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Ultracold polarons and impurities in one-dimensional optical lattices

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Ultracold polarons and impurities

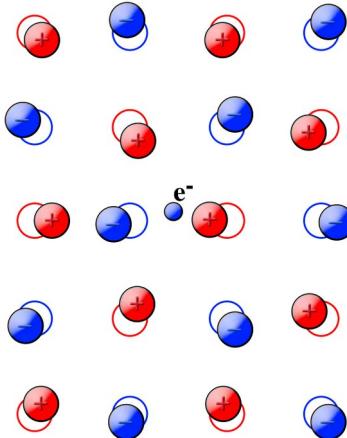
1. Polarons and **impurities** in **ultracold atomic systems**.
2. One-dimensional **harmonically confined lattice polarons and counterflows**.
3. Mobile **impurity** interacting with a **Hubbard chain**.
4. Summary and **future work**.

Ultracold polarons and impurities

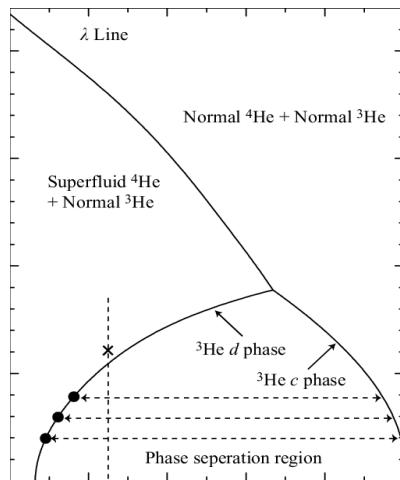
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Polarons and impurities

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

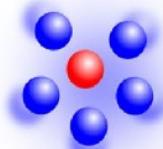


Electrons in an ionic crystal
L. Landau and S. Pekar, Zh. Eksp. Teor. Fiz. 18, 419 (1948).

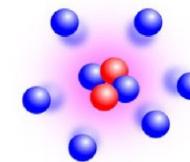


^3He impurities in ^4He
G. Baym and C. Pethick, "Landau Fermi-Liquid Theory: Concepts and Application" (1991).

Polaronic proton



Polaronic alpha particle



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

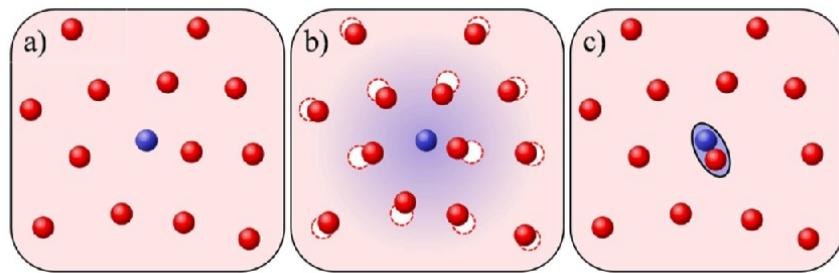
- Such **impurities** often **form** dressed **quasiparticles** referred to as **polarons**.

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**.

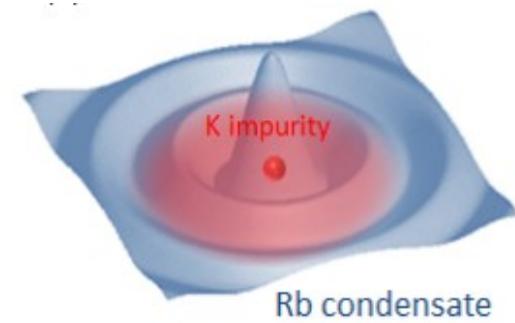
C. Baroni, G. Lamporesi and M. Zaccanti, Nat. Rev. Phys. **6**, 736 (2024).

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.

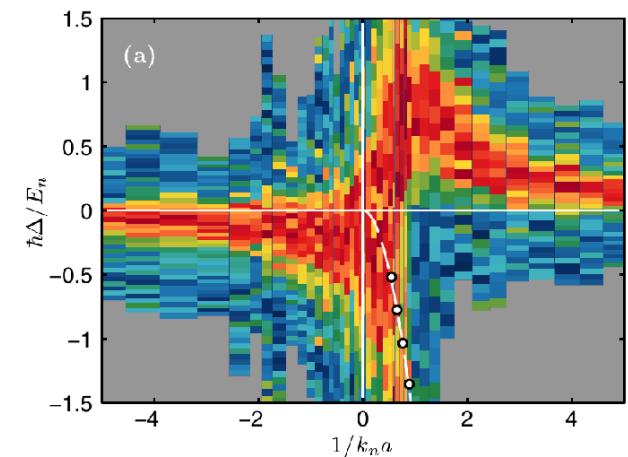
P. Massignan *et al.*, Rep. Prog. Phys. **77** 034401 (2014).

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

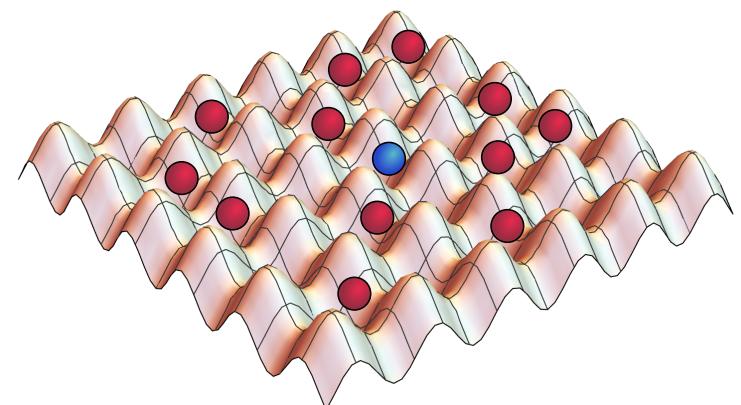
N. B. Jørgensen, et al., PRL 117, 055302 (2016).

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.

Ultracold polarons and impurities

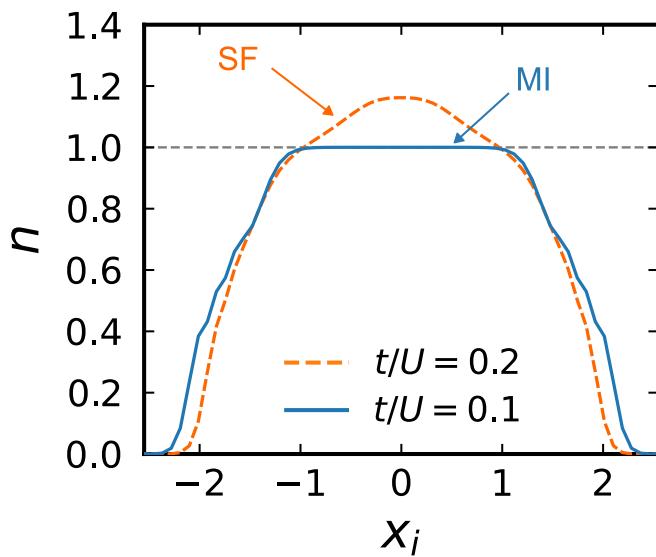
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Phys. Rev. Lett. **135**, 023404 (2025)

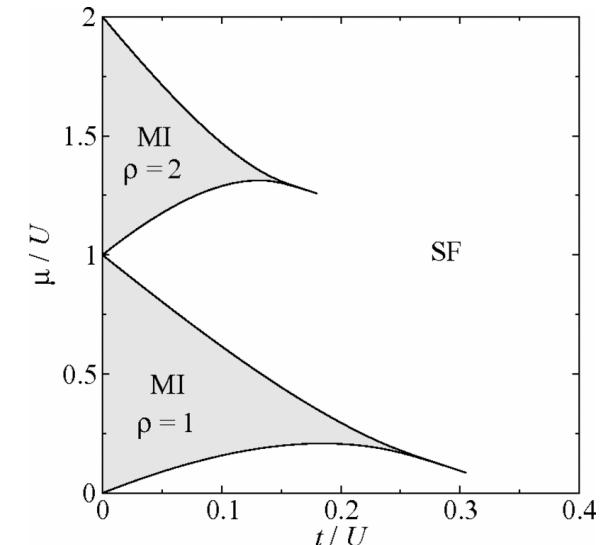
Bosons in optical lattices

- 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).



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



Phase diagram of the 1D BH model.

S. Ejima et al., PRA **85**, 053644 (2012).

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

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

Tunnelling

$$+ \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1).$$

Harmonic trap

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**.

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

Tunnelling

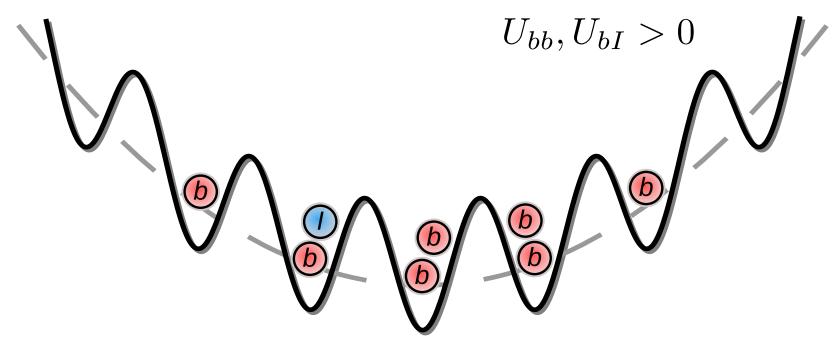
$$+ V_{\text{ho}} \sum_i \sum_{\sigma=b,I} i^2 \hat{n}_{i,\sigma}$$

Harmonic trap

$$+ \frac{U_{bb}}{2} \sum_i \hat{n}_{i,b} (\hat{n}_{i,b} - 1) + U_{bI} \sum_i \hat{n}_{i,b} \hat{n}_{i,I}.$$

Boson-boson repulsion

Bath-impurity repulsion

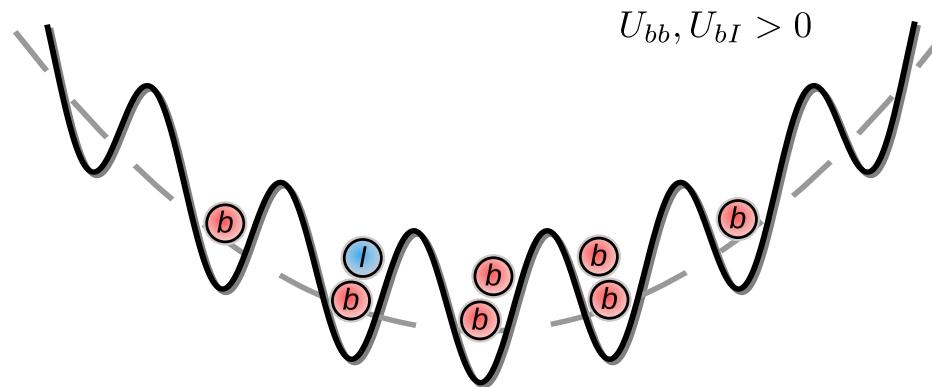


- We employed the **density matrix renormalisation group (DMRG)** for **large lattices** with a **large number of particles**.

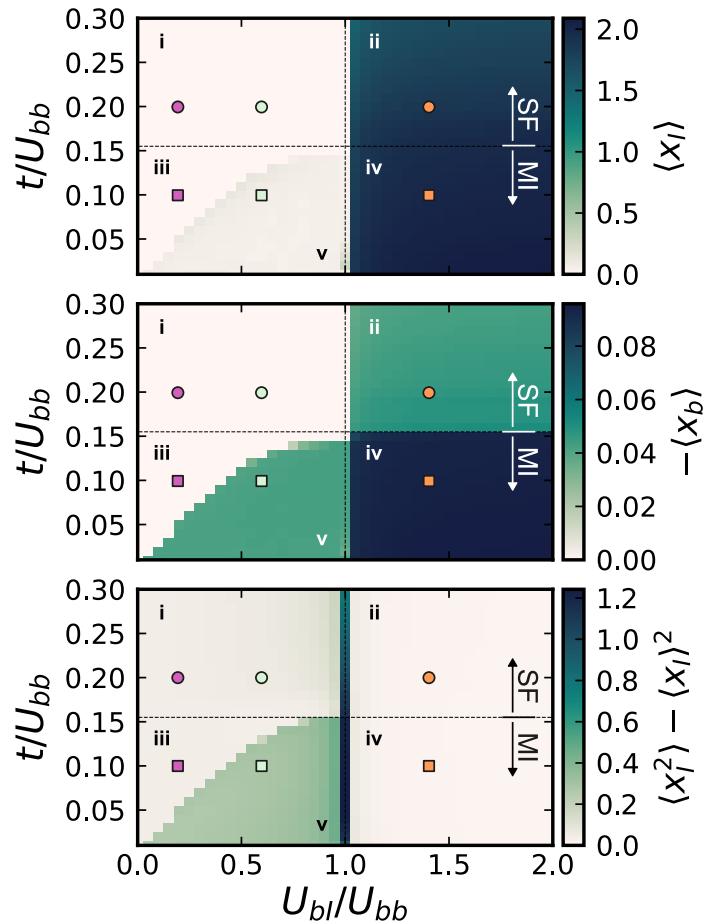
S. R. White, Phys. Rev. Lett. **69**, 2863 (1992). U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).

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:

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

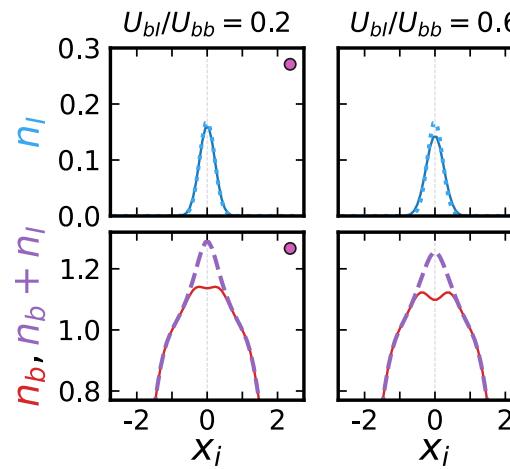
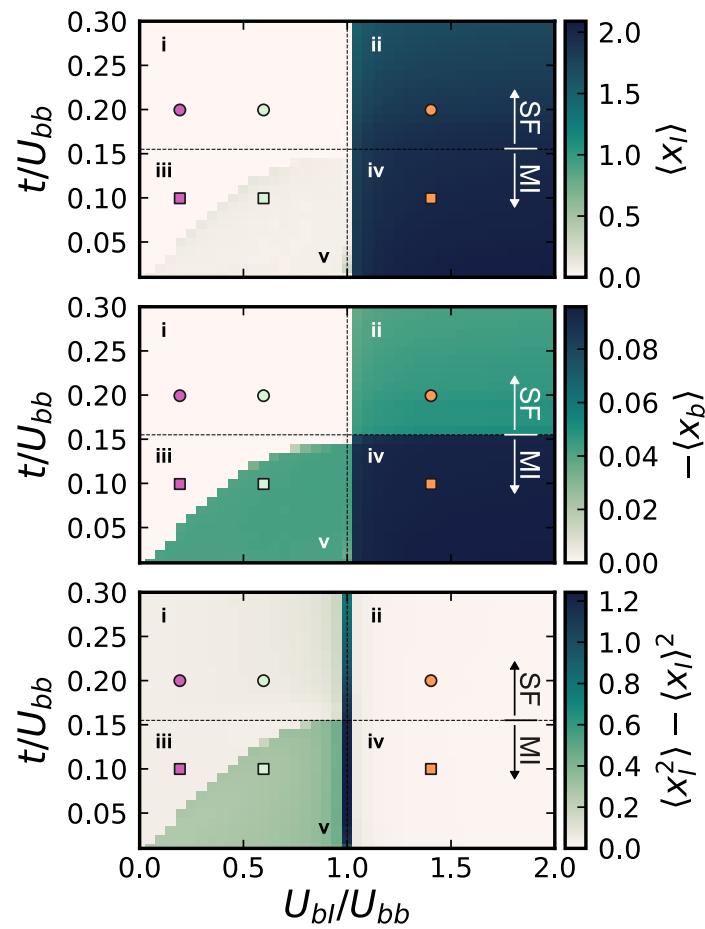
Impurity cloud:

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

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

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

Density profiles



$t/U_{bb} = 0.2$

Density profiles:

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

Average position:

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

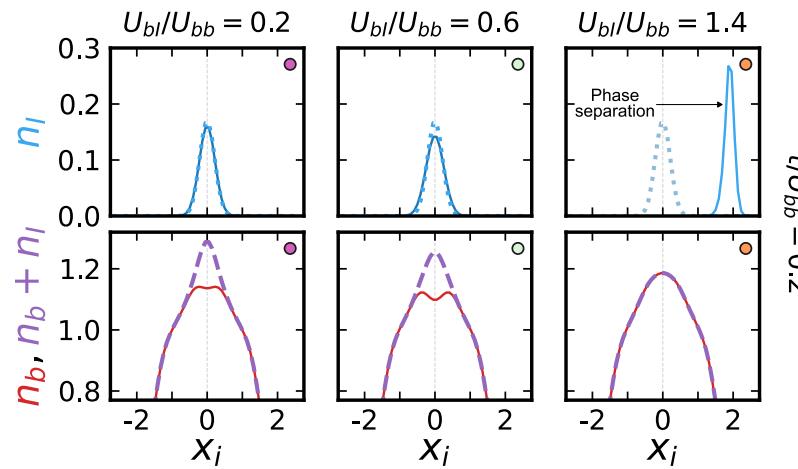
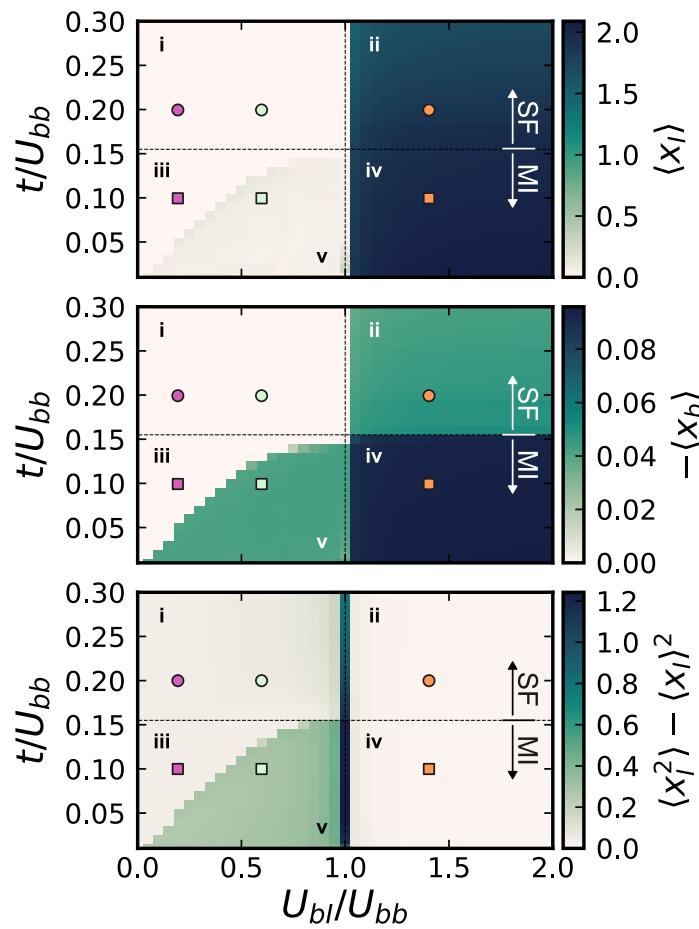
Impurity cloud:

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

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

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

Density profiles



Density profiles:

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

Average position:

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

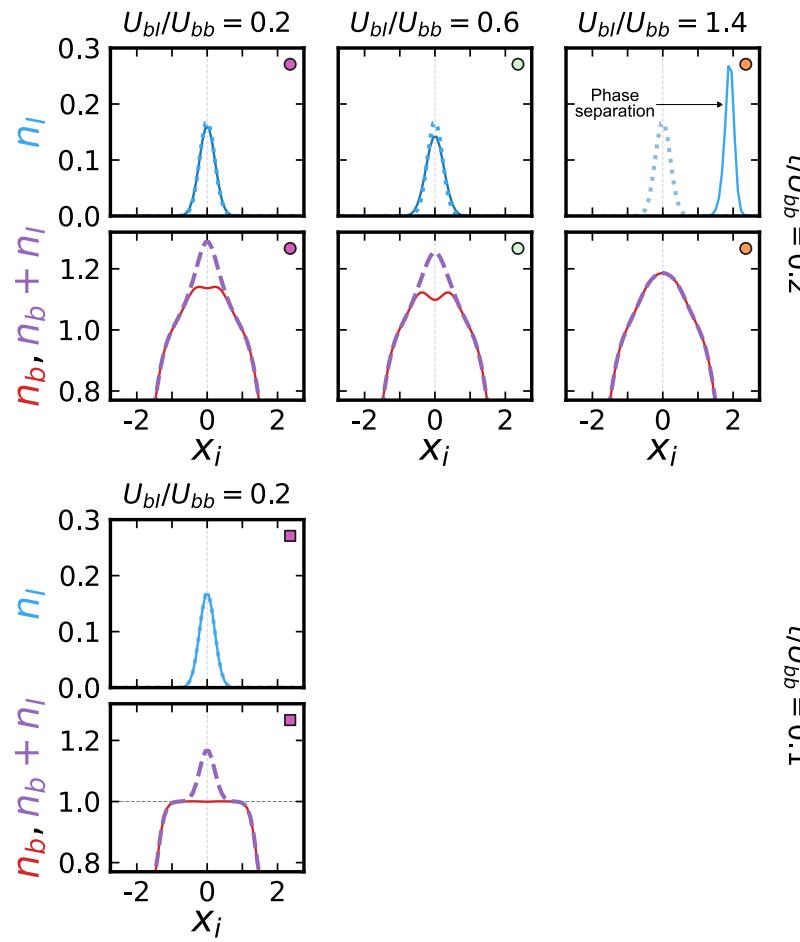
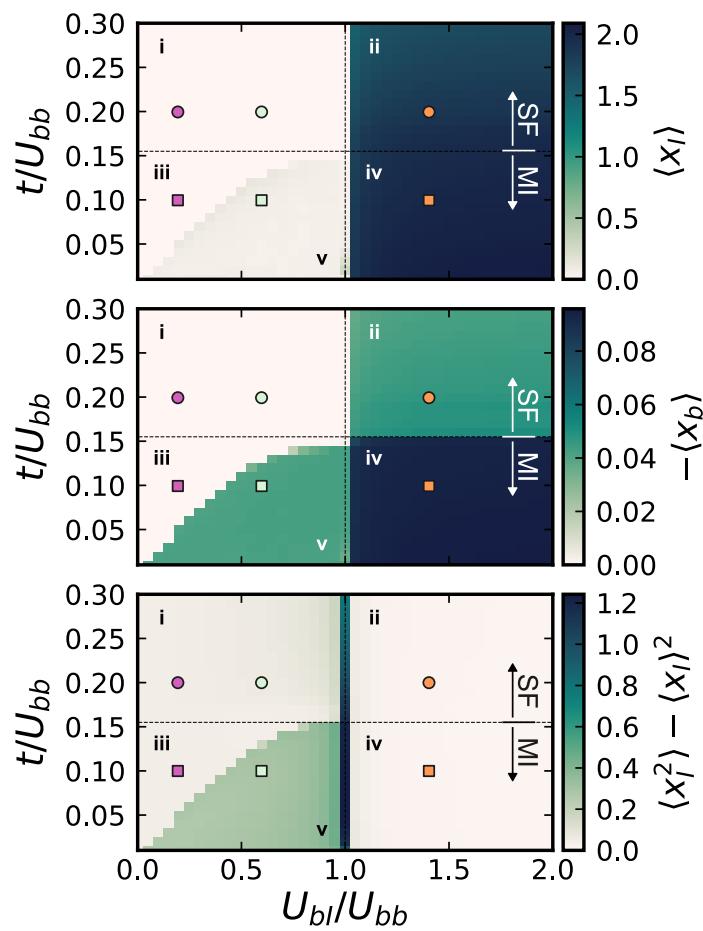
Impurity cloud:

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

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

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

Density profiles



Density profiles:

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

Average position:

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

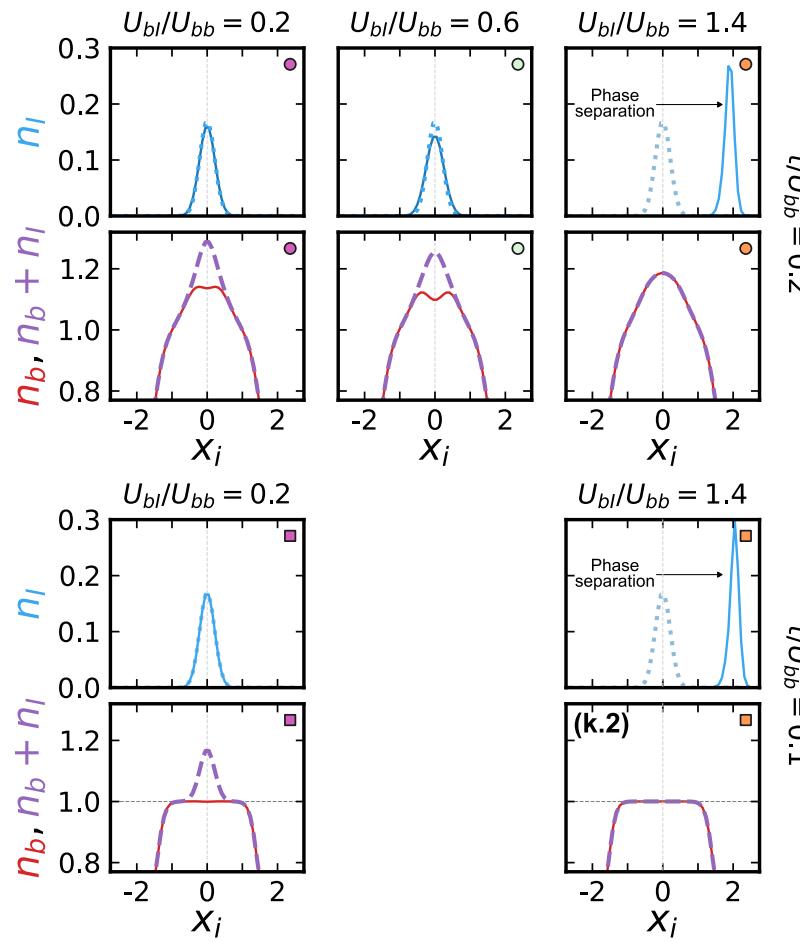
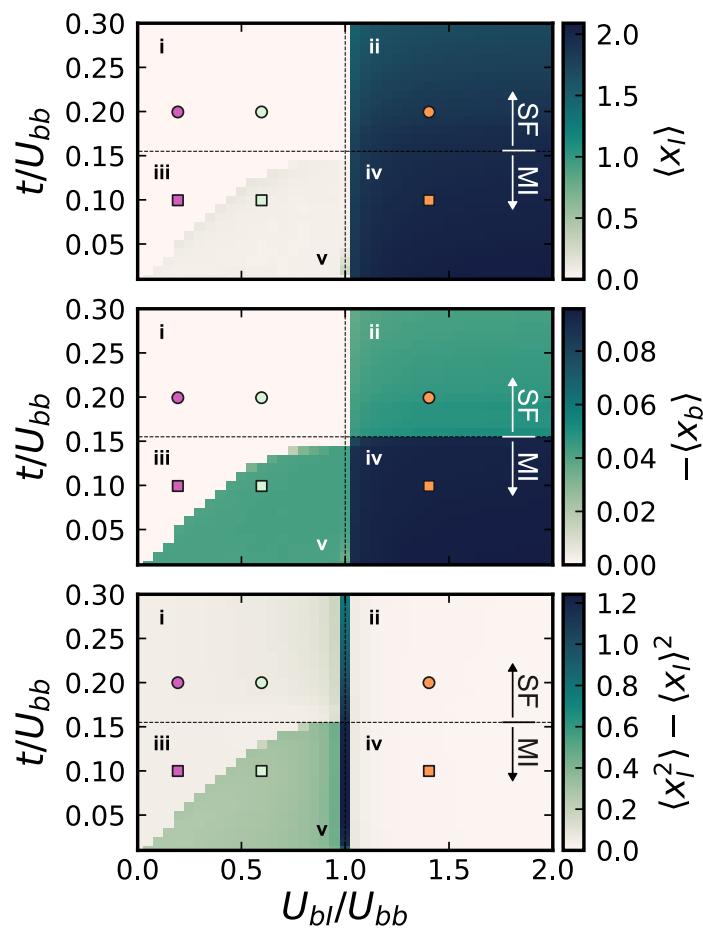
Impurity cloud:

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

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

- **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:

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

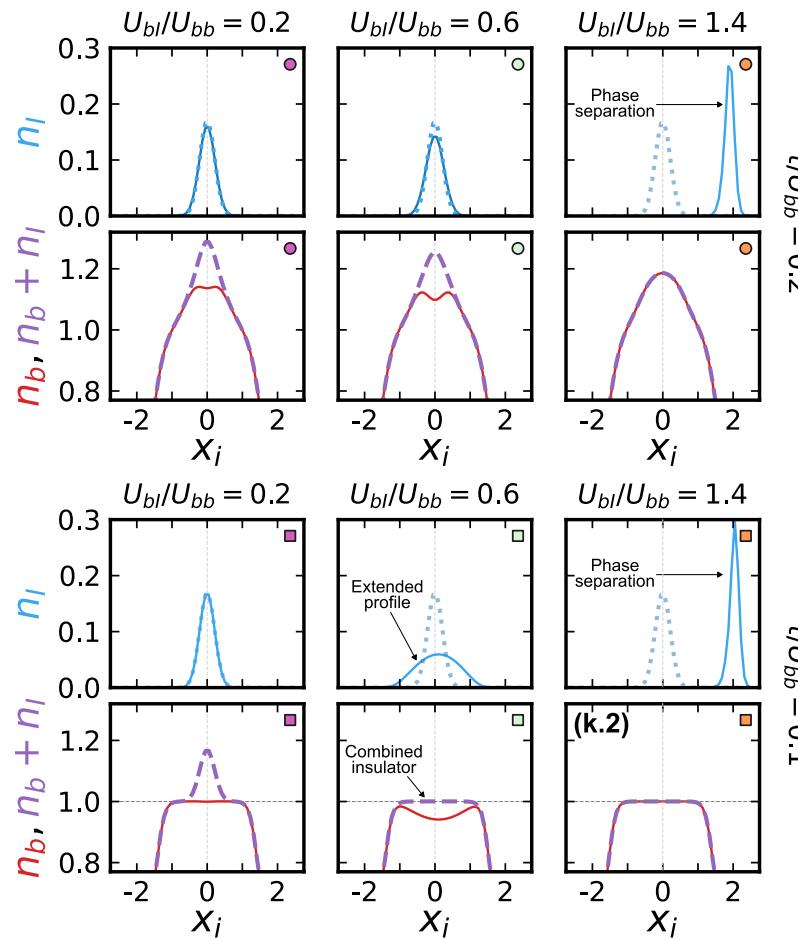
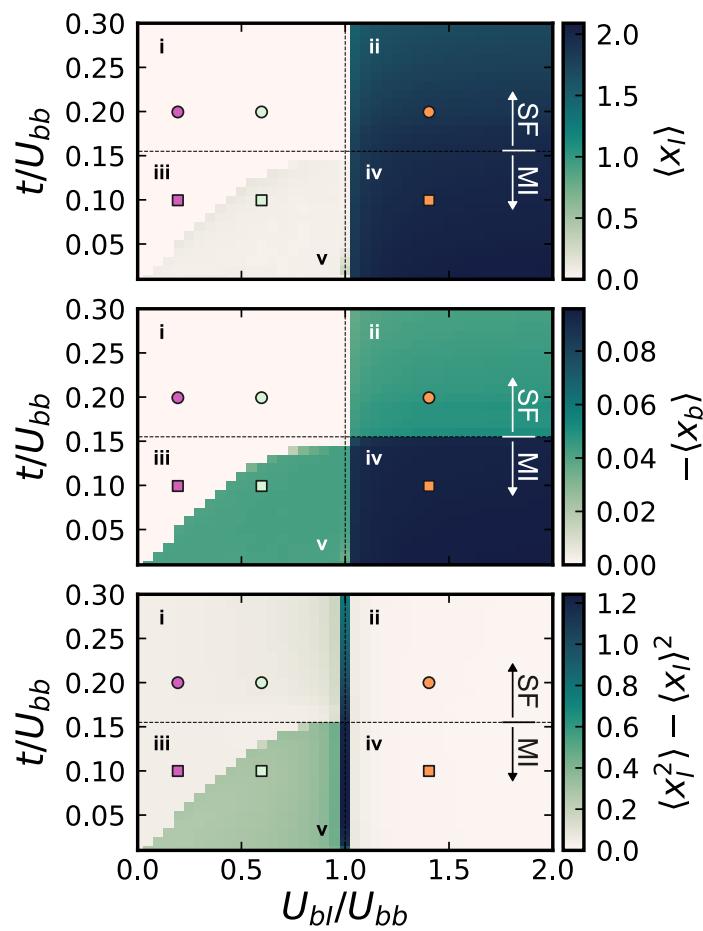
Impurity cloud:

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

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

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

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:

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

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

- **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

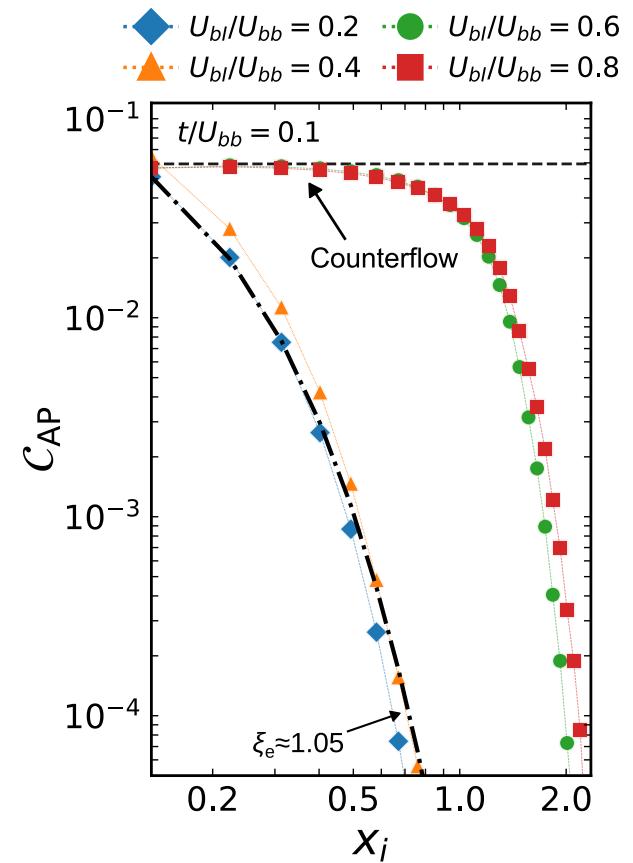
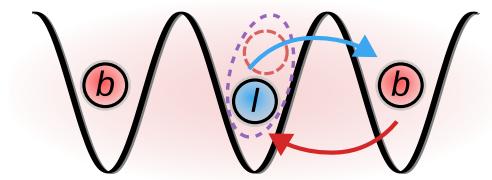
- The new state corresponds to a **counterflow phase**.
- It shows **anti-pair order**

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

- Counterflows were **realised experimentally** very recently with **binary Mott insulators**.

Y.-G. Zheng *et al.*, Nat. Phys. **21**, 208 (2025).

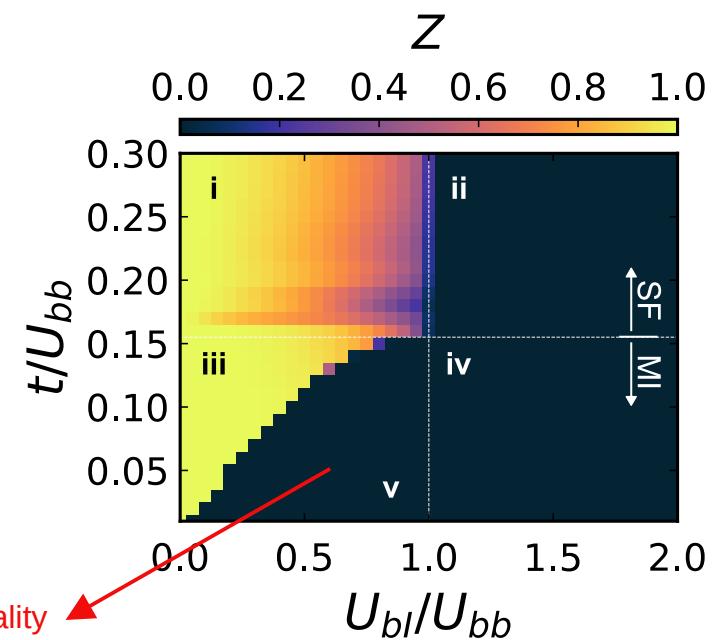
- Our results show that **counterflows appear for large population imbalances**.
- **Counterflows show properties of insulators.**



Counterflow

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

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



Counterflow

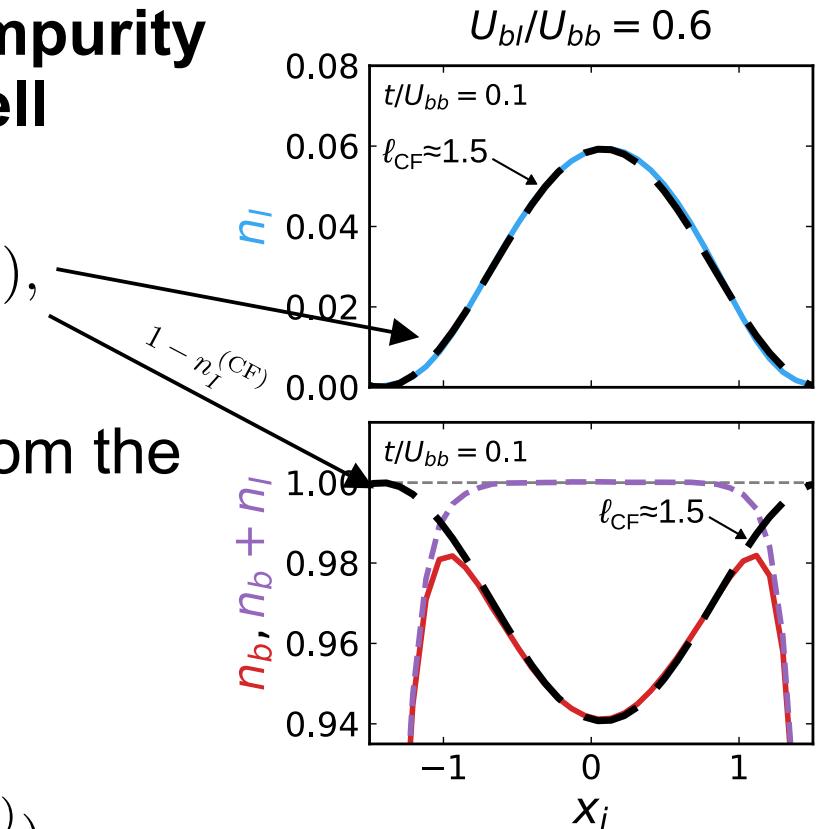
- We have found that the **profile of the impurity** is that of a **free particle in a square well**

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

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

- The **width** is given by:

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



Counterflow

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

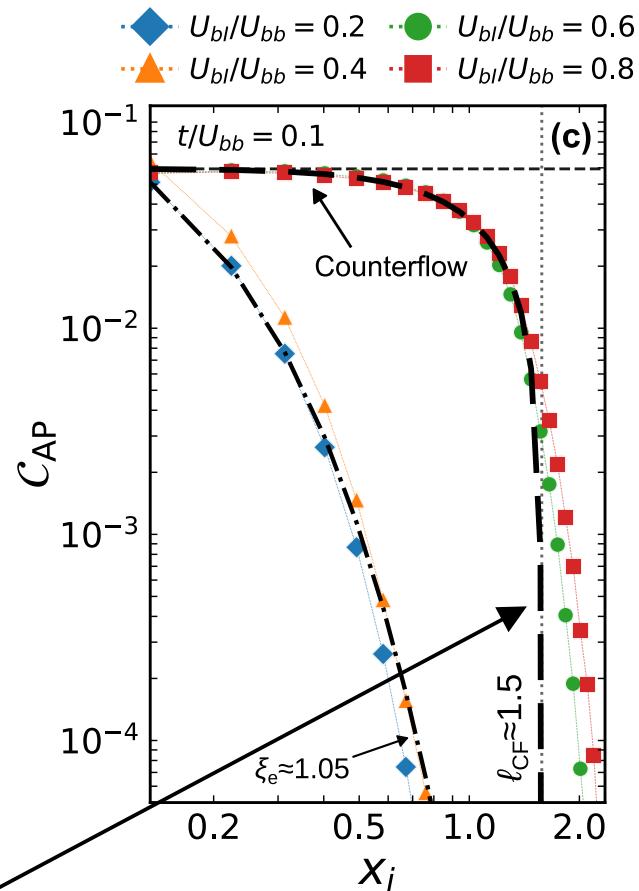
$$|\text{MI}\rangle = \prod_i \hat{a}_{i,b}^\dagger |\emptyset\rangle \quad \rightarrow \quad |\Psi_{\text{CF}}\rangle = \sum_i \alpha_i |i_{\text{IH}}\rangle.$$

$$|i_{\text{IH}}\rangle = \hat{a}_{i,I}^\dagger \hat{a}_{i,b} |\text{MI}\rangle$$

- After some algebra, one gets that $n_I(i) = |\alpha_i|^2$.
- From imposing the **square-well solution**, the **correlator** takes the form

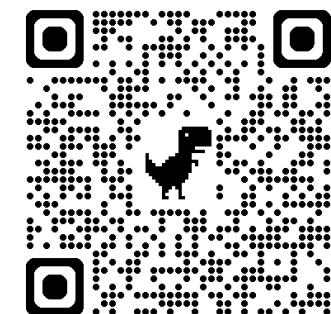
$$C_{(\text{AP})} = n_I^{(0)} \cos(i\pi(x_i - \langle x_I \rangle)/\ell_{\text{CF}}),$$

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:

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

Tunnelling fermion-fermion repulsion

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

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

- 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

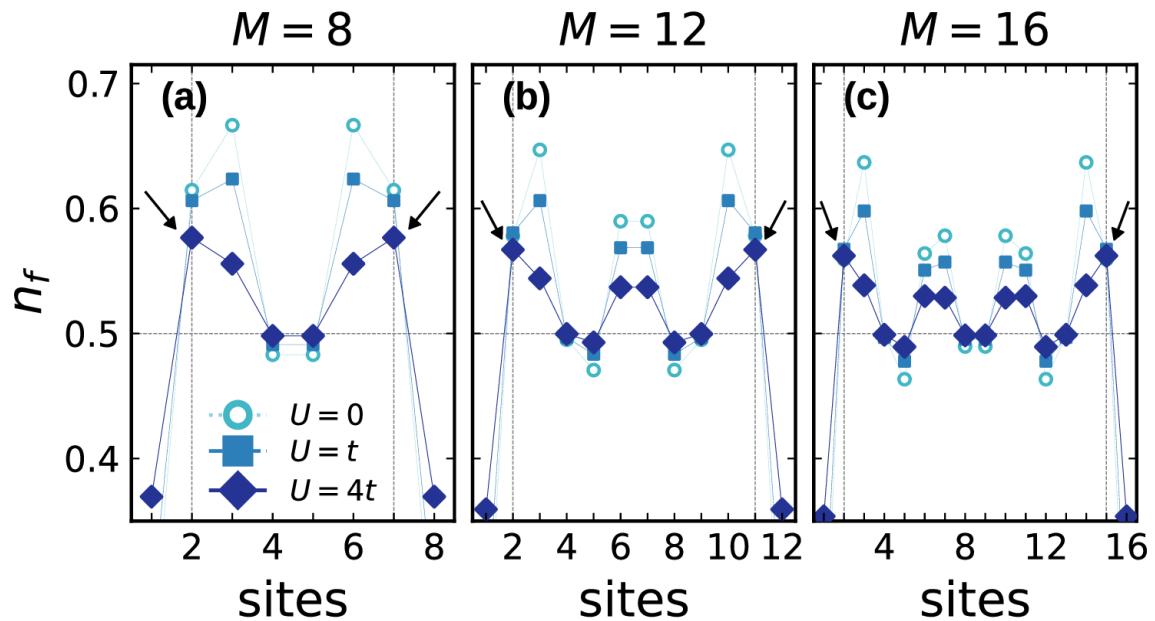
- An open chain with $\nu_f \neq 1/2$ features Friedel oscillations.

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**.

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

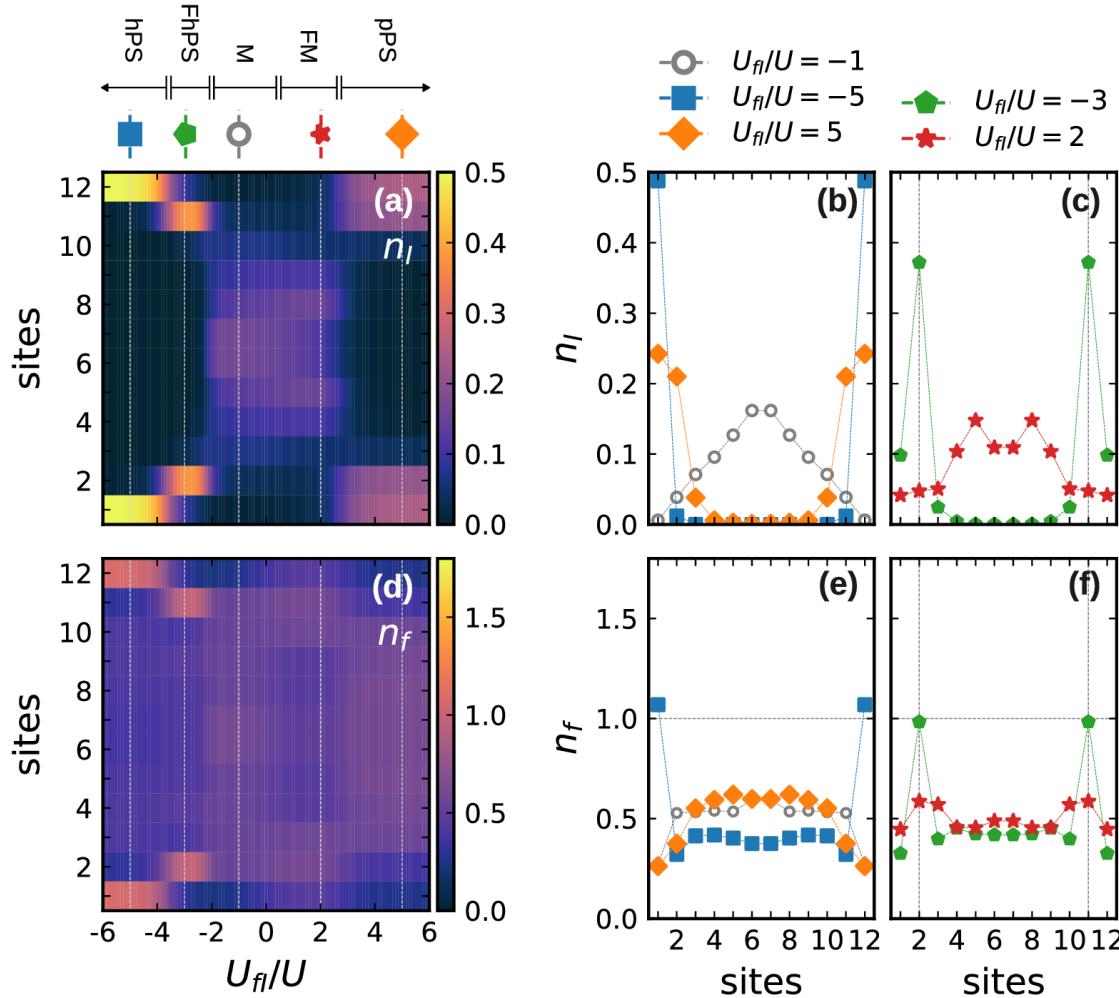
Tunnelling fermions fermion-fermion repulsion

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

Tunnelling impurity fermion-impurity interaction

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

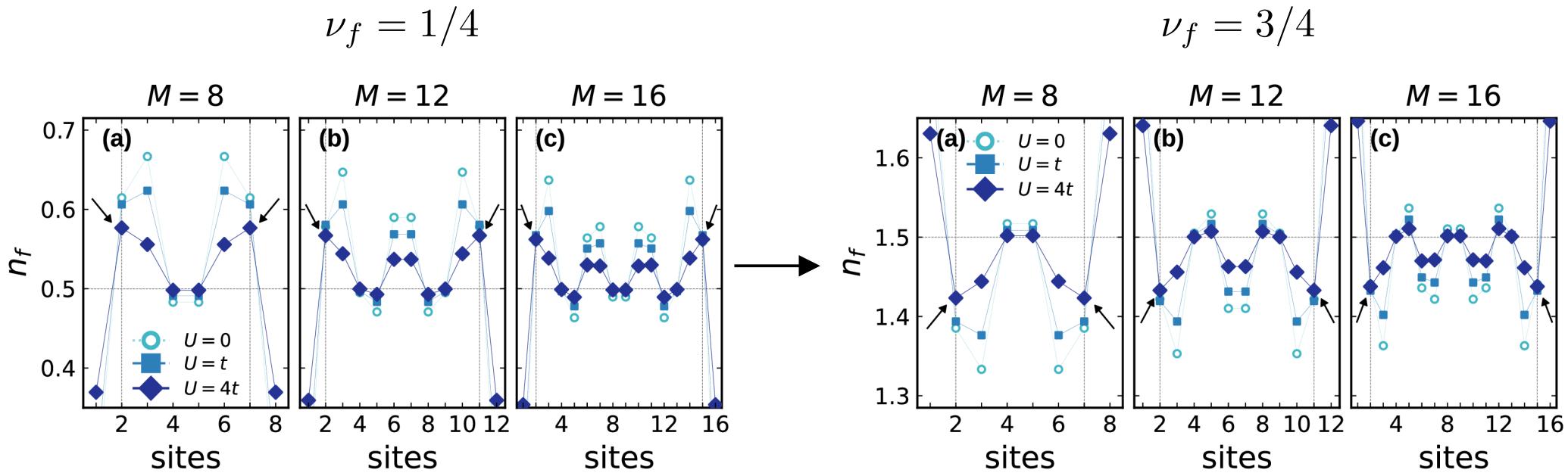
Density profiles $\nu_f=1/4$



- 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**.

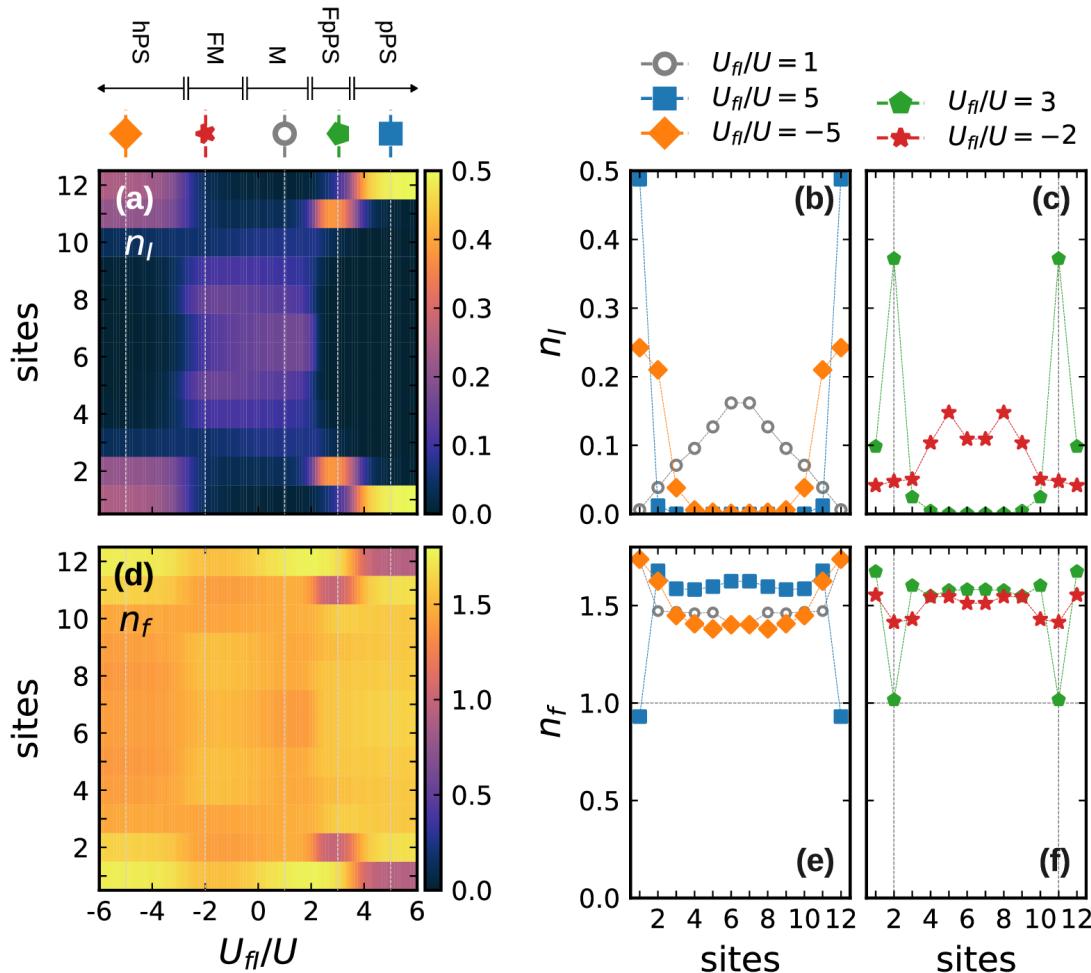
Spin 1/2 fermions in optical lattices

- 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:

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

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**.

Collaborators



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PUC Chile



Duc Tuan Hoang
OIST



Thomás Fogarty
OIST



Thomas Busch
OIST

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FONDECYT Postdoctorado
No. 3230023

THANK YOU!