Ultracold polarons and impurities in one-dimensional optical lattices

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Ultracold polarons and impurities

1. Polarons and **impurities** in **ultracold atomic** systems.
2. One-dimensional **harmonically confined lattice polarons** and **counterflows.**
3. Mobile **impurity** interacting with a **Hubbard chain**.
4. Summary and **future work**.

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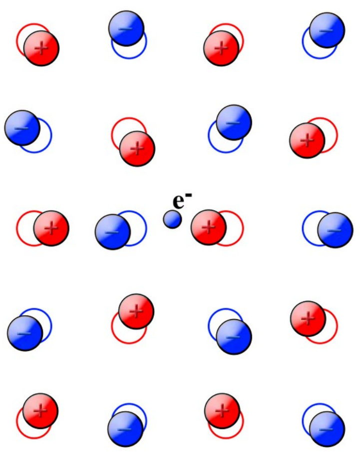
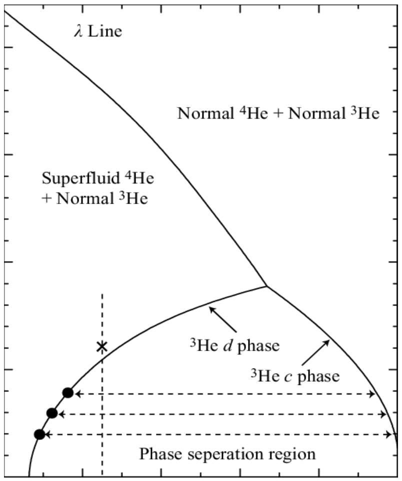
Polarons and impurities

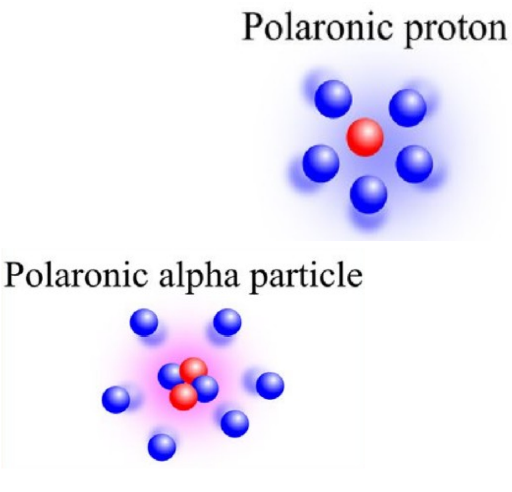
- The study of **impurities** immersed in a **quantum medium** has a **long history** and is **relevant** in **many fields** of physics.



Electrons in an ionic crystal
L. Landau and S. Pekar, Zh. Eksp. Teor. Fiz **18**, 419 (1948).



^{3}He impurities in ^{4}He
G. Baym and C. Pethick, *"Landau Fermi-Liquid Theory: Concepts and Application"* (1991).



Impurities in nuclear systems
Tajima *et al.*, AAPPS Bulletin, **34**, 9 (2024).

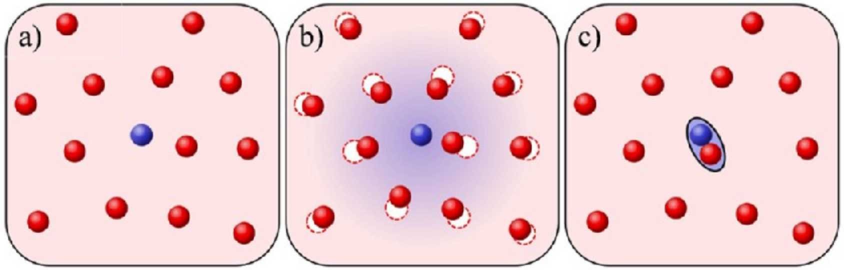
- Such **impurities** often **form** dressed **quasiparticles** referred to as **polarons**.

Polarons in ultracold atomic gases

- The **study of polarons** has been **revitalised** thanks to their **experimental realisation** in **ultracold atomic gases**.
- Impurities are realised with **highly imbalanced** atomic **mixtures**.

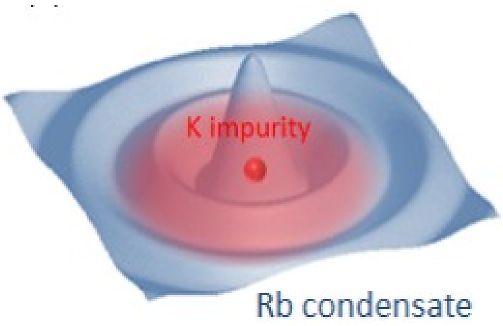
C. Baroni, G. Lamporesi and M. Zaccanti, Nat. Rev. Phys. **6**, 736 (2024).

Fermi polaron



A. Schirotzek *et al*., PRL **102**, 230402 (2009).

Bose polaron



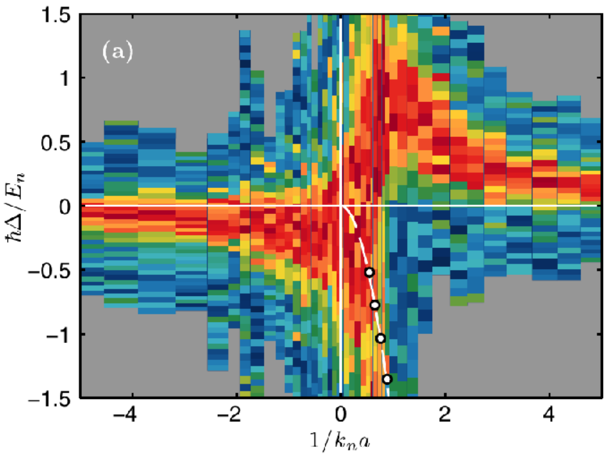
M.-G. Hu *et al*., PRL **117**, 055301 (2016).

- **Ultracold atoms** offer **high controllability**, being an ideal platform for studying impurities and polarons.

P. Massignan *et al*., Rep. Prog. Phys. **77** 034401 (2014).
F. Grusdt *et al*. Rep. Prog. Phys. **88**, 066401 (2025).
P. Massignan *et al*., arXiv:2501.09618 (2025).

Polarons in ultracold atomic gases

- Several properties can be examined:
  - → **Polaron energies**, **residue**, effective masses, etc.
- Impurities can be used to **probe** and **manipulate** quantum systems:
  - → Transport properties, **phase transitions**, **mediated interactions**, etc.
- Theoretical techniques:
  - → Variational approaches, QMC, ED, RG, Tensor Networks, etc.



Spectral response of an impurity In a BEC

N. B. Jørgensen, *et al.*, PRL **117**, 055302 (2016).

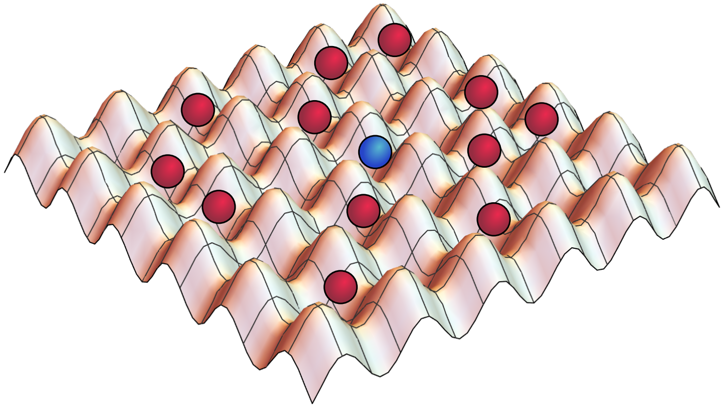
Lattice polarons

- A **rich platform** for **studying** ultracold atomic **impurities** is **optical lattices**.
  M. Lewenstein *et al.*, *Ultracold Atoms in Optical Lattices: Simulating Quantum Many-Body Systems* (Oxford, 2012).
  C. Gross and I. Bloch, Science **357**, 995 (2017).

- Such impurities are now referred to as **lattice polarons**.

- Ultracold atoms in **tight lattices** can be modelled with a **Hubbard-**based Hamiltonian.

- Recent theoretical studies have considered both
  - → a bosonic medium*,
    V. Colussi, C. Menotti C and A. Recati, PRL **130**, 173002 (2023).
    M. Santiago-García, S. Castillo-López and A. Camacho-Guardian, NJP **26,** 063015 (2024).
    F. Gómez-Lozada, H. Hiyane, T. Busch, T. Fogarty, PRR **7**, 023053 (2025).
  - → and a fermionic medium*.
    I. Amelio and N. Goldman, Scipost Physics **16**, 056 (2024).
    H. Hu, J. Wang, X.-J. Liu, PRA, **110**, 023314 (2024).
    G. Pascual, J. Boronat, K. Van Houcke, PRR **7**, L042024 (2025).



* Non-comprehensive list.

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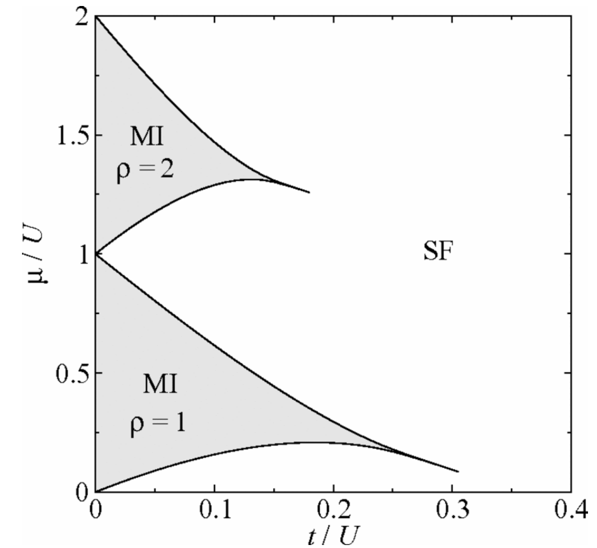
Phys. Rev. Lett. **135**, 023404 (2025)

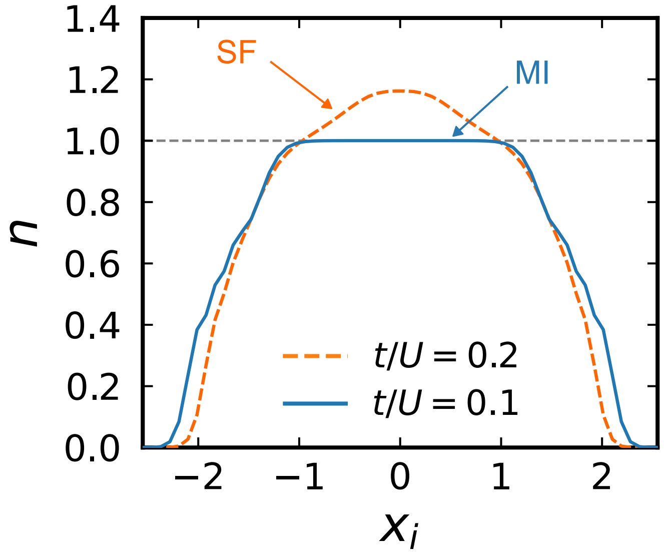
Bosons in optical lattices

- Bosons in optical lattices feature a **superfluid-to-Mott insulator** (SF-MI) transition.
- The study of **impurities across** this **SF-MI transition** has attracted increasing attention.

V. E. Colussi, F. Caleffi, C. Menotti, and A. Recati, Phys. Rev. Lett **130**, 173002 (2023).
R. Alhyder, V. E. Colussi, M. Čufar, J. Brand, A. Recati, G. M. Bruun, SciPost Phys. **19**, 002 (2025).



Phase diagram of the 1D BH model.
S. Ejima *et al.*, PRA **85**, 053644 (2012).



Density profiles of bosons in a 1D optical lattice with harmonic confinement.

- Bosons in tight lattices are described by the **Bose-Hubbard model**:

$$\hat{H} = \underbrace{-t \sum_i \left(\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.} \right)}_{\text{Tunnelling}} + \underbrace{V_{\text{ho}} \sum_i i^2 \hat{n}_i}_{\text{Harmonic trap}}$$

$$+ \underbrace{\frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)}_{\text{Boson-boson repulsion}}.$$

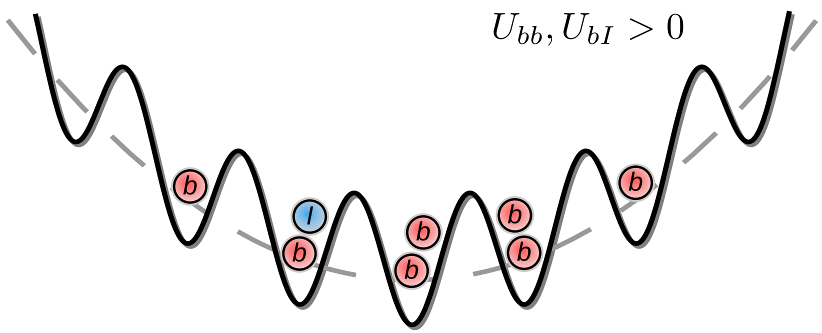
Harmonically confined lattice polarons

- We studied a **single impurity** interacting with a **bosonic bath** in a **one-dimensional harmonically confined optical lattice**.

$$\hat{H} = \underbrace{-t \sum_{\sigma=b,I} \sum_i \left(\hat{a}^{\dagger}_{i,\sigma} \hat{a}_{i+1,\sigma} + \text{h.c.} \right)}_{\text{Tunnelling}}$$

$$+ \underbrace{V_{\text{ho}} \sum_i \sum_{\sigma=b,I} i^2 \hat{n}_{i,\sigma}}_{\text{Harmonic trap}}$$

$$+ \underbrace{\frac{U_{bb}}{2} \sum_i \hat{n}_{i,b} \left(\hat{n}_{i,b} - 1 \right)}_{\text{Boson-boson repulsion}} + \underbrace{U_{bI} \sum_i \hat{n}_{i,b} \hat{n}_{i,I}}_{\text{Bath-impurity repulsion}} .$$

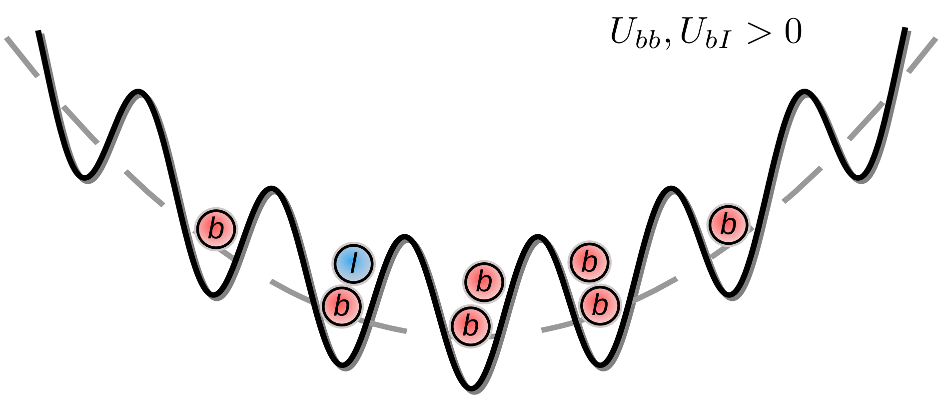


- We employed the **density matrix renormalisation group (DMRG)** for **large lattices** with a **large number of particles**.

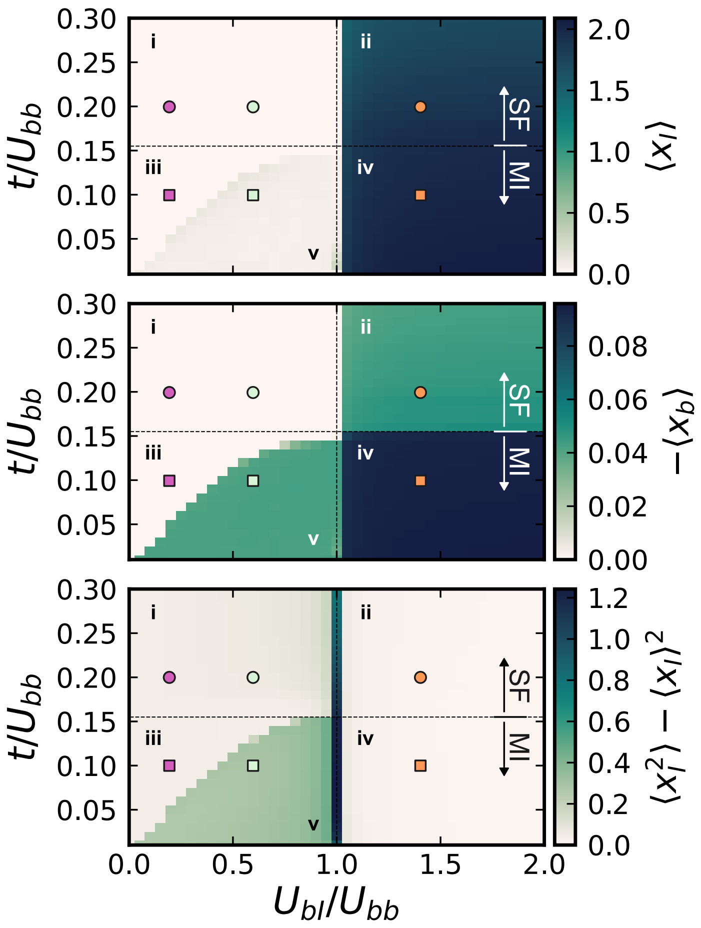
S. R. White, Phys. Rev. Lett. **69**, 2863 (1992). U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).

Harmonically confined lattice polarons

- We **considered** a **bath** that is **completely SF** for $t/U_{bb}>0.155$ and that has a **MI domain** of **unity filling** for $t/U_{bb}<0.155$.
- The main **DMRG simulations** considered $N_b=40$ bosons.
- However, we obtained **identical results** for **other choices**, and even a **qualitative agreement** with **ED**.



Density profiles



Density profiles:

$$n_\sigma(i) = \langle \hat{n}_{i,\sigma} \rangle$$

Average position:

$$\langle x_\sigma \rangle = \frac{1}{N_\sigma} \sum_i x_i n_\sigma(i)$$

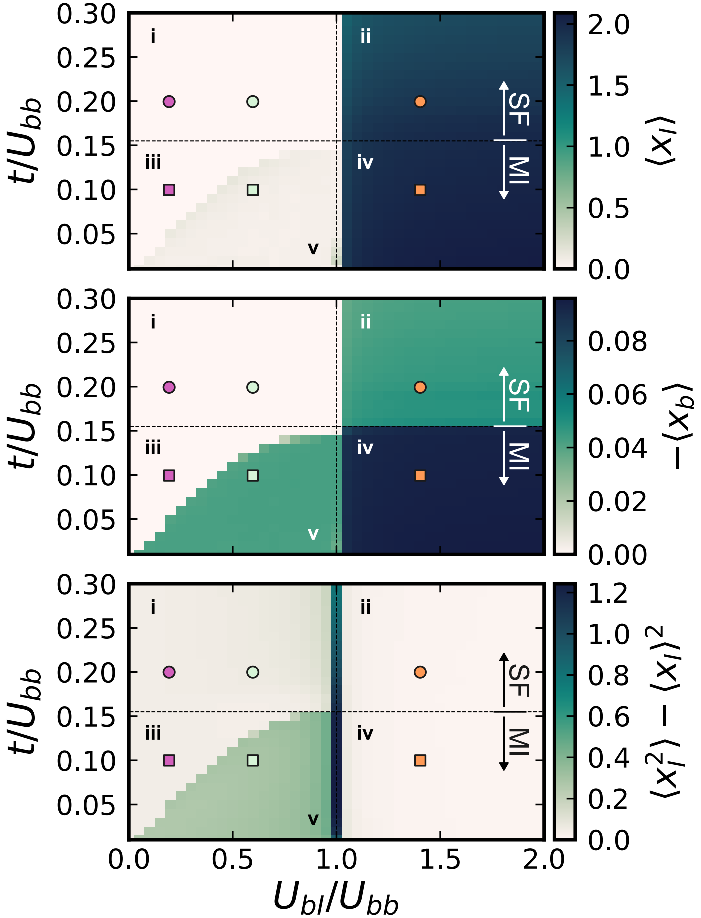
Impurity cloud:

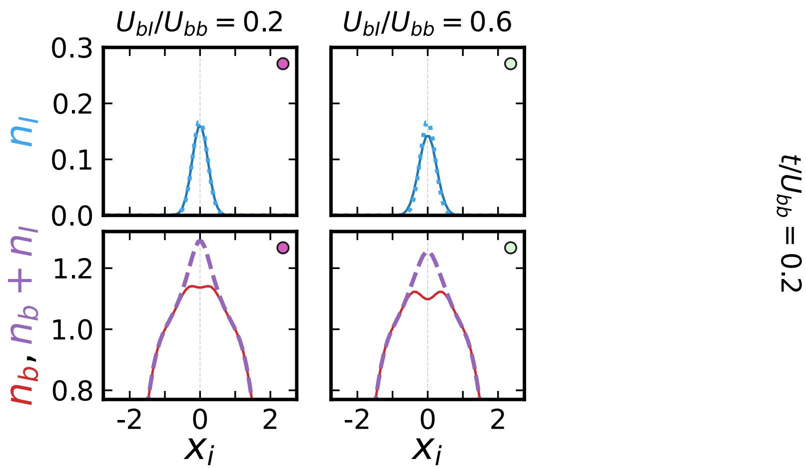
$$\langle x_I^2 \rangle = \frac{1}{N_\sigma} \sum_i x_i^2 n_I(i)$$

$$x_i = i\, d/\xi, \quad \xi = d\sqrt{t/V_{\rm ho}}.$$

- The system shows **well-defined phases**.

Density profiles





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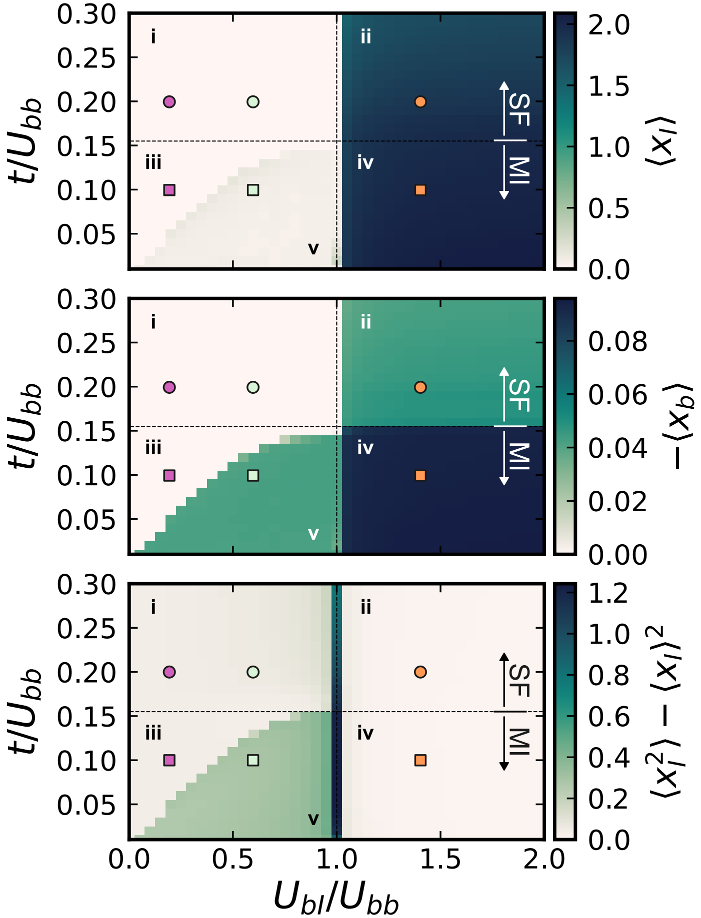
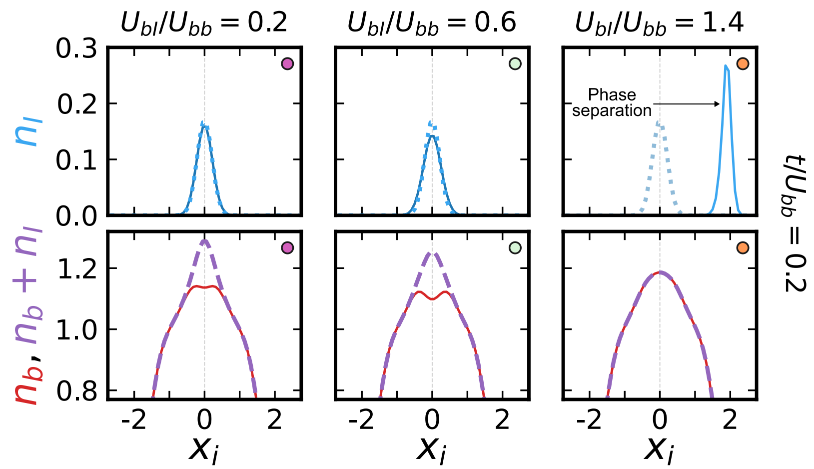
$$x_i = i\, d/\xi, \quad \xi = d\sqrt{t/V_{\rm ho}}.$$

- **Region i** is a **miscible** phase where the **impurity repels** the **compressible SF bath**.

Density profiles





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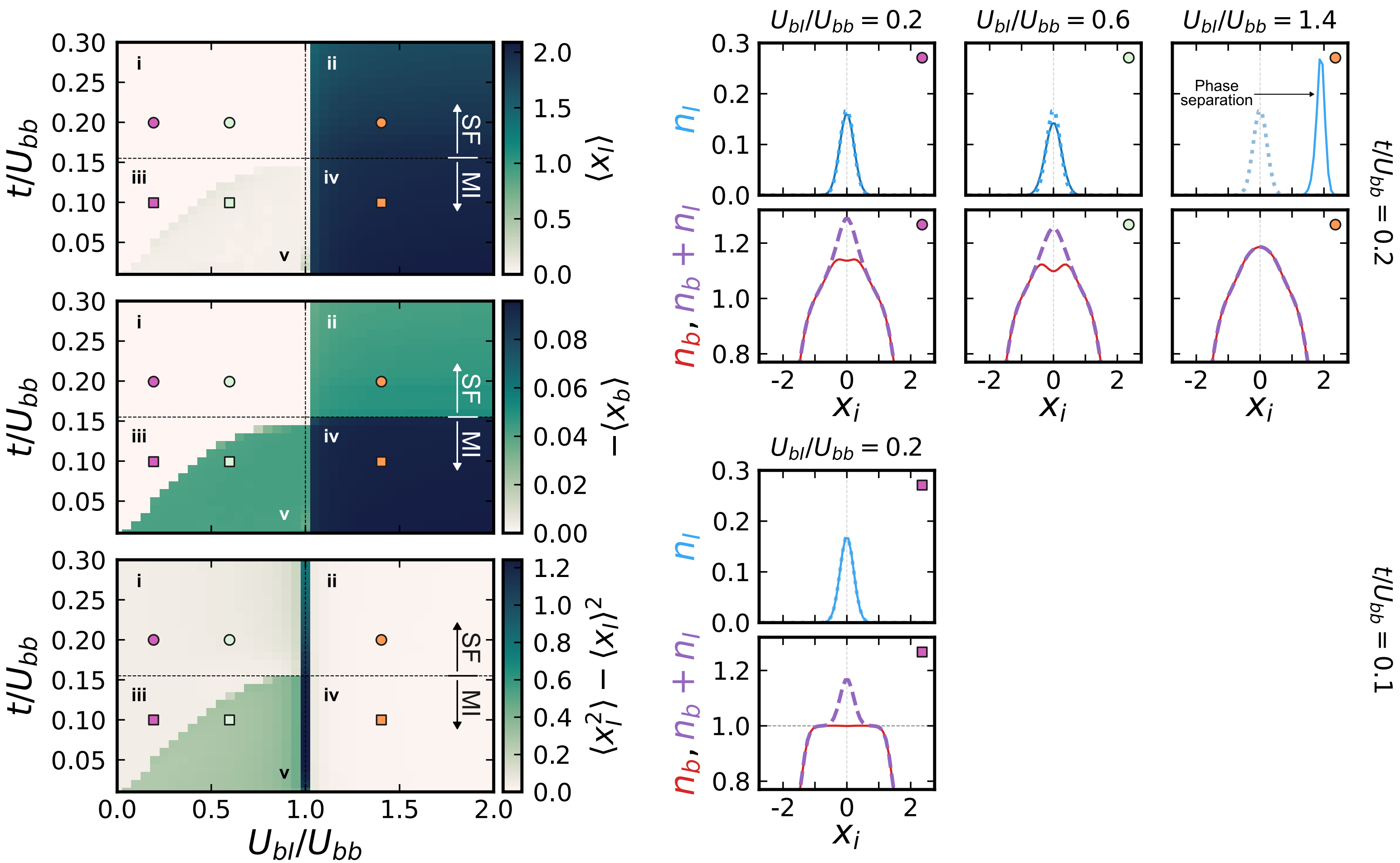
$$x_i = i\, d/\xi, \quad \xi = d\sqrt{t/V_{\mathrm{ho}}}.$$

- **Region ii** is simply a **phase-separated** configuration.

Density profiles



Density profiles:

$$n_\sigma(i) = \langle \hat{n}_{i,\sigma} \rangle$$

Average position:

$$\langle x_\sigma \rangle = \frac{1}{N_\sigma} \sum_i x_i n_\sigma(i)$$

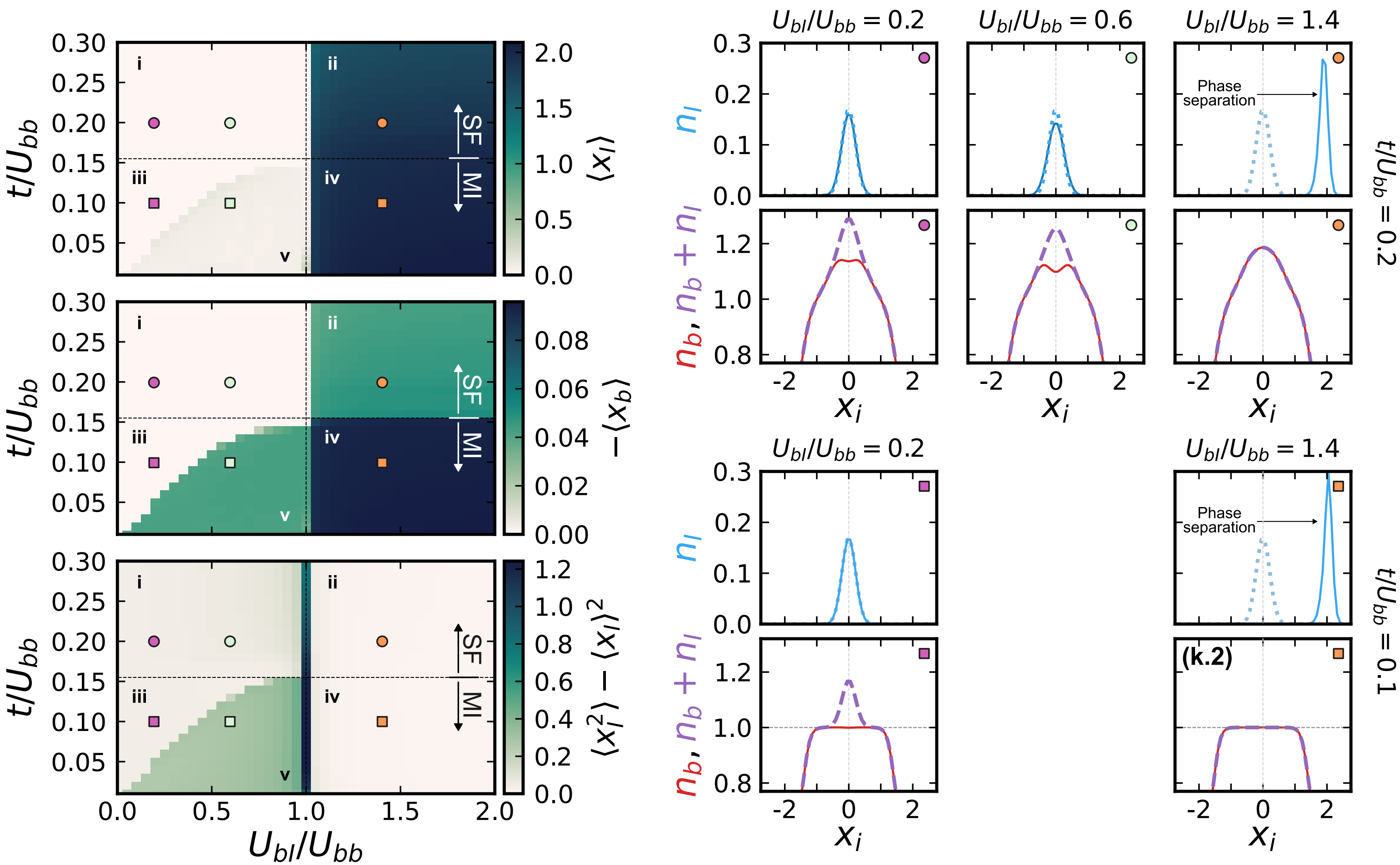
Impurity cloud:

$$\langle x_I^2 \rangle = \frac{1}{N_\sigma} \sum_i x_i^2 n_I(i)$$

$$x_i = i\, d/\xi, \quad \xi = d\sqrt{t/V_{\rm ho}}.$$

- **Region iii** is another **miscible phase**. The **MI bath** remains **undisturbed** due to its **incompressibility**.

Density profiles



Density profiles:

$$n_\sigma(i) = \langle \hat{n}_{i,\sigma} \rangle$$

Average position:

$$\langle x_\sigma \rangle = \frac{1}{N_\sigma} \sum_i x_i n_\sigma(i)$$

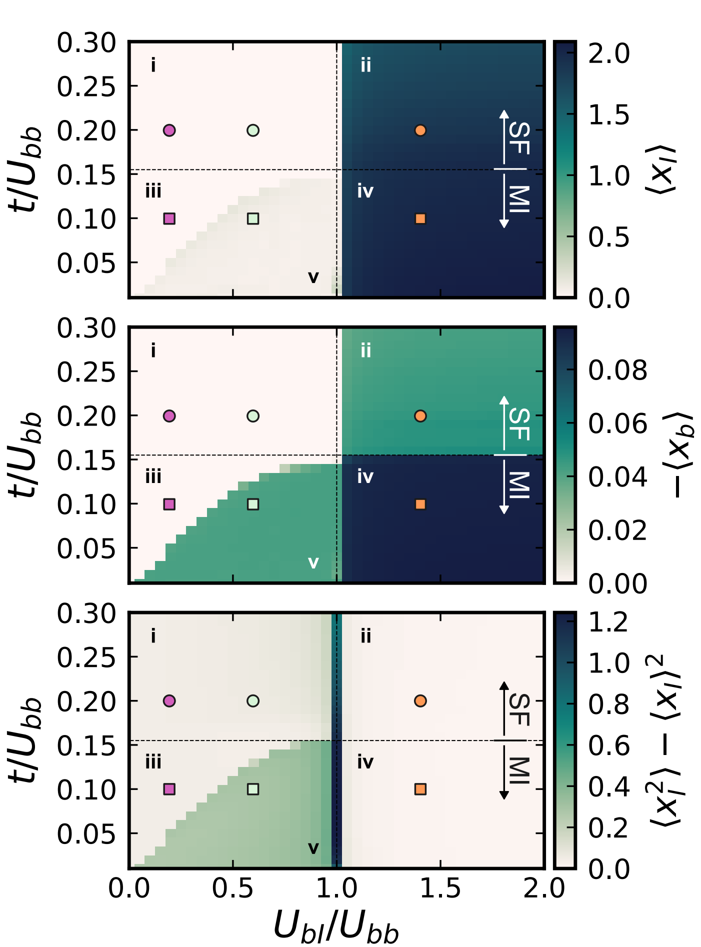
Impurity cloud:

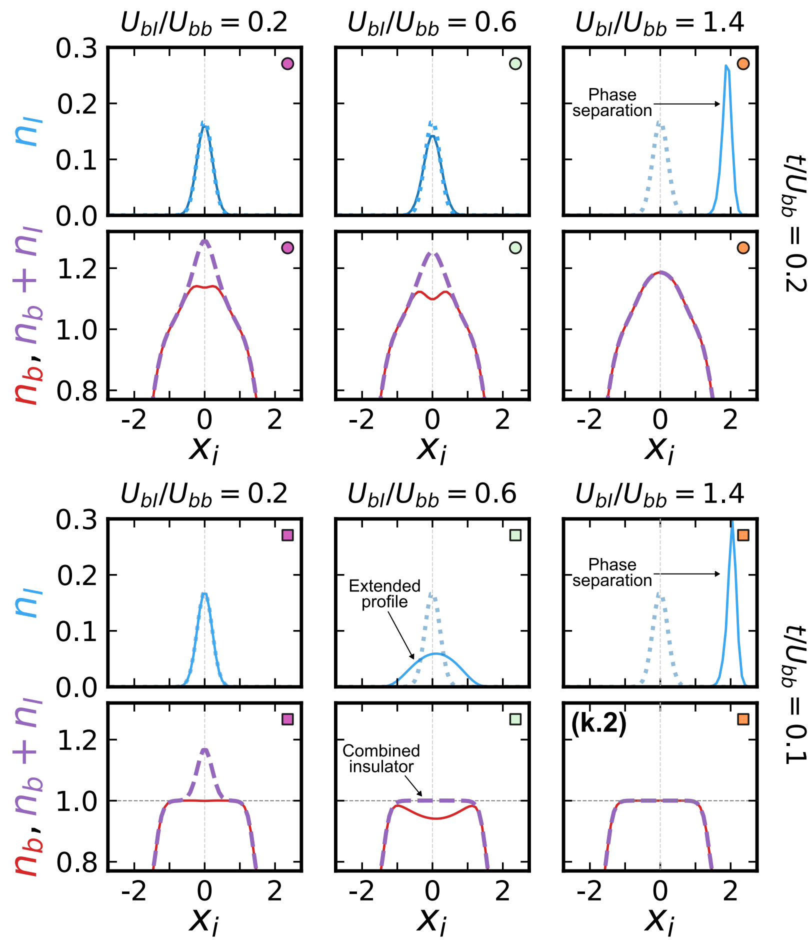
$$\langle x_I^2 \rangle = \frac{1}{N_\sigma} \sum_i x_i^2 n_I(i)$$

$$x_i = i\, d/\xi, \quad \xi = d\sqrt{t/V_{\rm ho}}.$$

- **Region iv** is another **phase-separated** configuration. The MI bath moves further away than an SF bath.

Density profiles





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Average position:

$$\langle x_\sigma \rangle = \frac{1}{N_\sigma} \sum_i x_i n_\sigma(i)$$

Impurity cloud:

$$\langle x_I^2 \rangle = \frac{1}{N_\sigma} \sum_i x_i^2 n_I(i)$$

$$x_i = i\, d/\xi, \quad \xi = d\sqrt{t/V_{\rm ho}}.$$

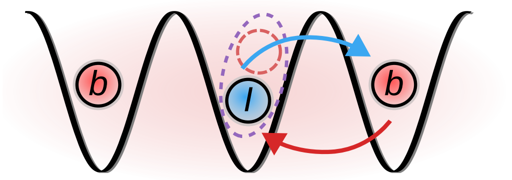
- **Region v** is a non-trivial phase where the **impurity** exhibits an **extended profile**, and the **combined profile** of the bath and impurity displays a domain of **unity filling**.

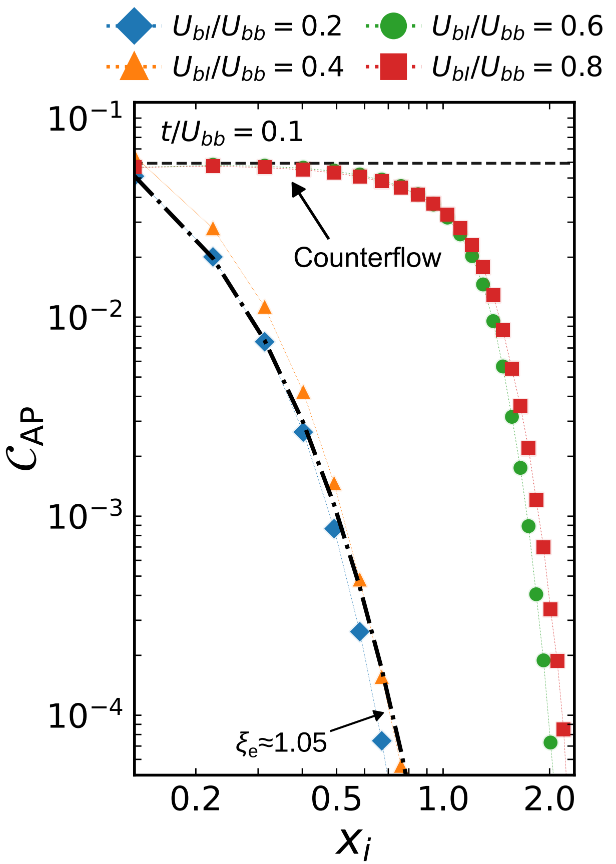
Counterflow

- The new state corresponds to a **counterflow phase**.
- It shows **anti-pair order**

$$\mathcal{C}_{\mathrm{AP}} = \langle \hat{a}_{0,I} \hat{a}^{\dagger}_{0,b} \hat{a}^{\dagger}_{i,b} \hat{a}_{i,I} \rangle.$$

- Counterflows were **realised experimentally** very recently with **binary Mott insulators**.
  Y.-G. Zheng *et al.*, Nat. Phys. **21**, 208 (2025).
- Our results show that **counterflows** appear for **large population imbalances**.
- **Counterflows** show properties of **insulators**.

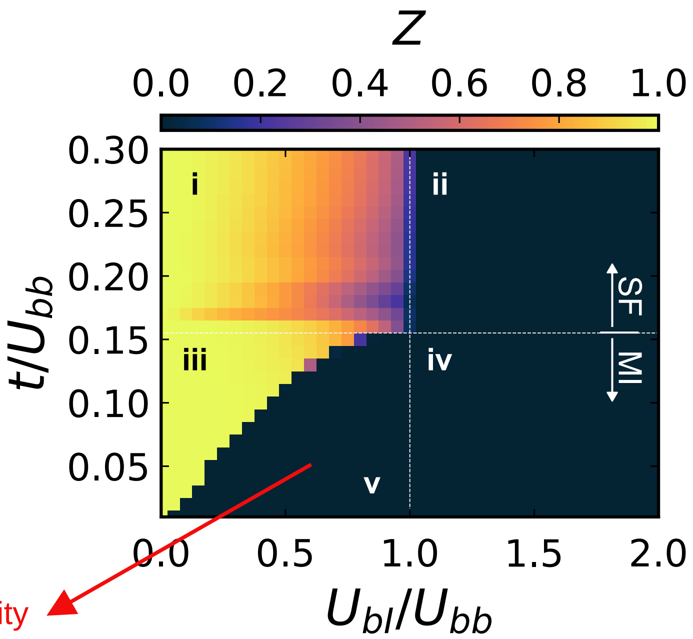




Counterflow

- The **impurity forms** this **correlated state** with (almost) the **whole insulating bath**.
- The **residue** abruptly **vanishes** at the **phase transition**.

$$Z(U_{bI}) = |\langle \Psi(U_{bI} = 0) | \Psi(U_{bI}) \rangle|^2.$$



Orthogonality

Counterflow

- We have found that the **profile** of the **impurity** is that of a **free particle** in a **square well**

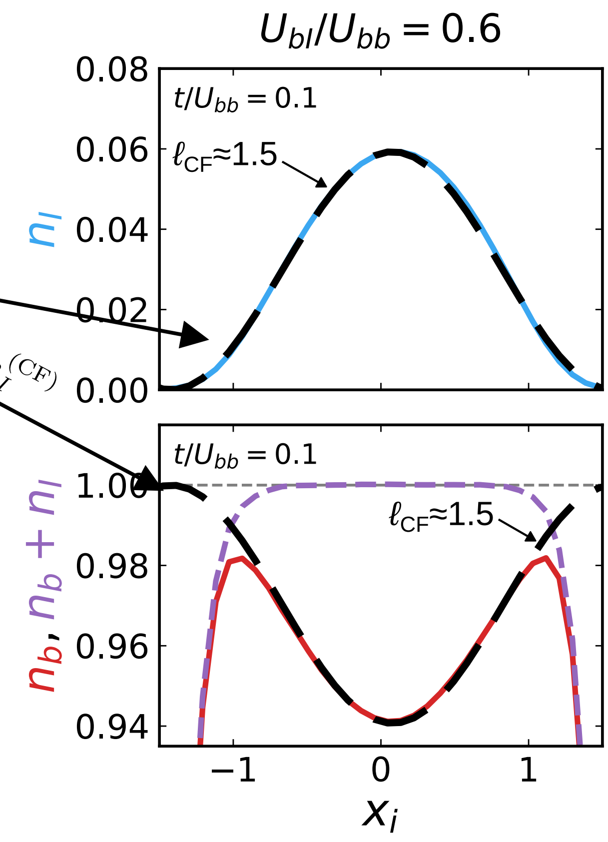
$$n_I^{(\mathrm{CF})}(x_i) = n_i^{(0)} \cos^2(\pi(x_i - \langle x_I \rangle)/\ell_{\mathrm{CF}}),$$

where only $n_I^{(0)}$ and $\langle x_I \rangle$ are extracted from the calculations.

- The **width** is given by:

$$\sum_i n_I^{(\mathrm{CF})} = 1 \quad \longrightarrow \quad \ell_{\mathrm{CF}} = 2/(\xi n_I^{(0)}).$$

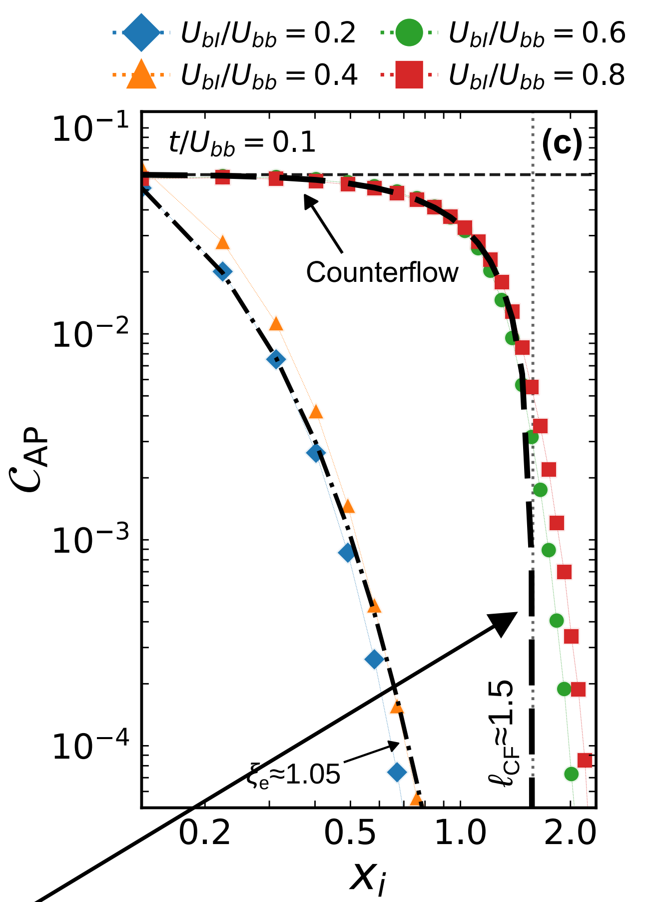
$1 - n_I^{(\mathrm{CF})}$



Counterflow

- We have developed a simple **analytical model** to describe the **counterflow** based on **impurity-hole pairs**

$$|\mathrm{MI}\rangle = \prod_i \hat{a}^\dagger_{i,b}|\emptyset\rangle \qquad \qquad |\Psi_{\mathrm{CF}}\rangle = \sum_i \alpha_i |i_{\mathrm{IH}}\rangle.$$
$$|i_{\mathrm{IH}}\rangle = \hat{a}^\dagger_{i,I}\hat{a}_{i,b}|\mathrm{MI}\rangle \longrightarrow$$



- After some algebra, one gets that $n_I(i) = |\alpha_i|^2$.

- From imposing the **square-well solution**, the **correlator** takes the form

$$C_{(\mathrm{AP})} = \sqrt{n_I^{(0)}}\cos(i\pi(x_i - \langle x_I\rangle)/\ell_{\mathrm{CF}}),$$

which **agrees** with the **numerical solution**.

Harmonically confined lattice polarons: Outlook

- An **impurity** can form a correlated **counterflow state** with a **bosonic bath** in harmonically confined optical lattices.

- This shows that **counterflows** can **form** in **mixtures** with **high population imbalance**.

- Ideas for future work in harmonically confined lattices:
  - ➔ Study dynamics.
  - ➔ Consider multiple impurities.
  - ➔ Bose-Bose and Bose-Fermi mixtures.
  - ➔ Bath with spin-1/2 fermions.

Phys. Rev. Lett. **135**, 023404 (2025)

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Spin ½ fermions in optical lattices

- **Spin ½ fermions** in an **optical lattice** are described by the (Fermi) **Hubbard model**. Thus, a Hubbard chain is described by:

$$\hat{H} = \underbrace{-t \sum_{\sigma=\uparrow,\downarrow} \sum_{i} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i+1,\sigma} + \text{h.c.} \right)}_{\text{Tunnelling}} + \underbrace{U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}}_{\text{fermion-fermion repulsion}}.$$

- In **balanced systems**, $N_f{=}N_{\uparrow}{=}N_{\downarrow}$, the **filling factor** is defined as

$$\nu_f = N_f/M. \qquad M : \text{Number of sites}$$

- At **half filling**, $\nu_f{=}1/2$, and $U{>}0$, the lattice features an **insulating state** where each site is occupied only by one fermion.

Spin ½ fermions in optical lattices

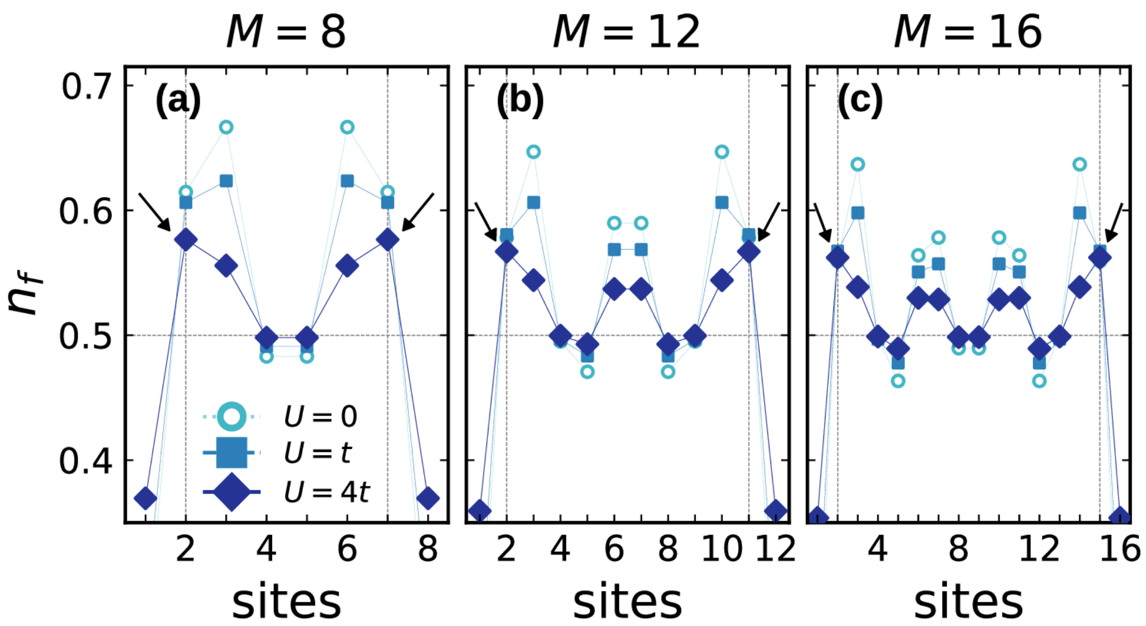
- An **open chain** with $\nu_f \neq 1/2$ features **Friedel oscillations**.

G. Bedürftig B. Brendel H. Frahm R. M. Noack, Phys. Rev. B **58**, 10225 (1998).

$$N_f = N_\uparrow = N_\downarrow$$

$$\nu_f = \frac{N_f}{M} = \frac{1}{4}$$

$$n_f(i) = \langle \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow} \rangle$$



- For $\nu_f < 1/2$, the number of peaks is equal to the number of fermions of each spin N_f.

Impurity interacting with an open Hubbard chain

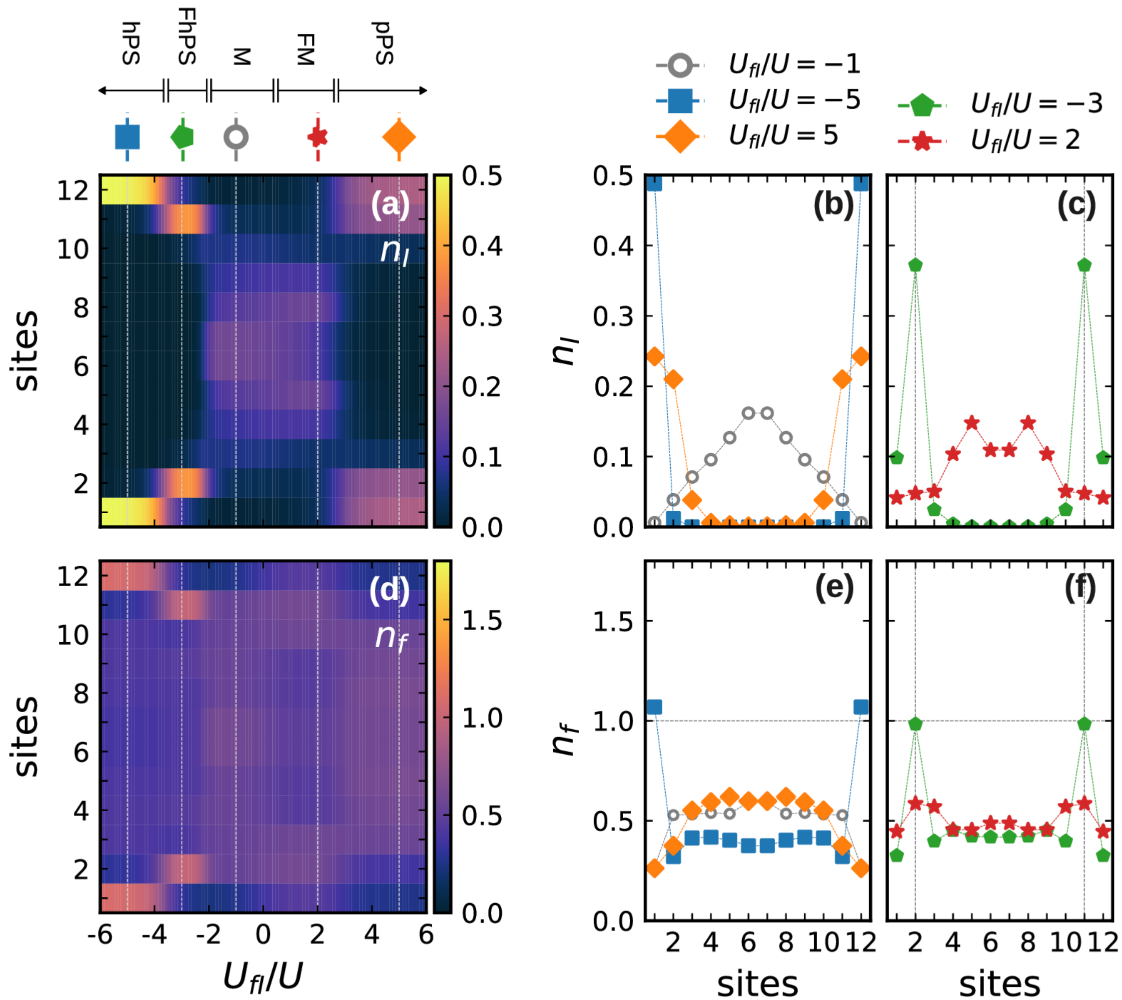
- We consider a **single impurity** interacting with **spin ½ fermions** in a **one-dimensional open optical lattice**.

$$\hat{H} = \underbrace{-t \sum_{\sigma=\uparrow,\downarrow} \sum_i \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i+1,\sigma} + \text{h.c.} \right)}_{\text{Tunnelling fermions}} + \underbrace{U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}}_{\text{fermion-fermion repulsion}}$$

$$\underbrace{-t \sum_i \left(\hat{a}^{\dagger}_i \hat{a}_{i+1} + \text{h.c.} \right)}_{\text{Tunnelling impurity}} + \underbrace{U_{fI} \sum_{\sigma=\uparrow,\downarrow} \sum_i \hat{n}_{i,\sigma} \hat{n}_{i,I}}_{\text{fermion-impurity interaction}}.$$

- We use the **exact diagonalisation** method for small lattices with a few particles.

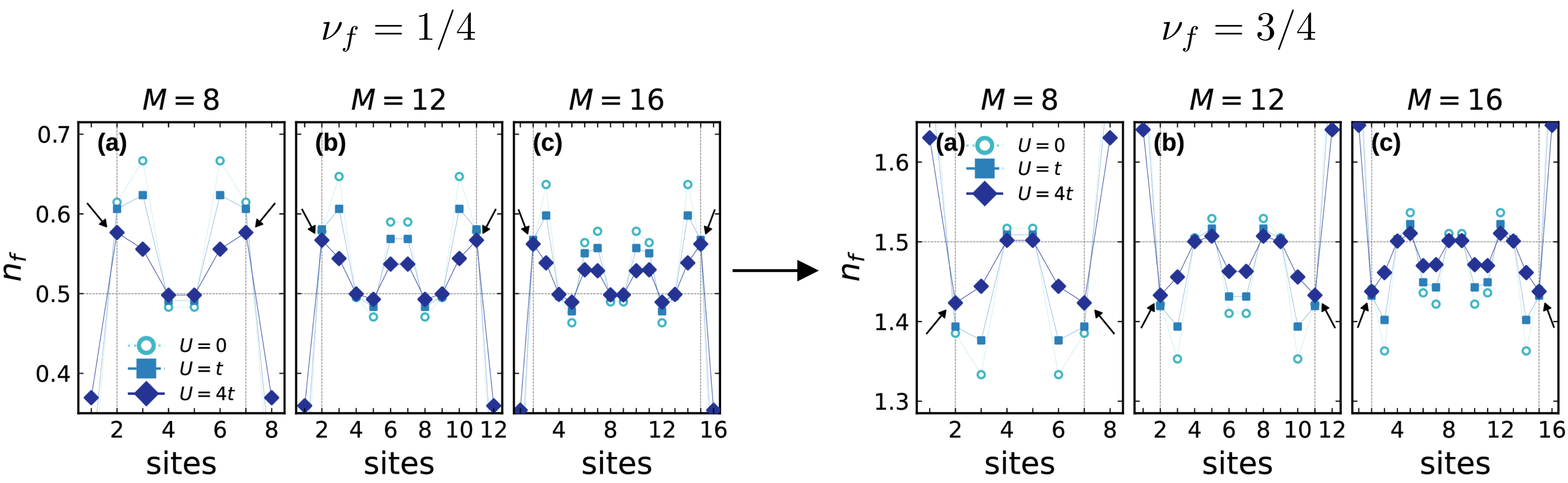
Density profiles $\nu_f = 1/4$



- The system undergoes **phase separations** between the impurity and either the **holes or the fermions**.
- The **position of the impurity** can be influenced by the **Friedel oscillations**.

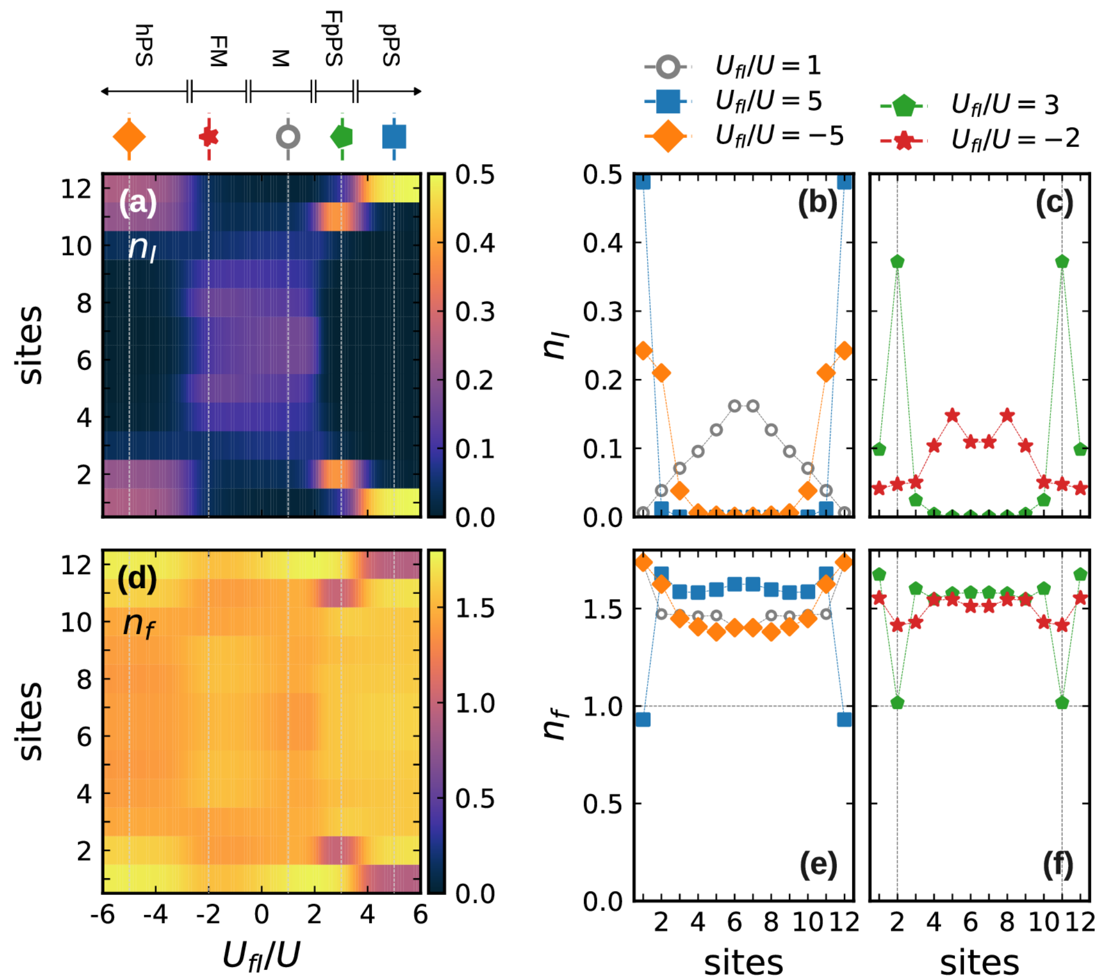
Spin ½ fermions in optical lattices

- For $\nu_f > 1/2$, the Hubbard model shows **Friedel oscillations** with a number of **local minima** equal to the number of holes $1 - N_f$.



- This is due to the **particle-hole symmetry** of the Hubbard model.

Density profiles $\nu_f = 3/4$



- The **particle-hole symmetry** imposes:

$$n_f(i; U_{fI}, \nu_f) + n_f(i; -U_{fI}, 1-\nu_f) = 2, \qquad n_I(i; U_{fI}, \nu_f) = n_I(i, -U_{fI}, 1-\nu_f).$$

Impurity interacting with a Hubbard chain: Outlook

- The system can undergo a **phase separation** between the impurity and either the **fermions or the holes**.
- The **Friedel oscillations** induce an **unusual localisation** of the impurity for intermediate interactions.
- Similar physics can be found at other fillings $\nu_f \neq 1/2$.
- Future work:
  - Larger lattices.
  - Lattice with harmonic confinement.

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Summary

- Polarons and **impurities** offer very **rich physics** in **optical lattices**.
- We have found the onset of a correlated **counterflow** bath-impurity state in **harmonically confined optical lattices**.
- **Friedel oscillations** can have an **impact** on the behaviour of **impurities**.
- Future work:
  - Further studies of **impurities** and **mixtures** in **harmonically confined optical lattices**.

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