Ultracold polarons and impurities

From lattice polarons to effective field theories

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Ultracold polarons and impurities

1. Quantum **polarons and impurities** in ultracold atomic systems.
2. One-dimensional **harmonically confined lattice polarons** and **counterflows.**
3. Polaron physics with the **functional renormalisation group**.
4. Summary and **future work**.

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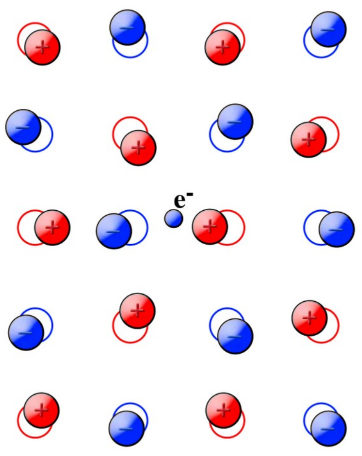
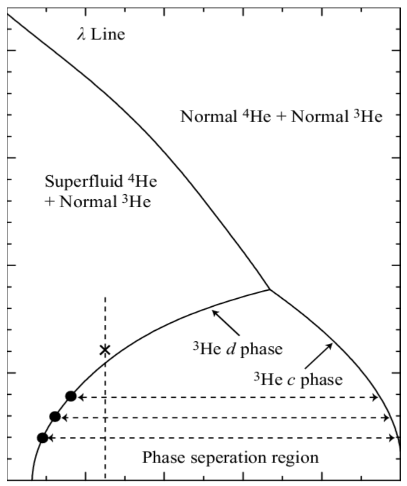
Polarons and impurities

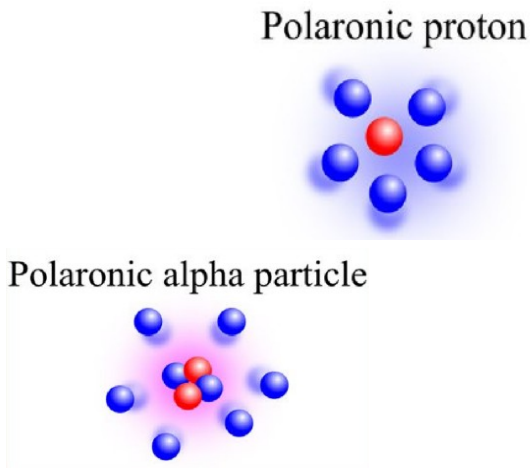
- The study of **impurities** immersed in **quantum mediums** has a **long history** and is **relevant** in **many fields** of physics.



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 mixtures** with a **high population imbalance**.
  P. Massignan *et al*., Rep. Prog. Phys. **77**, 034401 (2014). F. Grusdt *et al*. Rep. Prog. Phys. **88**, 066401 (2025).

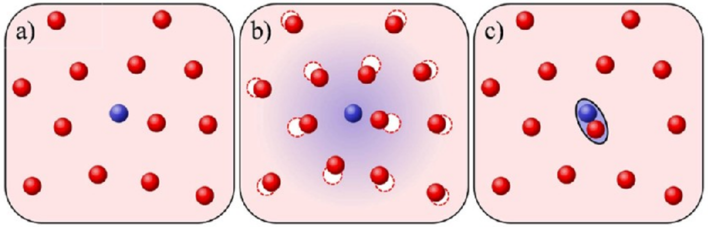


Illustration of a Fermi Polaron
A. Schirotzek *et al*., PRL **102**, 230402 (2009).

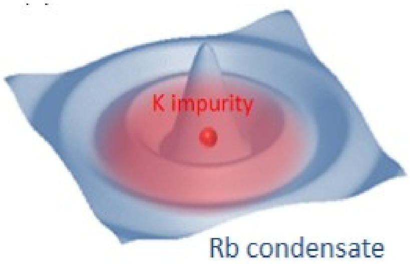


Illustration of a Bose Polaron
M.-G. Hu *et al*., PRL **117**, 055301 (2016).

- Several relevant properties can be examined: quasiparticle or **polaron energies**, **residue** and **orthogonality catastrophe**, coherence, effective masses, etc.
- They could also be used to **probe** and **manipulate** quantum **many-body systems**: transport properties, **phase transitions**, **mediated interactions**, etc.

Polarons in ultracold atomic gases

- Different configurations can be studied:
  - **Statistics**: Fermi and Bose polarons.
  - **Number of impurities**: Bipolarons and multipolarons.
  - **Confinement**: Optical lattices, harmonic traps, dimensionality.
  - **Stationary properties** or **dynamics**.
- Well-posed problem:
  - Variational approaches, Quantum Monte-Carlo (QMC), Exact Diagonalisation (ED), Tensor Networks, Effective Field Theories (EFT), amongst others.
- **Polarons** offer a **rich combination** of **few- and many-body physics**, and they are also a **starting point** to **study more complicated configurations**.

Ultracold polarons and impurities

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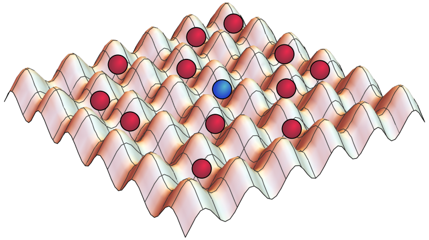
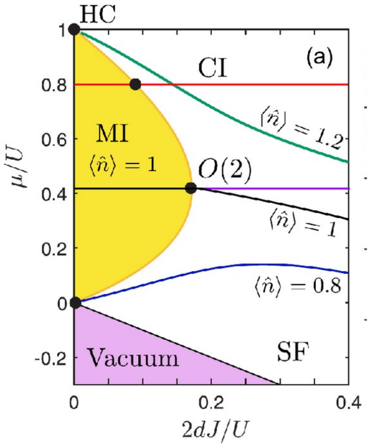
4. Summary and **future work**.

Lattice polarons

- A **rich platform** for **studying** ultracold atomic **impurities** is tight **optical lattices**.
  M. Lewenstein *et al.*, *Ultracold Atoms in Optical Lattices: Simulating Quantum Many-Body Systems* (Oxford, 2012).
- Such impurities are now referred to as **lattice polarons**.
- The study of **lattice polarons** in **bosonic mediums** has gained significant attention in the past few years.
- One relevant question is how the **polaron properties** change **across** the **superfluid-to-Mott insulator** (SF-MI) **transition**.
- We have tried to address this question in **one-dimensional lattices** with **numerical techniques**.





V. E. Colussi, F. Caleffi, C. Menotti, and A. Recati, Phys. Rev. Lett **130**, 17, 3002 (2023).

Harmonically confined lattice polarons

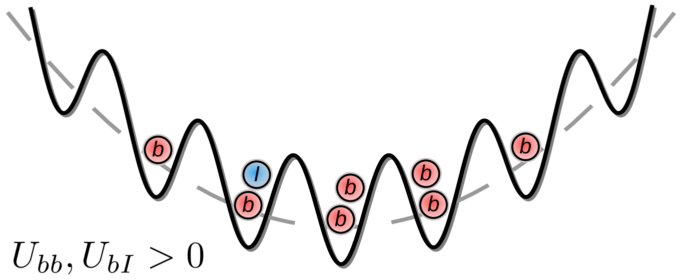
- We have recently studied a **single impurity** interacting with a **bosonic bath** in a **one-dimensional harmonically confined optical lattice**.

$$\hat{H} = -t \sum_{\sigma=b,I} \sum_{i} \left(\hat{a}^{\dagger}_{i,\sigma} \hat{a}_{i+1,\sigma} + \mathrm{h.c.} \right) + V_{\mathrm{ho}} \sum_{i,\sigma=b,I} i^2 \hat{n}_{i,\sigma}$$

Tunnelling — Harmonic trap

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

Boson-boson repulsion — Bath-impurity repulsion



- We have investigated this system using 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).

- The latter enables us to examine **sharp phase transitions** instead of the smooth crossovers observed for a few particles with ED.

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined Bose-Hubbard model

- But firstly, a reminder on **bosons** in a **harmonically confined optical lattice**.

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

Tunnelling | Harmonic trap | Boson-boson repulsion

- The system shows **SF and MI domains**.

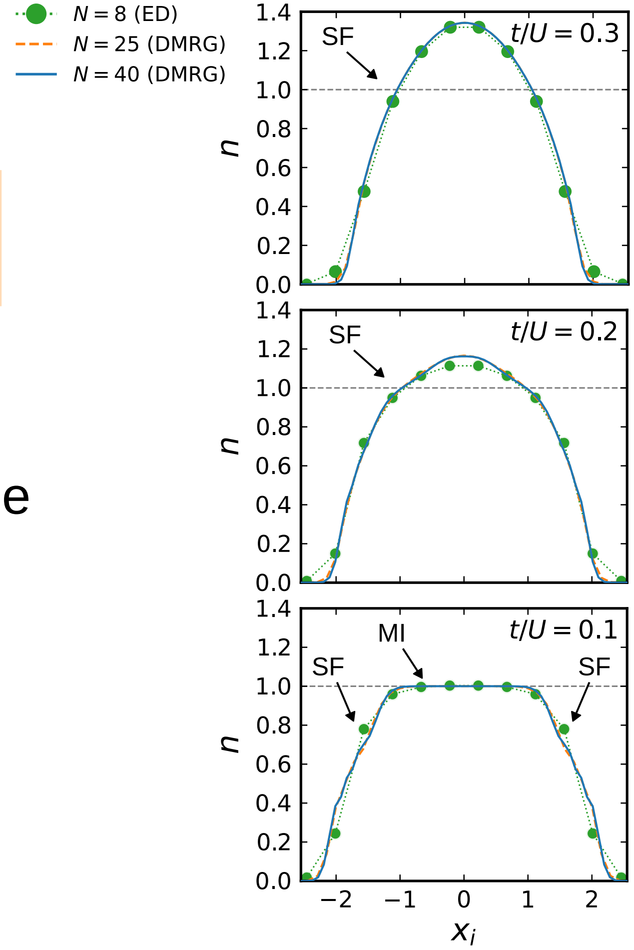
- For **large** enough **systems**, the properties become **invariant** for **equal characteristic density**

G. G. Batrouni *et al.*, Phys. Rev. A **78**, 023627 (2008)

$$\tilde{\rho} = dN/\xi, \qquad \xi = d\sqrt{t/V_{\text{ho}}}.$$

- The profiles scale with the **rescaled length**

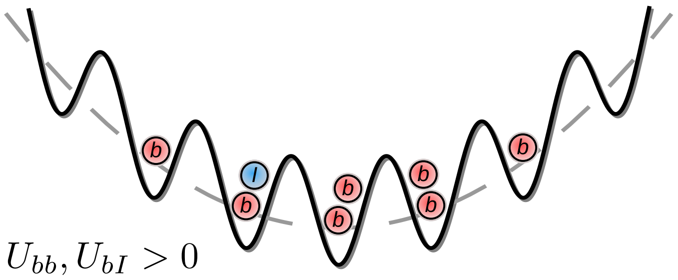
$$x_i = i\, d/\xi_i.$$



F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

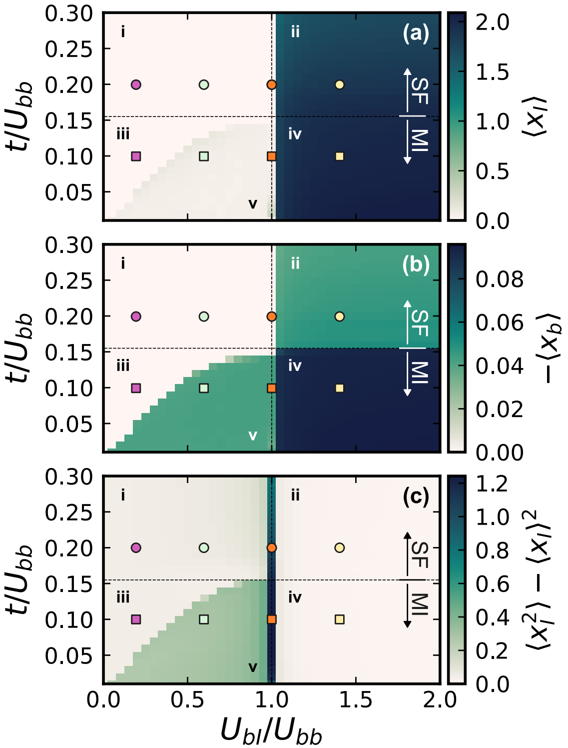
Harmonically confined lattice polarons

- We **considered** a **bath** with a characteristic density that is **completely SF** for $t/U_{bb}>0.155$ and that has a **MI domain** of **unity filling** for $t/U_{bb}<0.155$.
- This choice enables us to nicely **examine** the **behaviour of the impurity** across the **SF-MI phase transition**.
- We performed **DMRG simulations** for $N_b=40$ bosons. We also obtained **identical results** for **other choices**, and even a **qualitative agreement** with **ED**.



F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Density profiles



Density profiles:

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

Average position:

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

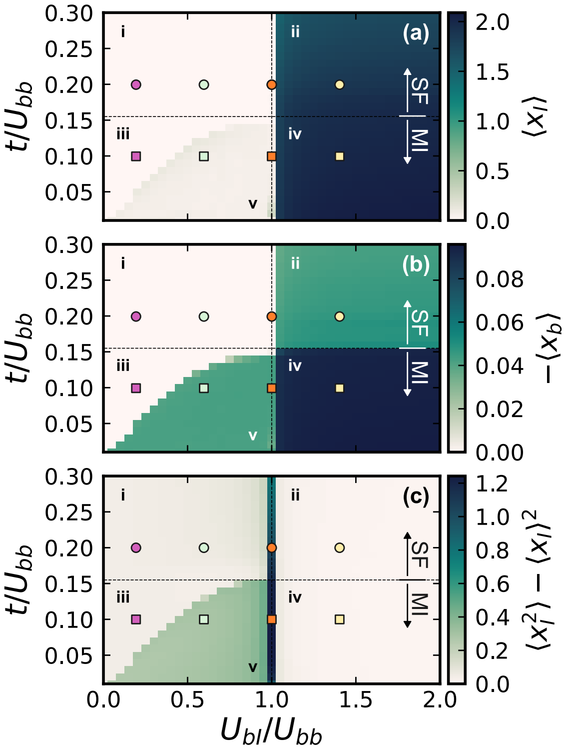
Impurity cloud:

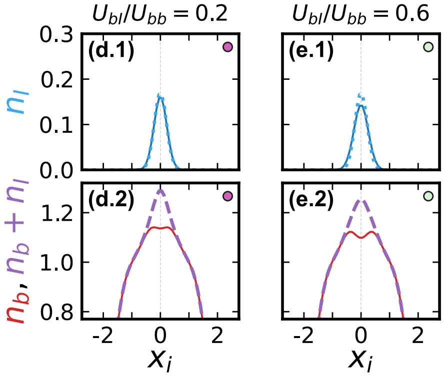
$$\langle x_I^2 \rangle = \frac{1}{N_\sigma} \sum_i x_i^2 n_\sigma(i)$$

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

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Density profiles





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Impurity cloud:

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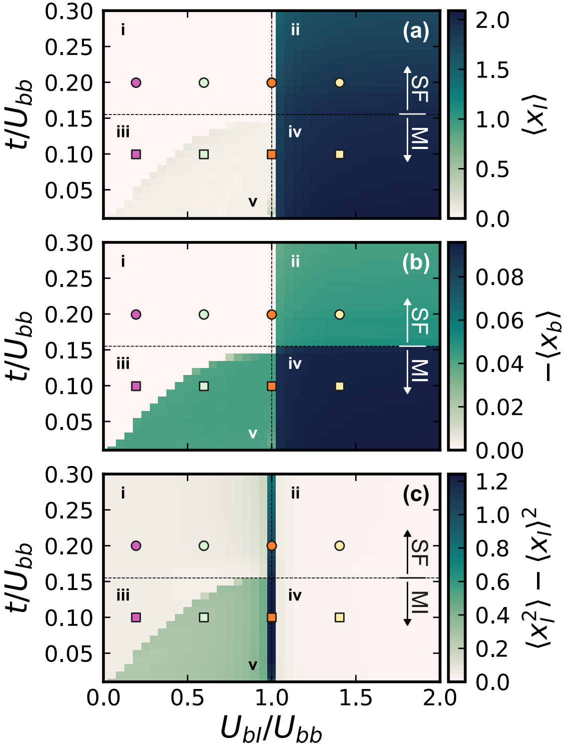
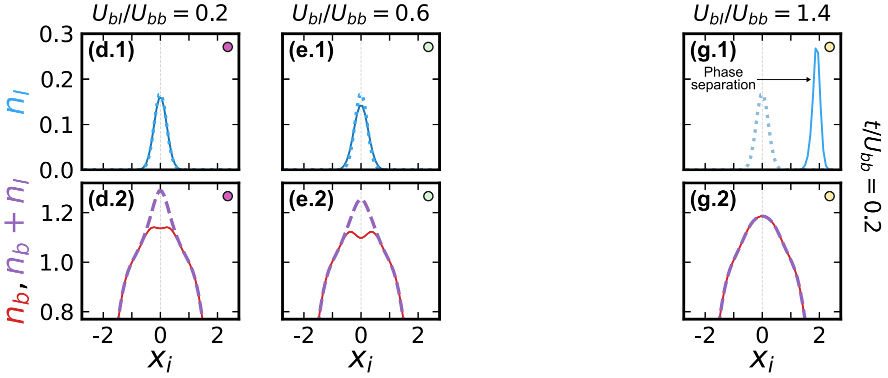
- **Region i** is a **miscible** phase where the **impurity repels** the **compressible SF bath**.

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Density profiles





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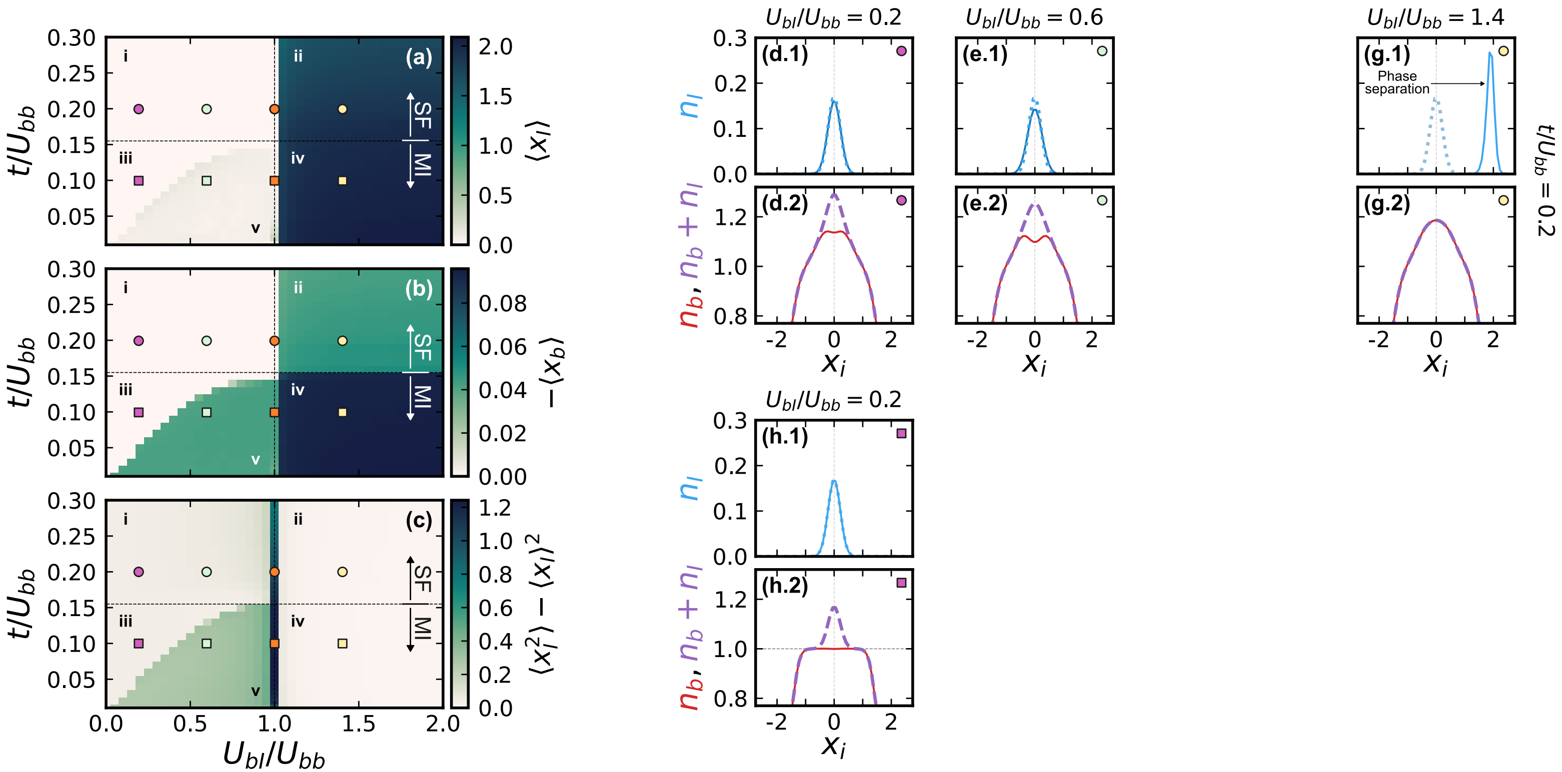
- **Region ii** is simply a **phase-separated** configuration.

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Density profiles



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Average position:

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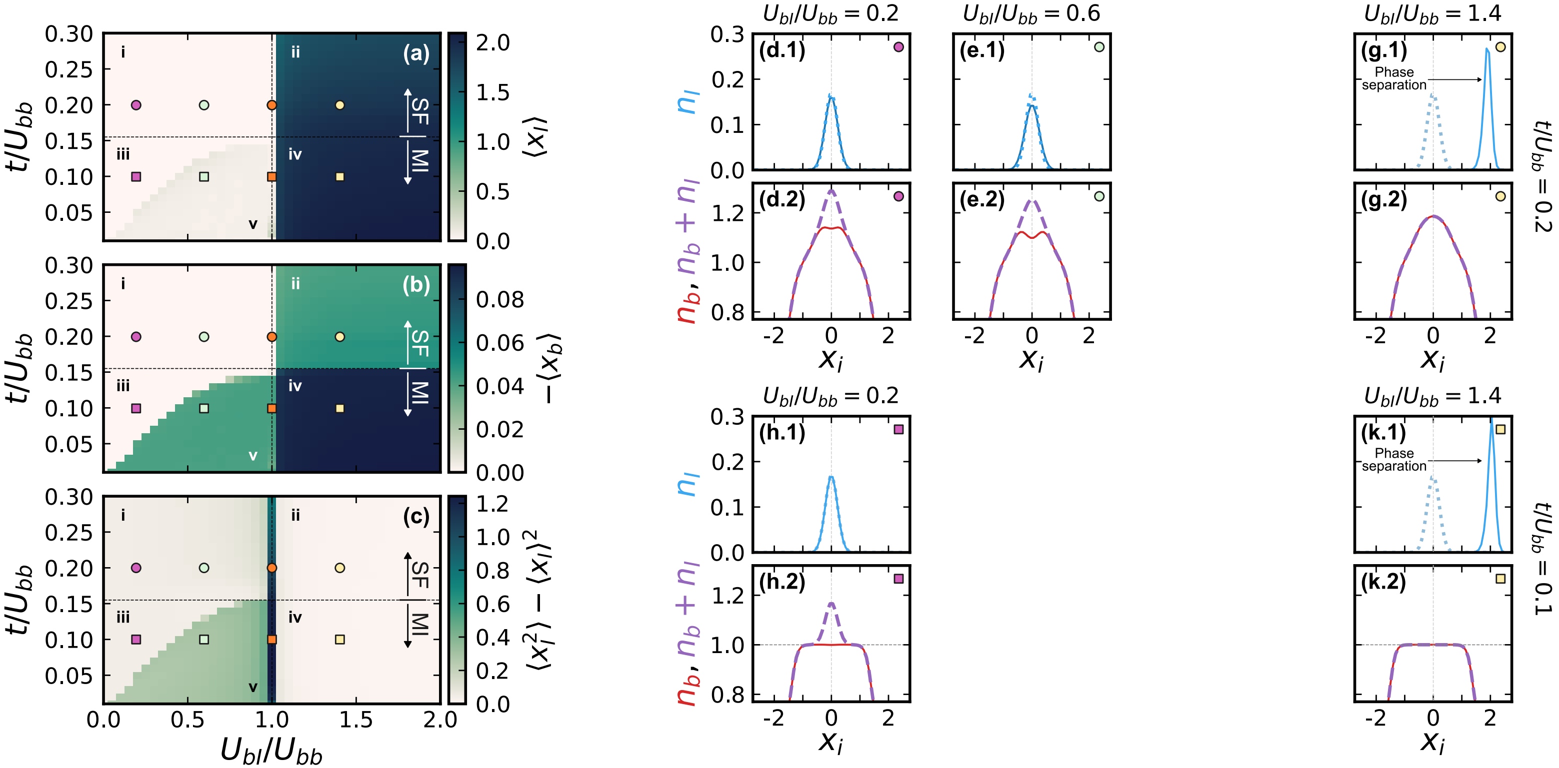
Impurity cloud:

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

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

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Density profiles



Density profiles:

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

Average position:

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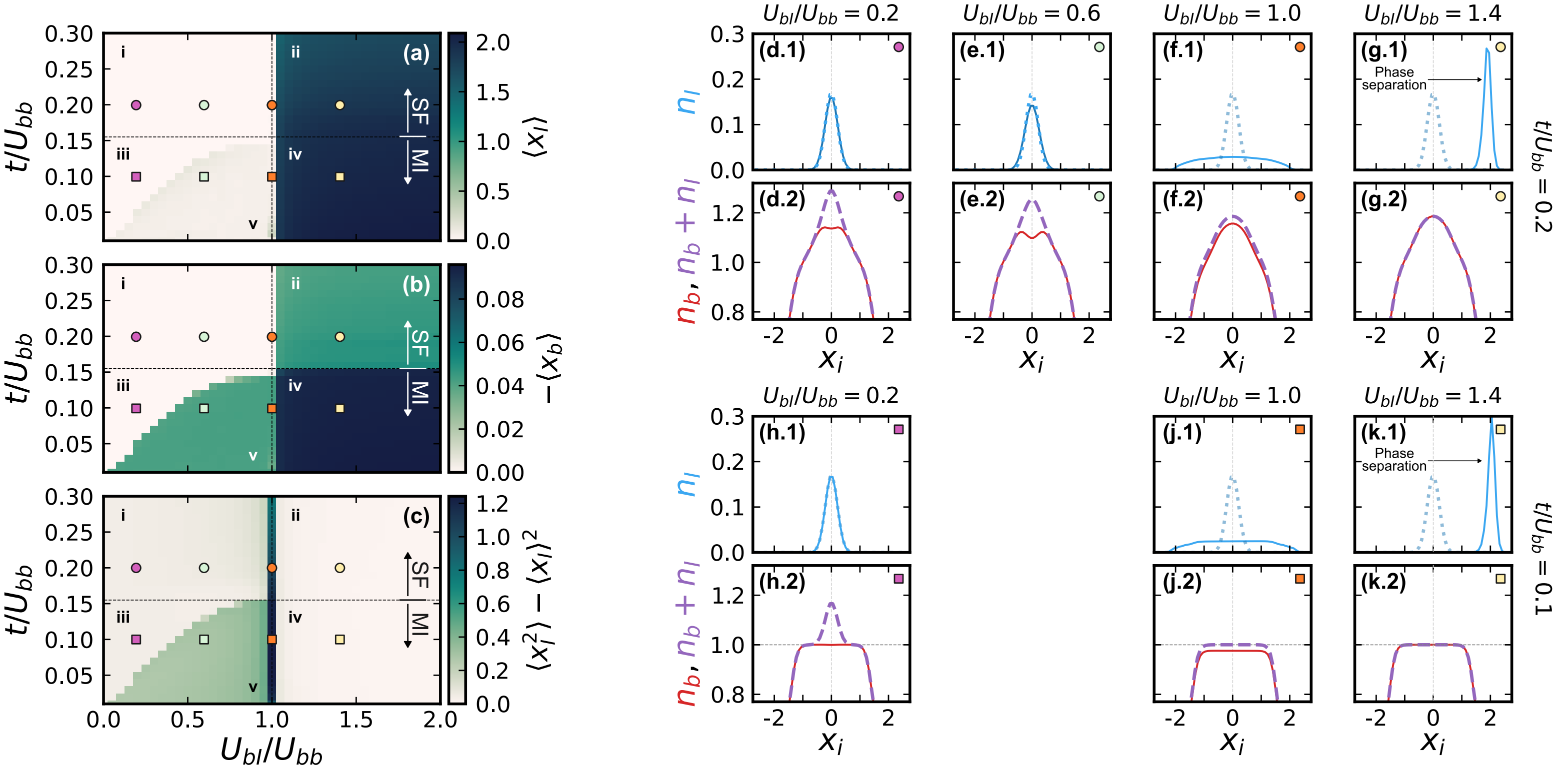
Impurity cloud:

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

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

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Density profiles



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Average position:

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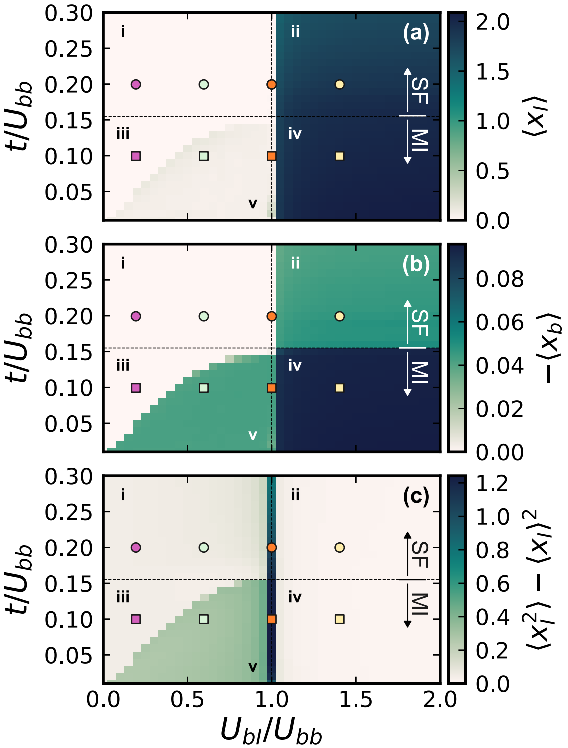
Impurity cloud:

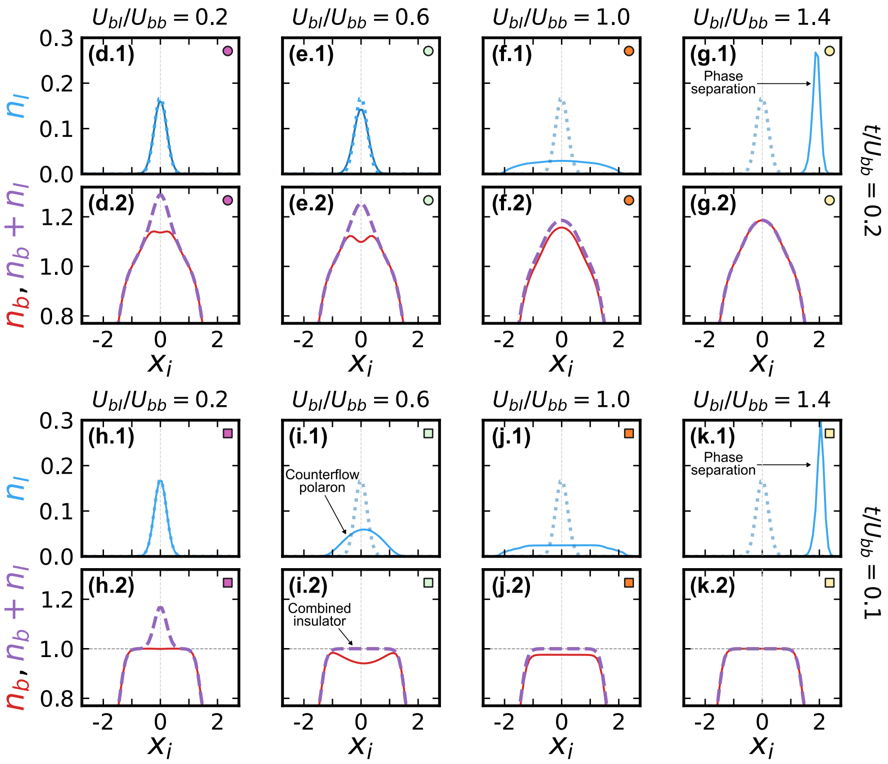
$$\langle x_I^2 \rangle = \frac{1}{N_\sigma} \sum_i x_i^2 n_\sigma(i)$$

- At U_{bI}=U_{bb} the impurity simply behaves as one particle in a **one-component system** with N_b+1 **bosons**.

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Density profiles





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Impurity cloud:

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

F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Counterflow

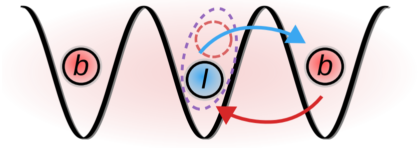
- The new state corresponds to a **counterflow phase**, which **only appears** with **harmonic confinement**.

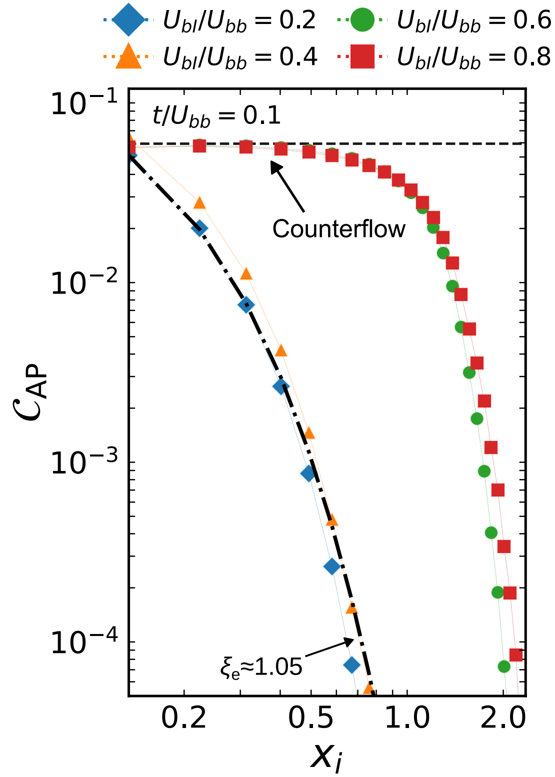
- It shows **long-range anti-pair order**

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

- **Supercounterflows** have been **studied theoretically** in the **past** in **two-component bosonic mixtures**.
  A. B. Kuklov and B. V. Svistunov, PRL **90**, 100401 (2003). C. Menotti and S. Stringari, PRA **81**, 045604 (2010).

- They were **realised experimentally** very recently with **binary Mott insulators**.
  Y.-G. Zheng *et al*., Nat. Phys. **21**, 208 (2025).



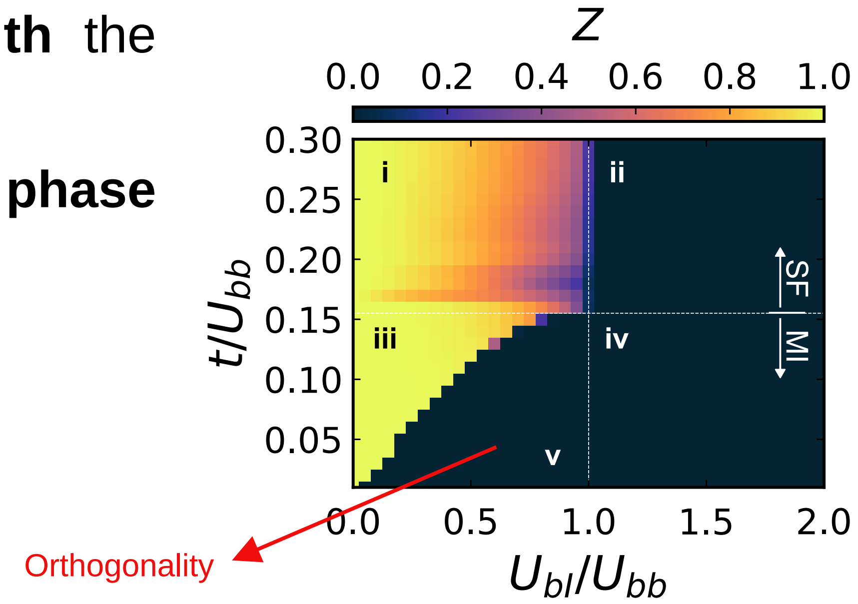


F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Counterflow

- **Counterflows** are **insulators**, explaining the combined insulator domain.
- **Counterflows require** commensurable filling or a **harmonic trap.**
- We showed that **counterflows** appear for **large population imbalance**.
- The **impurity forms** a **correlated state with** the **whole insulating bath**.
- The **residue** abruptly **vanishes** at the **phase transition**.

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



F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Counterflow

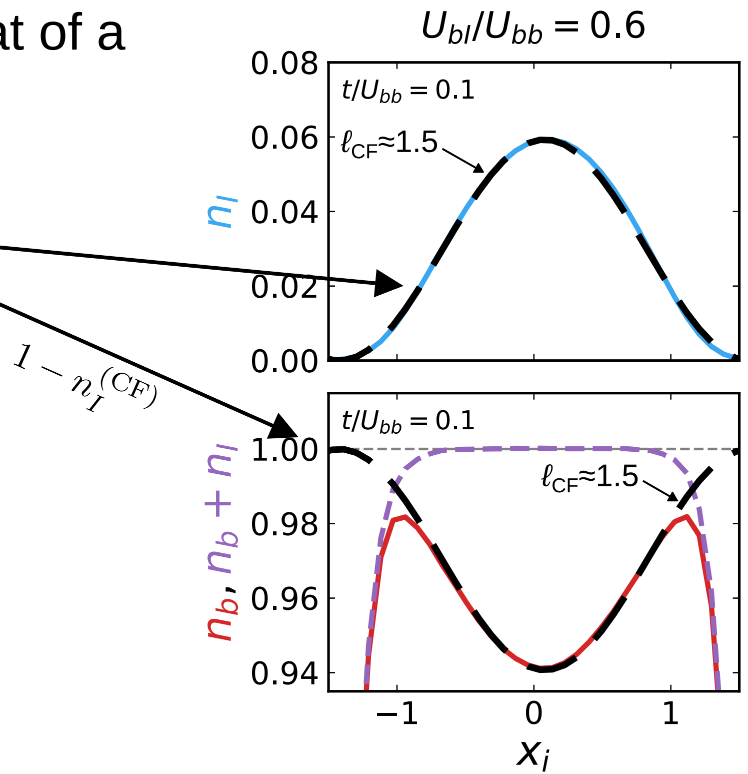
- We have found that the **profile** of the **impurity** is that of a **free particle** in a **square well**

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

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

- The **width** is given by:

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



F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Counterflow

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

$$|\mathrm{MI}\rangle = \prod_i \hat{a}^\dagger_{i,b}|\emptyset\rangle$$

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

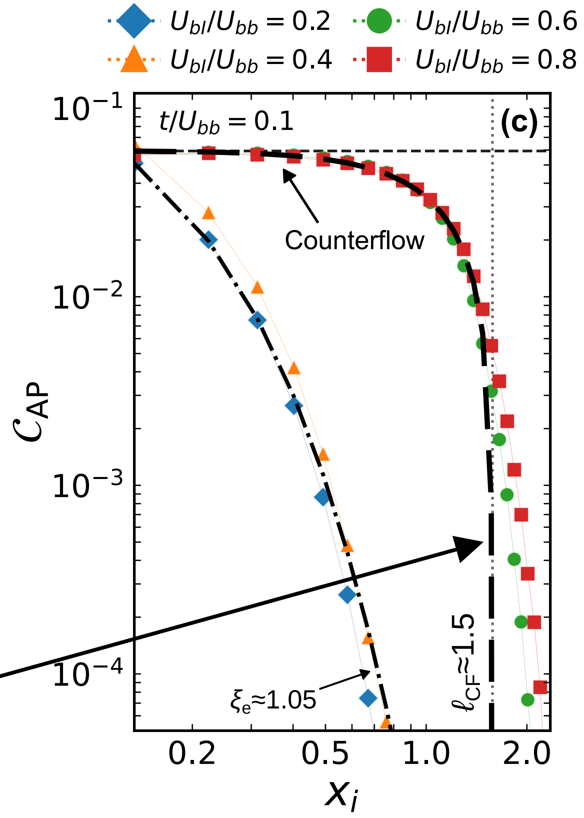
$$\longrightarrow \quad |\Psi_{\mathrm{CF}}\rangle = \sum_i \alpha_i |i_{\mathrm{IH}}\rangle.$$

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

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

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

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



F. Isaule, A. Rojo-Francàs, L. Morales-Molina and B. Juliá-Díaz, Phys. Rev. Lett. **135**, 023404 (2025)

Harmonically confined lattice polarons: Outlook

- An **impurity** forms a **correlated counterflow state** with an **insulating bath** in **harmonically confined optical lattices**.
- The **impurity** behaves as a **free particle** in a **square well**.
- Ideas for **future work** in **harmonically confined lattices**:
  - ➔ Study **dynamics**.
  - ➔ Consider **multiple impurities**.
  - ➔ Examine the **attractive branch** (molecule formation?).
  - ➔ Study balanced **binary mixtures** (droplets, supercounterflows, etc).

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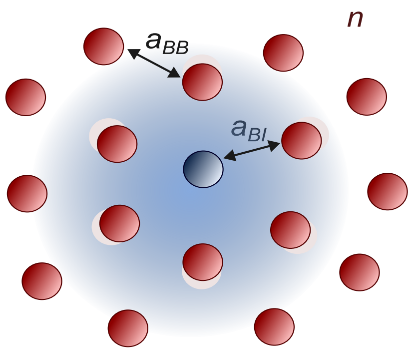
Bose polarons

- A **Bose polaron** is the quasiparticle formed by an **impurity** interacting with a **weakly-interacting Bose gas** (BEC).



$$\hat{H} = \sum_{k,\sigma=B,I} (\varepsilon_{k,\sigma} - \mu_\sigma)\hat{b}^\dagger_{k,\sigma}\hat{b}_{k,\sigma} + \frac{g_{BB}}{2\mathcal{V}} \sum_{kk'k''} \hat{b}^\dagger_{k,B}\hat{b}^\dagger_{k',B}\hat{b}_{k'-k'',B}\hat{b}_{k'-k'',B}$$

$$+ \frac{g_{BI}}{\mathcal{V}} \sum_{kk'k''} \hat{b}^\dagger_{k,B}\hat{b}^\dagger_{k',I}\hat{b}_{k'-k'',I}\hat{b}_{k'-k'',B}$$

Kinetic energy — Chemical potential — Boson-boson repulsion — Bath-impurity interaction

$$\varepsilon_{\boldsymbol{k},\sigma} = \frac{\boldsymbol{k}^2}{2m_\sigma}$$

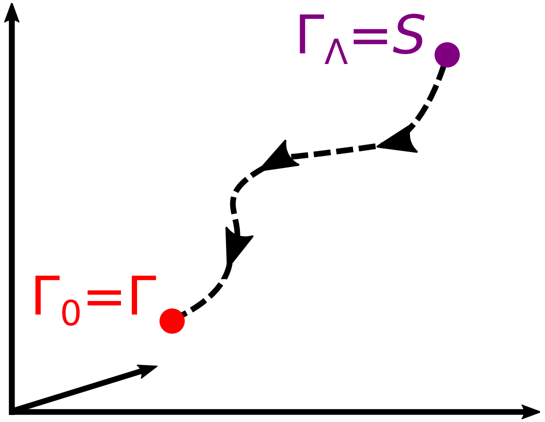
- Bose polarons were **achieved experimentally** in **2016**.

N. Jørgensen *et al.*, Phys. Rev. Lett. **117**, 055302 (2016), M. Hu *et al.*, Phys. Rev. Lett. **117**, 055301 (2016).

- The branch of **attractive bath-impurity interactions** offers **rich physics**:
  - **Strong coupling** regime (Unitary limit $a_{BI} \to \infty$), **three-** and more-**body correlations**, Efimov physics, finite temperatures.

The functional renormalisation group

- **Bose polarons** have been studied with a variety of techniques such as **Quantum MonteCarlo**, variational ansatzë, Frölich model, etc.
- In general, one needs to rely on **non-perturbative methods** to theoretically study the **strongly-interacting regime**.
- One such technique is the **functional renormalisation group** (FRG).
  N. Dupuis *et al.*, Phys. Rep. **910**, 1 (2021).
- The objective of the FRG is to compute an **effective action** Γ (IR) from a microscopic action $\mathcal{S}$ (UV).



Wetterich equation:

$$\partial_k \Gamma_k = \frac{1}{2} \mathrm{tr} \left[\partial_k R_k (\Gamma^{(2)} + R_k)^{-1} \right]$$

C. Wetterich, Phys. Lett. B **301**, 90 (1993)

Regulator ("cutoff")

$$\mathcal{Z}[\varphi] = \int D\varphi e^{-\mathcal{S}[\varphi]} \longrightarrow \Omega_G = -\frac{1}{\beta} \ln \mathcal{Z} = \frac{1}{\beta} \Gamma[\varphi_{\mathrm{cl},0}]$$

The functional renormalisation group

- The FRG is useful to study **strongly correlated systems** and critical phenomena.

- It has been used in different problems in **ultracold atomic** systems:

  - One-component Bose gases
    S. Floerchinger and C. Wetterich, Phys. Rev. A **77**, 053603 (2008). Phys. Rev. A **79**, 013601 (2009).

  - Fermi gases: BCS-BEC crossover
    S. Floerchinger *et al.*, Phys. Rev. A **81**, 063619 (2010). I. Boettcher *et al.*, Phys. Rev. A **89**, 053630 (2014).

  - Bose gases in optical lattices
    A. Rançon and N. Dupuis, Phys. Rev. A **85**, 063607 (2012), Phys. Rev. A **86**, 043624 (2012).

  - Few bosons: Efimov physics
    S. Floerchinger *et al*., Few-Body Syst. **51**, 153 (2011). R. Schmidt and S. Moroz, Phys. Rev. A **81**, 052709 (2010).

  - Fermi polaron
    R. Schmidt and T. Enss, Phys. Rev. A **83**, 063620 (2011). von Milczewski *et al*., Phys. Rev. A **105**, 013317 (2022).

Field-theory description of Bose Polarons

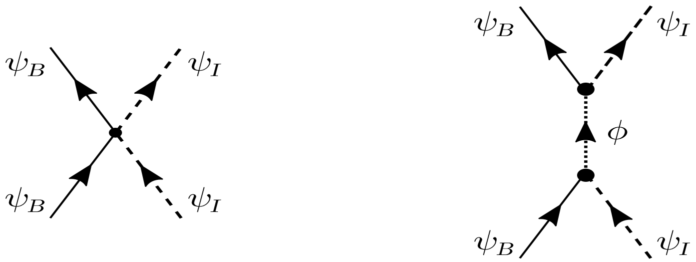
- The **microscopic model** for the **Bose polaron** problem reads

S. P. Rath and R. Schmidt, Phys. Rev. A **88**, 053632 (2013).

$$\mathcal{S} = \int_x \left[\sum_{\sigma=B,I} \psi_\sigma^\dagger \left(\partial_\tau - \frac{\nabla^2}{2m_\sigma} - \mu_\sigma \right) \psi_\sigma + \nu_\phi \phi^\dagger \phi + \frac{g_{BB}}{2} (\psi_B^\dagger \psi_B)^2 + h_\Lambda \left(\phi^\dagger \psi_B \psi_I + \phi \psi_B^\dagger \psi_I^\dagger \right) \right],$$

Kinetic energy | Chemical potential | Boson-boson repulsion | Bath-impurity interaction

where $\phi \sim \psi_B \psi_I$ are **auxiliary dimer fields** that **mediate** the **bath-impurity interaction**.



Hubbard-Stratonovich transformation

F. Isaule. I. Morera, P. Massignan, and B. Juliá-Díaz, Phys. Rev A. **104**, 023317 (2021).

FRG for Bose polarons

- We employ the following **ansatz** (shortened version):

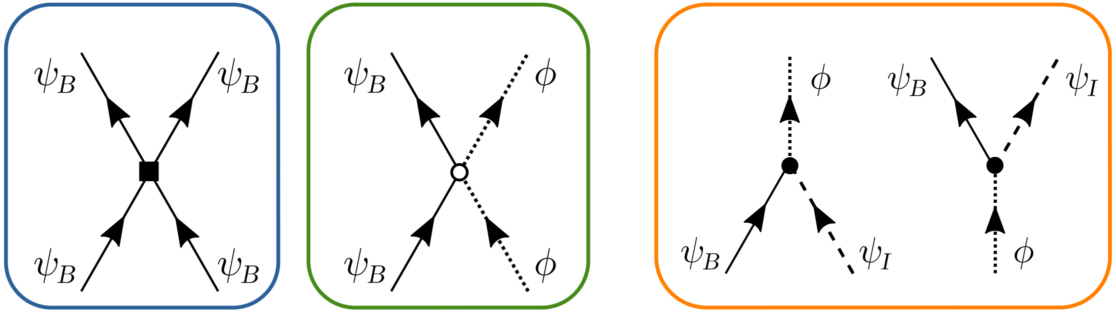
$$\Gamma_k = \int_x \Big[\psi_B^\dagger \left(S_B\partial_\tau - \frac{Z_B}{2m_B}\nabla^2\right)\psi_B + \psi_I^\dagger\left(S_I\partial_\tau - \frac{Z_I}{2m_I}\nabla^2 + m_I^2\right)\psi_I$$

$$+\phi^\dagger\left(S_\phi\partial_\tau - \frac{Z_\phi}{2m_\phi}\nabla^2 + m_\phi^2\right)\phi + U_B(|\psi_B|^2) + \lambda_{B\phi}|\psi_B|^2|\phi|^2 + h\left(\phi^\dagger\psi_B\psi_I + \phi\psi_B^\dagger\psi_I^\dagger\right)\Big].$$

Boson-boson repulsion

Three-body Bath-impurity interaction

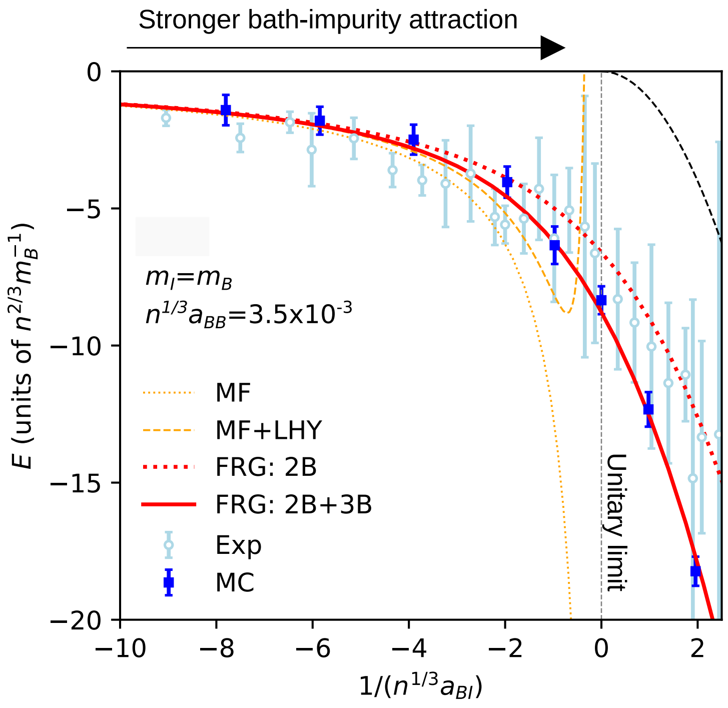
Two-body Bath-impurity interaction

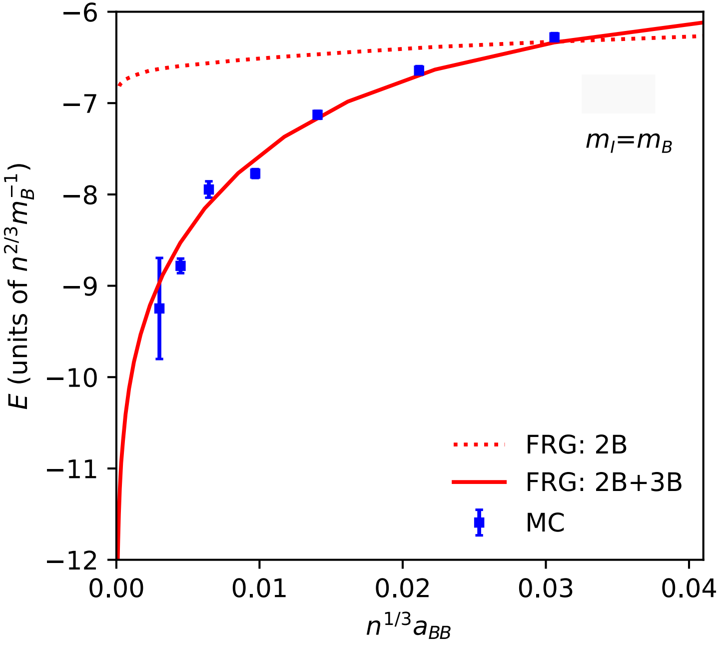


- **Multi-body correlations** can be added **systematically.**
- We **solved** the RG flow **with and without three-body correlations**.

F. Isaule. I. Morera, P. Massignan, and B. Juliá-Díaz, Phys. Rev A. **104**, 023317 (2021).

Polaron energy for the three-dimensional Bose Polaron





n: Bath density
a_{BB}: boson-boson scattering length
a_{BI}: bath-impurity scattering length

Exp (left): N.B Jørgensen *et al.*, PRL **117**, 055302 (2016).
QMC (left): L. Peña Ardila *et al.*, PRA **99**, 063607 (2019).
QMC (right): L. Peña Ardila and S. Giorgini, PRA **92**, 033612 (2015).

F. Isaule. I. Morera, P. Massignan, and B. Juliá-Díaz, Phys. Rev A. **104**, 023317 (2021).

FRG for Bose polarons

- The **FRG describes** with **high accuracy** the **Bose polaron**, giving a good agreement with Quantum Monte-Carlo.
- It allows us to **quantify** the effect of **three-body correlations** and add them systematically.
- Future work:
  - Polarons across the **BCS-BEC crossover**.
  - Efimov physics in Bose polarons.
  - Bipolarons in BECs.
  - **Bose-Fermi** mixtures.
  - Polarons in **optical lattices**.

Ultracold polarons and impurities

1. Quantum **polarons and impurities** in ultracold atomic systems.
2. One-dimensional **harmonically confined lattice polarons** and **counterflows.**
3. Polaron physics with the **functional renormalisation group**.
4. Summary and **future work**.

Summary

- We have **numerically** studied **impurities** interacting with **bosonic baths** in **optical lattices** across the **SF-MI transition**.
- We have found the onset of a correlated **counterflow** bath-impurity state in **harmonically confined optical lattices**.
- The **FRG** is a **powerful technique** to study **strongly-interacting polarons**.
- Future work:
  - Further studies of **impurities** and **mixtures** in **harmonically confined optical lattices**.
  - Employ the **FRG** to study **more complicated polaron** configurations.