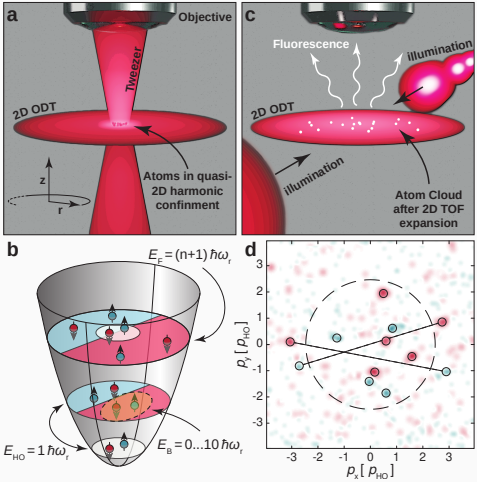
Density profiles and correlations of harmonically trapped ultracold fermions

Felipe Attanasio, **Marc Bauer**, J. M. Pawlowski

Heidelberg University

Why cold quantum gases?

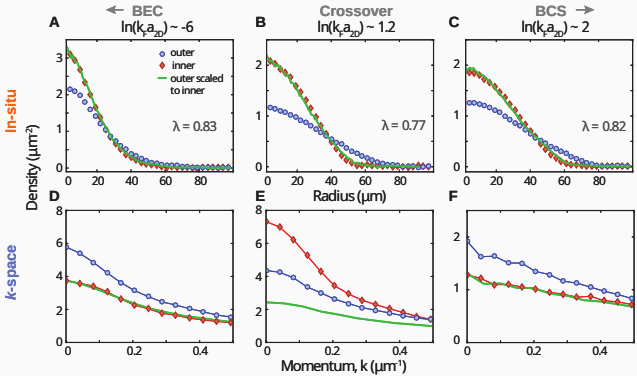
- Experiments with tunable Hamiltonians.
- Testing ground for theories.
- Relatively low cost of experimental setups.
- Access to lower dimensions via tuning of trapping frequency.



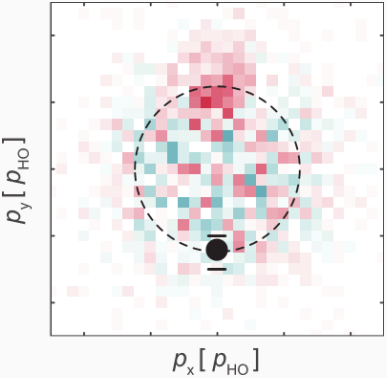
[Jochim et. al. 2021 arXiv:2109.11511]

Whats being done/can be done in experiment

Direct access to density profiles and correlations in position and momentum space.



[Jochim et. al. 2018 arXiv:1805.04734]



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Action and auxiliary field transform

Low energy action in 1+1 dimensions

$$S[\psi^\dagger, \psi] = \int_0^\beta dt \int dx \psi_\sigma^\dagger \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu_\sigma + V_t x^2\right) \psi_\sigma - \lambda \psi_\uparrow^\dagger \psi_\uparrow \psi_\downarrow^\dagger \psi_\downarrow$$

auxiliary field transform in density channel, large freedom to choose HS-transform

$$e^{\lambda \Delta t \hat{\psi}_\uparrow^\dagger \hat{\psi}_\uparrow \hat{\psi}_\downarrow^\dagger \hat{\psi}_\downarrow} = \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \left(1 + \hat{\psi}_\uparrow^\dagger \hat{\psi}_\uparrow A \sin\phi\right) \left(1 + \hat{\psi}_\downarrow^\dagger \hat{\psi}_\downarrow A \sin\phi\right)$$

$$A = \sqrt{2\left(e^{\lambda \Delta t} - 1\right)}$$

Integrating over the fermions yields

$$Z = \int \mathcal{D}\phi \det M_\uparrow[\phi] \det M_\downarrow[\phi]$$

The sign problem

$\lambda > 0$ attractive coupling $\longrightarrow A \in \mathbb{R}$.
In the balanced case $\mu_\uparrow = \mu_\downarrow$

$$\det M_\uparrow = \det M_\downarrow \in \mathbb{R} \longrightarrow \prod_\sigma \det M_\sigma \in \mathbb{R}_{\geq 0}$$

$\longrightarrow$ No sign problem!

Two cases of sign problems in the system:

Attractive, but imbalanced $\mu_\uparrow \neq \mu_\downarrow$

$$\det M_\uparrow \det M_\downarrow \in \mathbb{R}$$

$\longrightarrow$ Possible sign problem.

$\lambda < 0$ repulsive coupling $\longrightarrow A \in i\mathbb{R}$

$$\det M_\uparrow \det M_\downarrow \in \mathbb{C}$$

$\longrightarrow$ Sign problem (complex weights)!

Complex Langevin

Complexify:

Complex Langevin

$$\partial_\tau \operatorname{Re}\left[\phi_{t,x}\right] = -\operatorname{Re}\left[\frac{\partial S}{\partial \phi_{t,x}} + \sigma \phi_{t,x}\right] + \eta_{t,x}$$

$$\partial_\tau \operatorname{Im}\left[\phi_{t,x}\right] = -\operatorname{Im}\left[\frac{\partial S}{\partial \phi_{t,x}} + \sigma \phi_{t,x}\right]$$

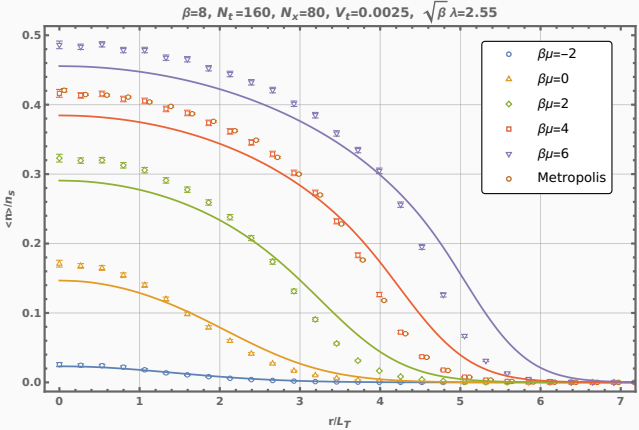
Gaussian regulator $\frac{\sigma}{2}\phi^2$ is added to the action. Typical value: $\sigma = 0.1$. [Loheac, Drut '17 arXiv: 1702.04666]

$\rightarrow$ Avoids sign problem in many situations.

Can have issues with wrong convergence in some cases.

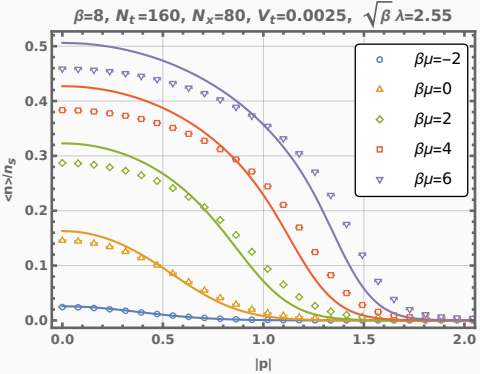
Attractive case density

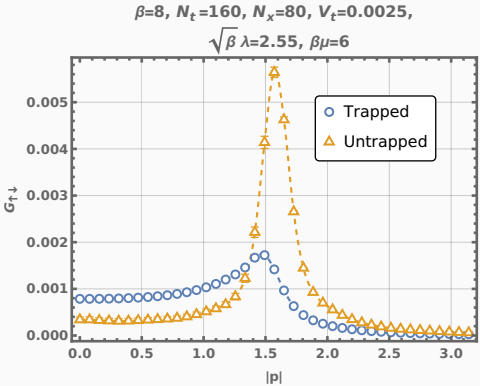
The characteristic length of the trap is given by $L_t = (2mV_t)^{-\frac{1}{4}}$.



Density profile for attractive interactions, solid line indicate free case tuned to average particle content of the interacting one.

Density correlations and momentum space





Density-density correlations at $(k, -k)$: $G_{\uparrow\downarrow}(k) = \langle n_\uparrow(k) n_\downarrow(-k)\rangle - \langle n_\uparrow(k)\rangle\langle n_\downarrow(-k)\rangle$.

Correlations indicate pairing around k_F.

Status of complex Langevin for cold atoms systems

Successes:

- Ground state studies of spin & mass imbalanced systems. [Rammelmüller et al., arXiv: 2003.06853]
- Repulsive systems at finite temperature & ground state (low to moderate couplings). [Rammelmüller et al., arXiv: 1708.03149]
- Computation of Virial coefficients via Fourier projection with complex μ [Shill, Drut, arXiv: 1808.07836]
- ...

Open Questions

- Finding a suitable regulator of larger repulsive couplings.
- What happens at lower temperature?
- Applicability in presence of Trapping potential.

Applicability of CL

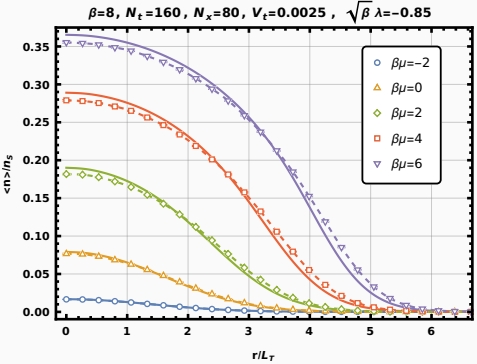
Attractive couplings:

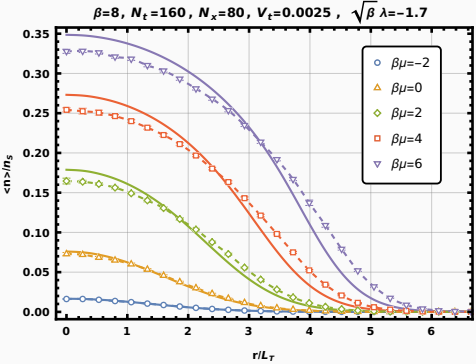
- Weight is real, but not necessarily positive.
- Problematic for drift based/Langevin methods. [M. Nagasawa, J. Math. Biol. 9, 213 (1980)]
- Problem for complex Langevin in particular. [Flower et al. Phys. Rev. D34 (1986) 598]

Repulsive couplings:

- In principal amenable to complex Langevin simulations under the usual constraints.
- Regulator necessary even at small couplings.
- Previous studies found correct results up to $\sqrt{\beta}\lambda = 2$. [Loheac, Drut '17 arXiv: 1702.04666]

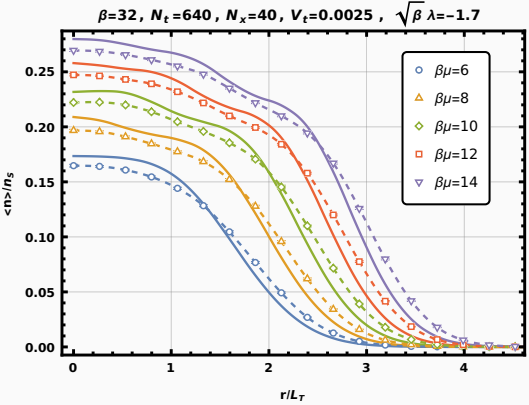
Repulsive density profiles

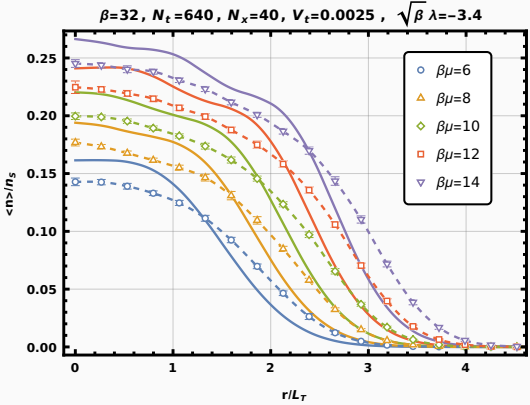




- Observables show stable convergence.
- Slight flattening distribution in comparison to the Free case at same average particle content.

Repulsive density profile at larger β

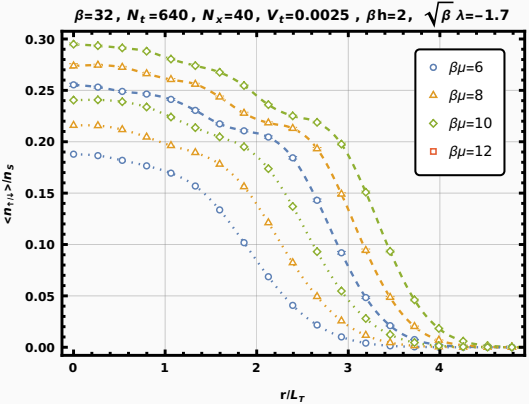


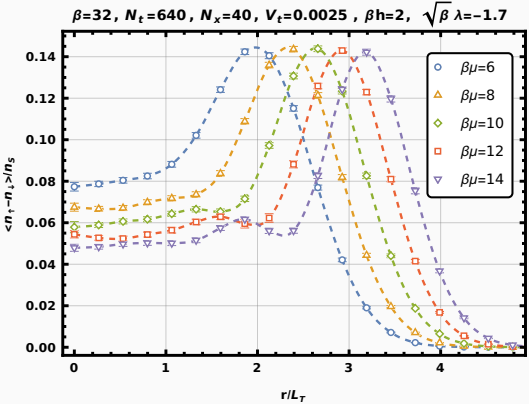


Slow decay in observables!

Repulsive and imbalanced

Introduce imbalance via h with $\mu_\uparrow = \mu + h$, $\mu_\downarrow = \mu - h$.





Summary & Outlook

Summary:

- Some first results for complex Langevin in harmonically trapped non-relativistic fermion systems.
- Applicable range appears similar to the untrapped case.

Future:

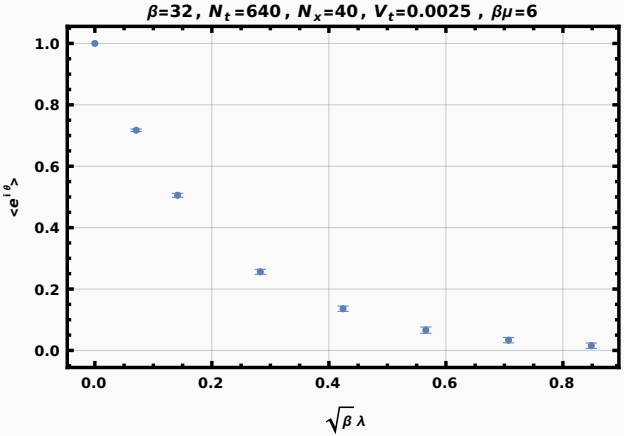
- Thorough analysis of boundary terms.
- Search for more sophisticated regulation.
- Projection to fixed particle number.

Thanks for your attention!

Backup: Average phase

We calculate the average phase of a metropolis simulation in the repulsive case as a function of the dimensionless coupling.

→ Strong sign problem at $\sqrt{\beta} = .8$ already



Backup: Attractive imbalanced, sign problem?

Attractive, imbalanced systems do not **necessarily** show a sign problem. Plot shows quenched Metropolis vs. Langevin at finite imbalance. No samples of negative weight are encountered.