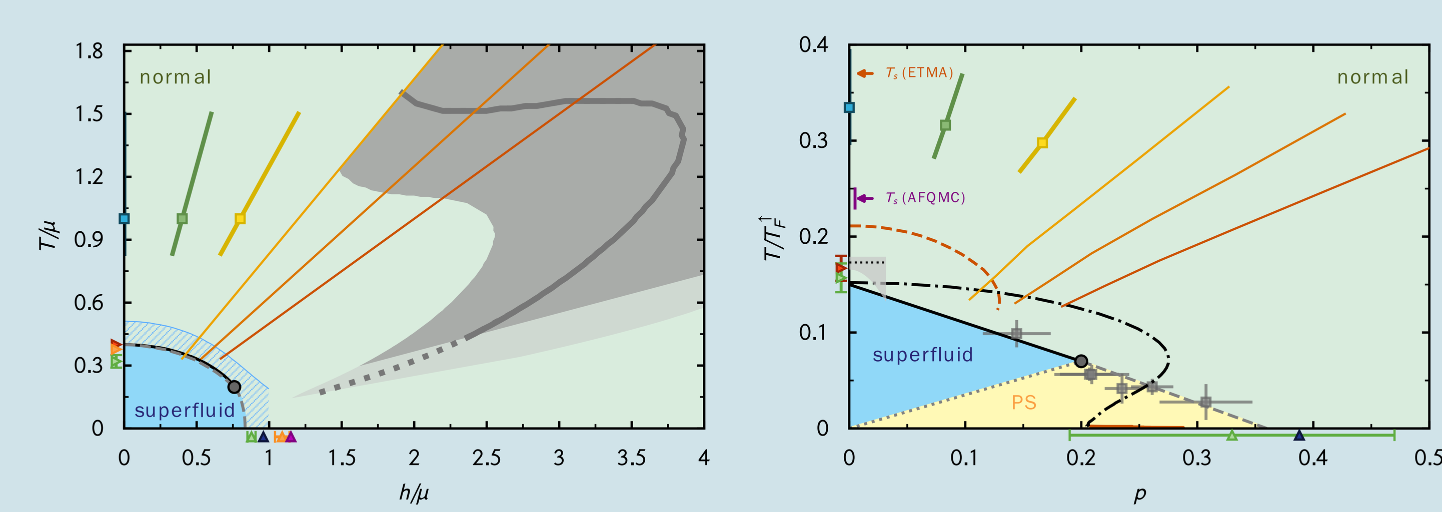
$$\mathcal{Z} = \mathrm{Tr}[\mathrm{e}^{-\beta(\hat{H} - \mu_\uparrow\hat{N}_\uparrow - \mu_\downarrow\hat{N}_\downarrow)}] = \mathrm{Tr}[\mathrm{e}^{-\beta(\hat{H} - \mu\hat{N} - h\hat{M})}]$$



thermodynamic properties

- balanced gas: excellent agreement with experimental results and state-of-the-art numerical data [experiment/BDMC: Van Houcke et al. '12; Ku et al. '12; DHMC: Drut, Lähde, Wlazlowski, Magierski '12; AFQMC: Richie-Halford,Drut,Bulgac '20; Jensen,Gilbreth,Alhassid '20; (E)TMA: Tajima et al. '14; Pantel et la. '14; LW: Enns,Haussmann '12; Frank et al. '20]
- low T: thermal wavelength λ_T increases, finite volume effects visible (currently $V = 11^3$)
- virial expansion (VE) & resummation: valid at high temperature ($\beta\mu < 0$), provides an important benchmark for polarized systems
- probe for pseudogap physics: anomalously suppressed spin-susceptibility above T_c would be indicative of pairing [PD: Boettcher et al. '14 (fRG); Shin et al. '08 (experiment)]
- CL suggests that pesudogap is absent for sizable imbalances, inconclusive for near-balanced systems





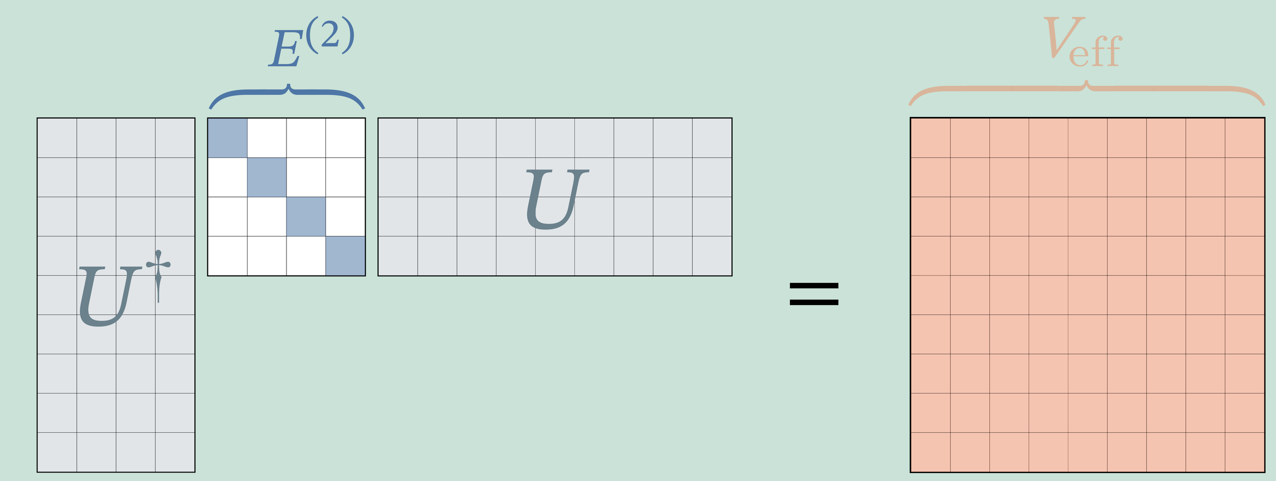
harmonically trapped 1D fermions with effective interaction

[LR, Huber, Hammer, Volosniev *in preparation*]

Here we show preliminary results for harmonically trapped fermions in 1D obtained with the full-configuration interaction (FCI) method, also known as exact diagonalization in a truncated basis. Generally, convergence with basis size is poor which limits computations to relatively small particle numbers. To mitigate this shortcoming, we can use a trick known in nuclear physics, namely an effective interaction, that dramatically speeds up calculations.

$$\hat{H}_{\mathrm{trap}} = \hat{H} + \sum_{s=\uparrow,\downarrow} \int \mathrm{d}^d x \, \hat{\psi}_s^\dagger(\vec{x}) \left(\frac{m\omega^2}{2} x^2\right) \hat{\psi}_s(\vec{x})$$

effective interaction



- use exact solution to fix lowest part of the spectrum (in this case by Busch-formula) [Rotureau '13; Busch et al. '98]
- essentially this is a particularly useful renormalization procedure that relates the spectrum to the scattering length
- convergence properties with basis cutoff n_b are drastically improved

benchmark against literature data

- compares well with $n_b \to \infty$ extrapolated data for $3\uparrow + 1\downarrow$ particles [Grining et al. '15;]
- relative error for energies $\lesssim 1\%$ already at $n_b \approx 15$
- accurate energies for experimentally relevant regimes for polaronic and paired systems [Heidelberg experiments: Wenz et al. '13; Zürn et al. '13]
- density profiles: converge slower as the common wisdom suggests, effective interaction shows excellent behavior
- efficiency: all computations have been done in $\lesssim 30$ minutes on a standard notebook, allows us to push particle number further than previously possible