improving the grasp of harmonically trapped fermions in low dimensions

[LR, D. Huber, H.W. Hammer, A.G. Volosniev, (arxiv:2106.XXXXX)]

Lukas Rammelmüller, LMU Munich

52nd DAMOP Meeting, June 04, 2021

nothing will be placed here

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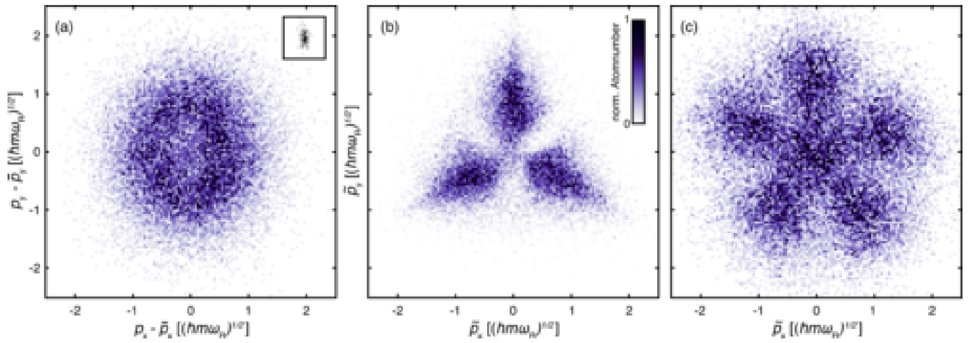
PHYSICAL REVIEW LETTERS

Featured in Physics | Editors' Suggestion

Observation of Pauli Crystals

Marvin Holten, Luca Bayha, Keerthan Subramanian, Carl Heintze, Philipp M. Preiss, and Selim Jochim
Phys. Rev. Lett. **126**, 020401 – Published 13 January 2021

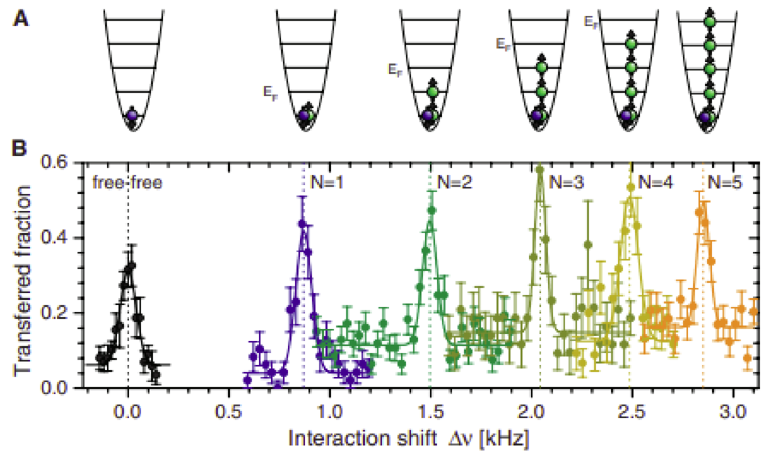


REPORT

From Few to Many: Observing the Formation of a Fermi Sea One Atom at a Time

A. N. Wenz[1,2,*,†], G. Zürn[1,2,†], S. Murmann[1,2], I. Brouzos[3], T. Lompe[1,2,4], S. Jochim[1,2,4]
+ See all authors and affiliations

Science 25 Oct 2013:

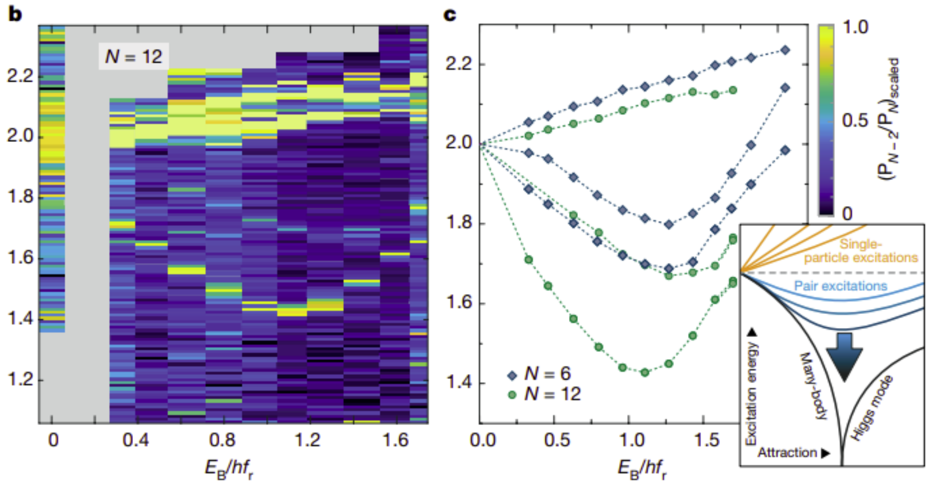


nature

Article | Published: 25 November 2020

Observing the emergence of a quantum phase transition shell by shell

Luca Bayha, Marvin Holten, Ralf Klemt, Keerthan Subramanian, Johannes Bjerlin, Stephanie M. Reimann, Georg M. Bruun, Philipp M. Preiss & Selim Jochim



PHYSICAL REVIEW LETTERS

Pairing in Few-Fermion Systems with Attractive Interactions

G. Zürn, A. N. Wenz, S. Murmann, A. Bergschneider, T. Lompe, and S. Jochim
Phys. Rev. Lett. **111**, 175302 – Published 22 October 2013

... and many more experiments!

[reviews: Guan,Batchelor,Lee '13; Sowiński,García-March '19]

outline

part I

theoretical description and **effective two-body interaction**

(how can proper renormalization help us with convergence?)

part II

application: **few 1D trapped fermions with magnetic impurity**

(emergence of a 1D quantum phase transition)

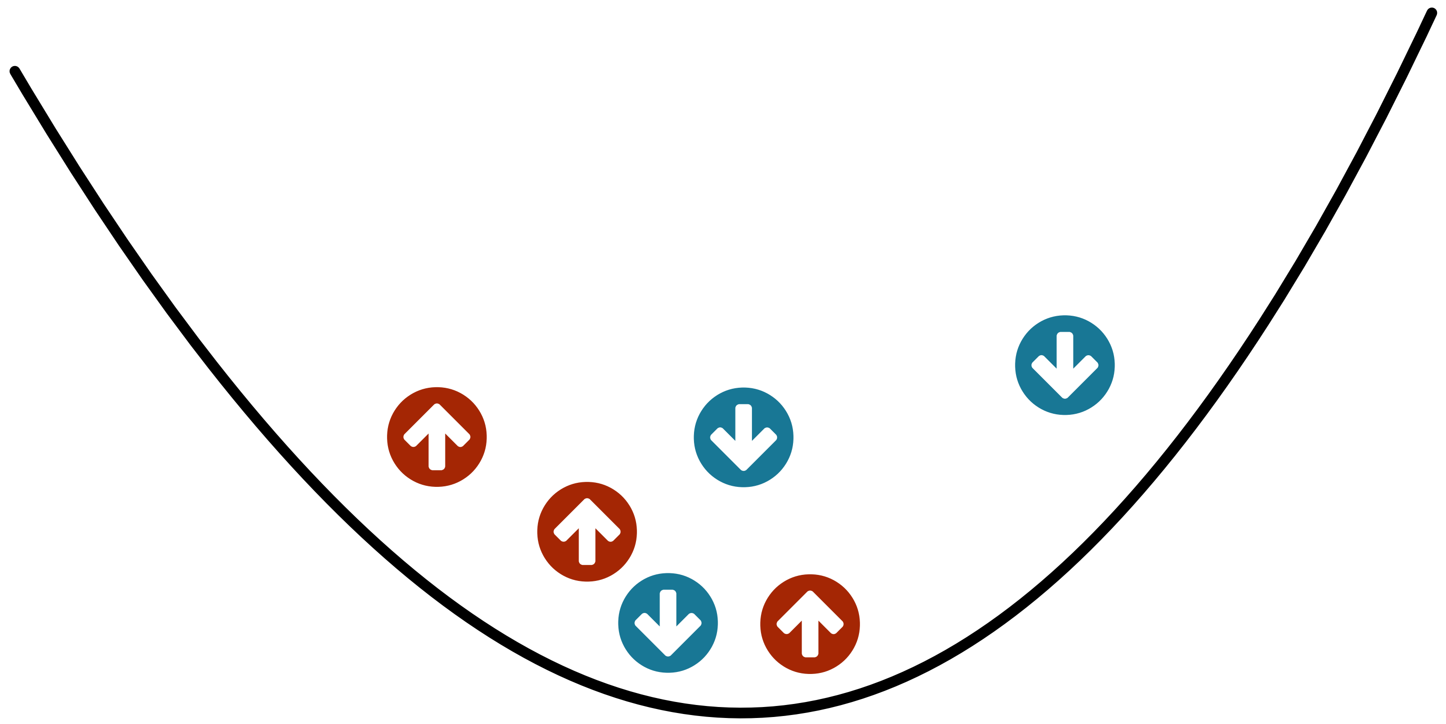
harmonically trapped fermions

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla^2_{\vec{x}_i} + \frac{m\omega^2}{2} x_i^2 \right) + g \sum_{i \neq j} \delta^{(d)} (\vec{x}_i - \vec{x}_j)$$

kinetic part

harmonic trap

contact interaction

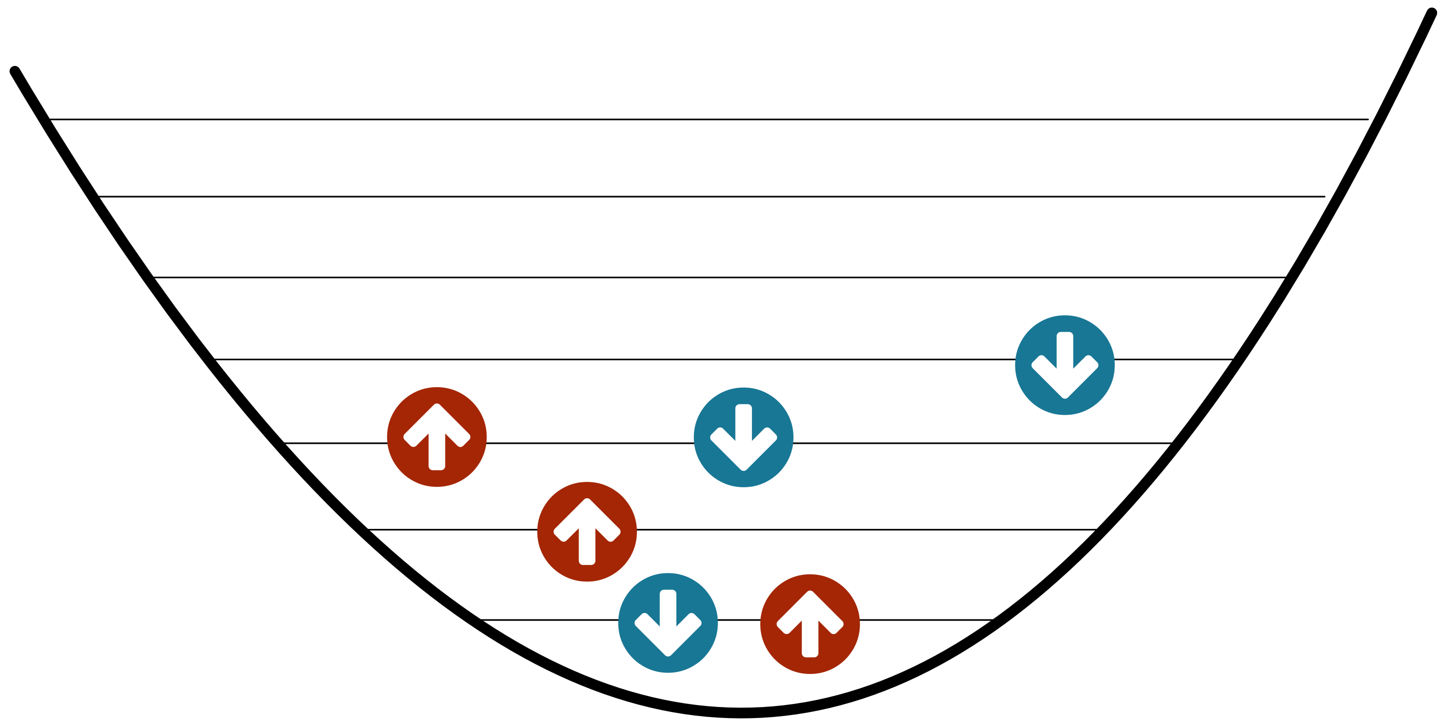


harmonically trapped fermions

$$\hat{H} = \sum_{i,\sigma} \varepsilon_{i\sigma} \, \hat{\psi}^\dagger_{i\sigma} \hat{\psi}_{i\sigma} + \sum_{ijkl} V_{ijkl} \, \hat{\psi}_{i\uparrow} \hat{\psi}_{j\downarrow} \hat{\psi}_{l\downarrow} \hat{\psi}_{k\uparrow}$$

diagonal in HO basis

(generic) all-to-all interaction



harmonically trapped fermions + FCI / ED

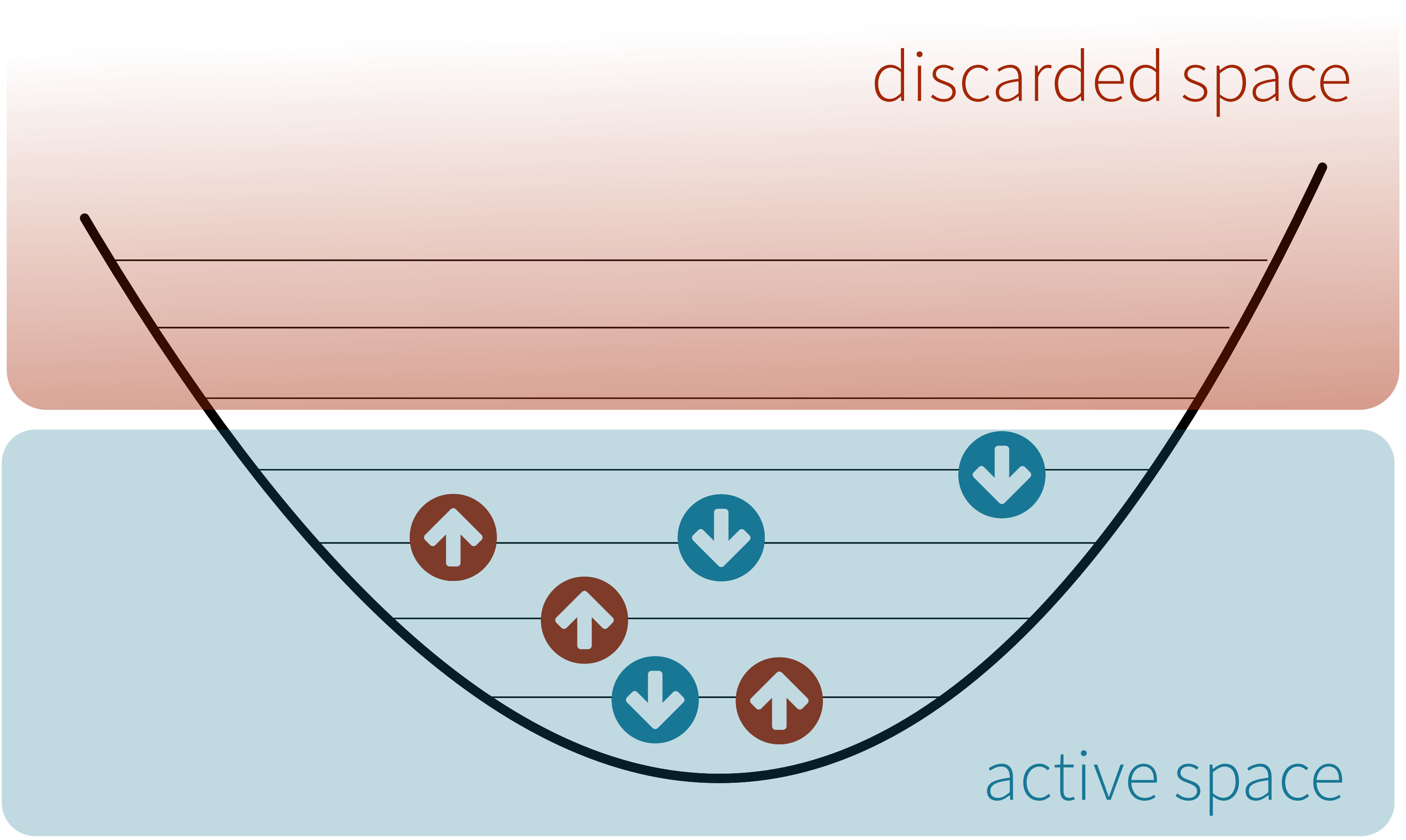
$$\hat{H} = \sum_{i,\sigma} \varepsilon_{i\sigma}\, \hat{\psi}^\dagger_{i\sigma}\hat{\psi}_{i\sigma} + \sum_{ijkl} V_{ijkl}\, \hat{\psi}_{i\uparrow}\hat{\psi}_{j\downarrow}\hat{\psi}_{l\downarrow}\hat{\psi}_{k\uparrow}$$

diagonal in HO basis

(generic) all-to-all interaction

standard approach: full-configuration interaction (FCI)

regularization through finite basis set (maximal single-particle orbital, energy cutoff etc.)



harmonically trapped fermions + FCI / ED

$$\hat{H} = \sum_{i,\sigma} \varepsilon_{i\sigma}\, \hat{\psi}^\dagger_{i\sigma}\hat{\psi}_{i\sigma} + \sum_{ijkl} V_{ijkl}\, \hat{\psi}_{i\uparrow}\hat{\psi}_{j\downarrow}\hat{\psi}_{l\downarrow}\hat{\psi}_{k\uparrow}$$

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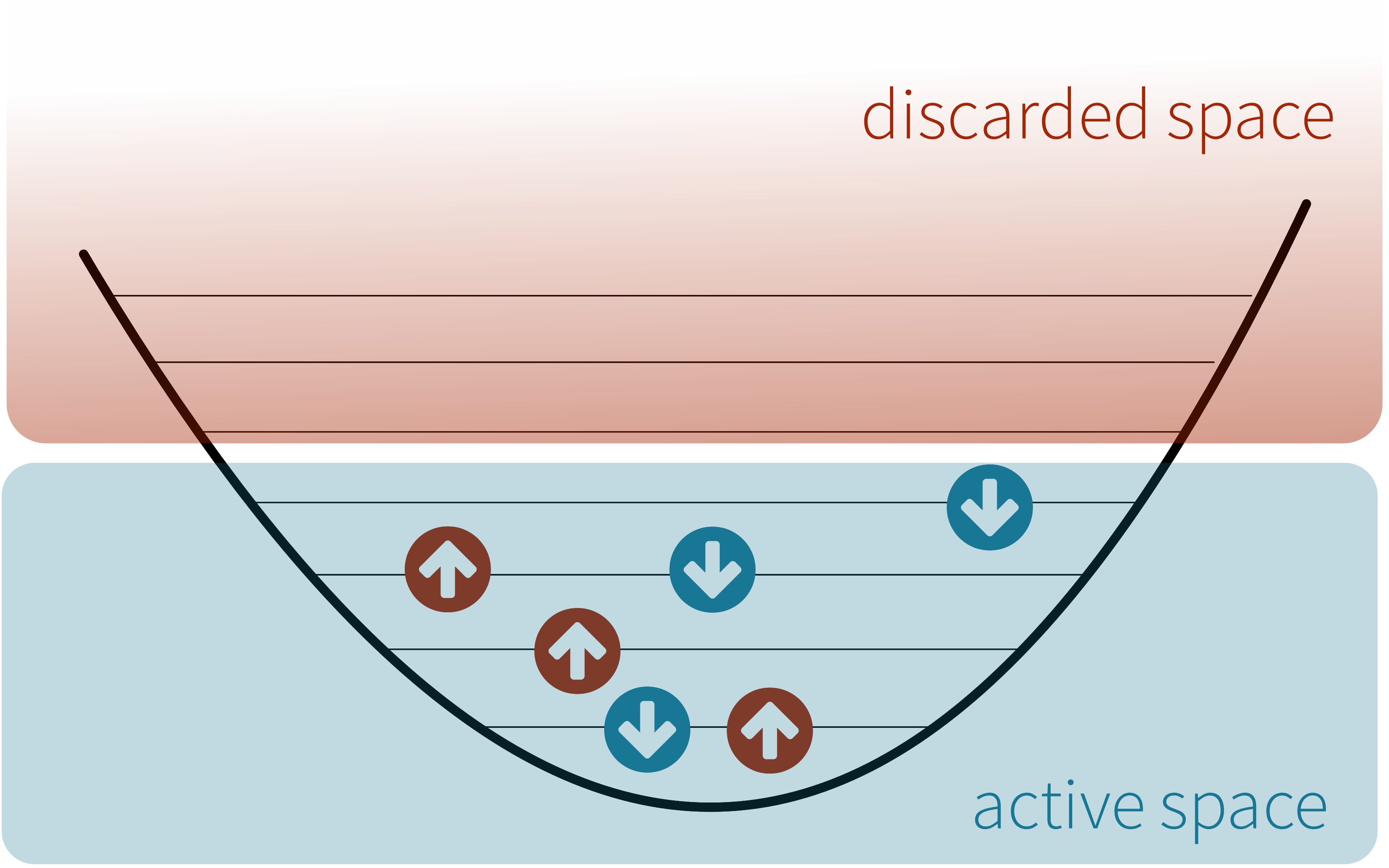


$$\dim \mathcal{H} = \binom{N_b}{N_\uparrow}\binom{N_b}{N_\downarrow}$$

main bottleneck:

can convergence be achieved?

effective two-body interaction

[Rotureau '13; Lindgren '14]

$$H_{ab}^{(2)} = \langle \psi_a | \hat{H}^{(2)} | \psi_b \rangle$$

$$= \sum_{n,m} \langle \Phi_a | \Psi_n \rangle \langle \Psi_n | \hat{H}^{(2)} | \Psi_m \rangle \langle \Psi_m | \Phi_b \rangle$$

$$= \sum_{n} \langle \Phi_a | \Psi_n \rangle \, \varepsilon_n^{(2)} \, \langle \Psi_n | \Phi_b \rangle \equiv U^\dagger E^{(2)} U$$

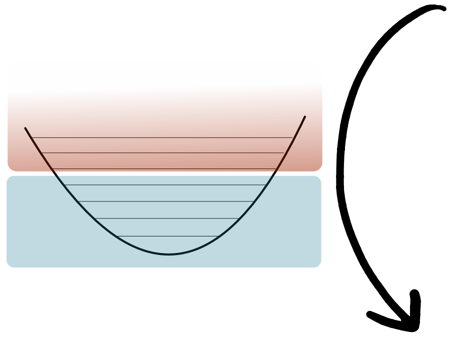
exact energies and eigenfunctions
from analytic solution of two-body problem
(Busch formula)

[Busch et al. '98]

effective two-body interaction

[Rotureau '13; Lindgren '14]

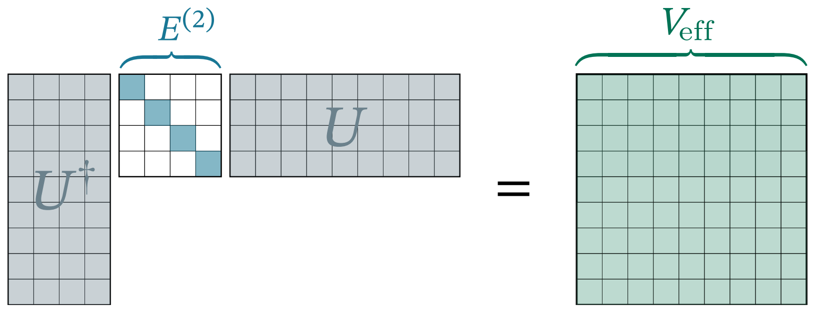
$$H^{(2)}_{ab} = \langle \psi_a | \hat{H}^{(2)} | \psi_b \rangle$$
$$= \sum_{n,m} \langle \Phi_a | \Psi_n \rangle \langle \Psi_n | \hat{H}^{(2)} | \Psi_m \rangle \langle \Psi_m | \Phi_b \rangle$$
$$= \sum_{n} \langle \Phi_a | \Psi_n \rangle \, \varepsilon^{(2)}_n \, \langle \Psi_n | \Phi_b \rangle \equiv U^\dagger E^{(2)} U$$



$$Q_{\mathcal{M}} = \frac{U_{\mathcal{M}\mathcal{M}}}{\sqrt{U^\dagger_{\mathcal{M}\mathcal{M}} U_{\mathcal{M}\mathcal{M}}}}$$

$$V^{(2)}_{\mathrm{eff}} = Q^\dagger_{\mathcal{M}} E^{(2)}_{\mathcal{M}} Q_{\mathcal{M}} - T^0_{\mathcal{M}}$$

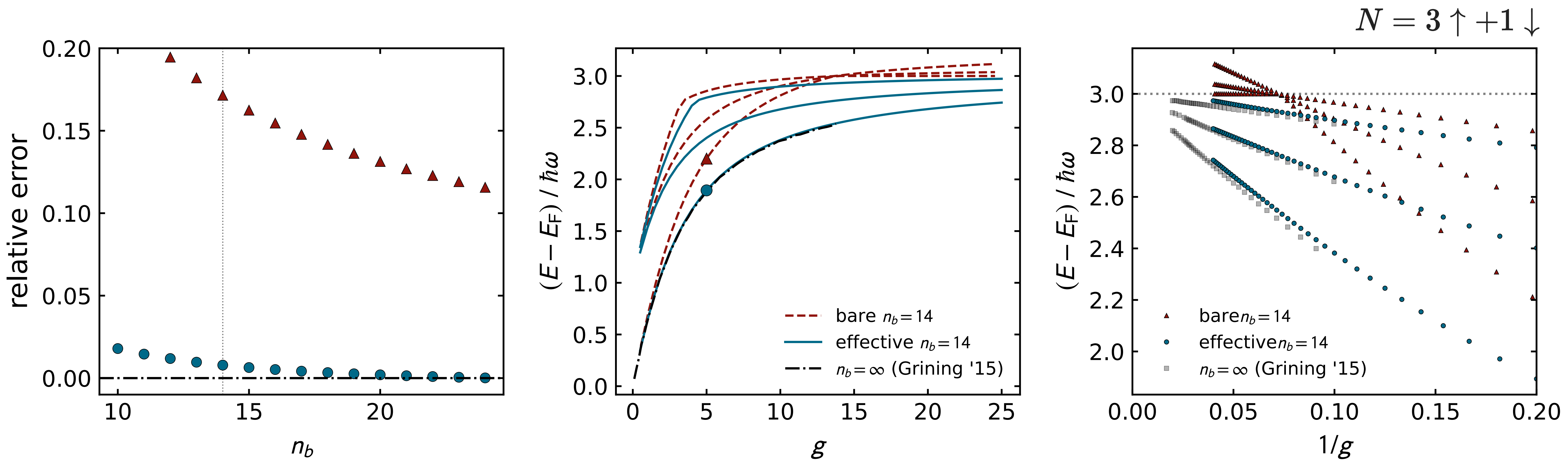
$$V_{ijkl} = \sum_b \alpha_{ij,(i+j-b)b} \, \alpha_{kl,(k+l-b)b} \, [V^{(2)}_{\mathrm{eff}}]_{(i+j-b)(k+l-b)}$$



optimized two-body interaction that **exactly** reproduces the two-body spectrum **already in the finite basis set $\mathcal{M}$**

few-body: benchmark vs. extrapolated values

[extrapolated FCI: Grining et al. '15]

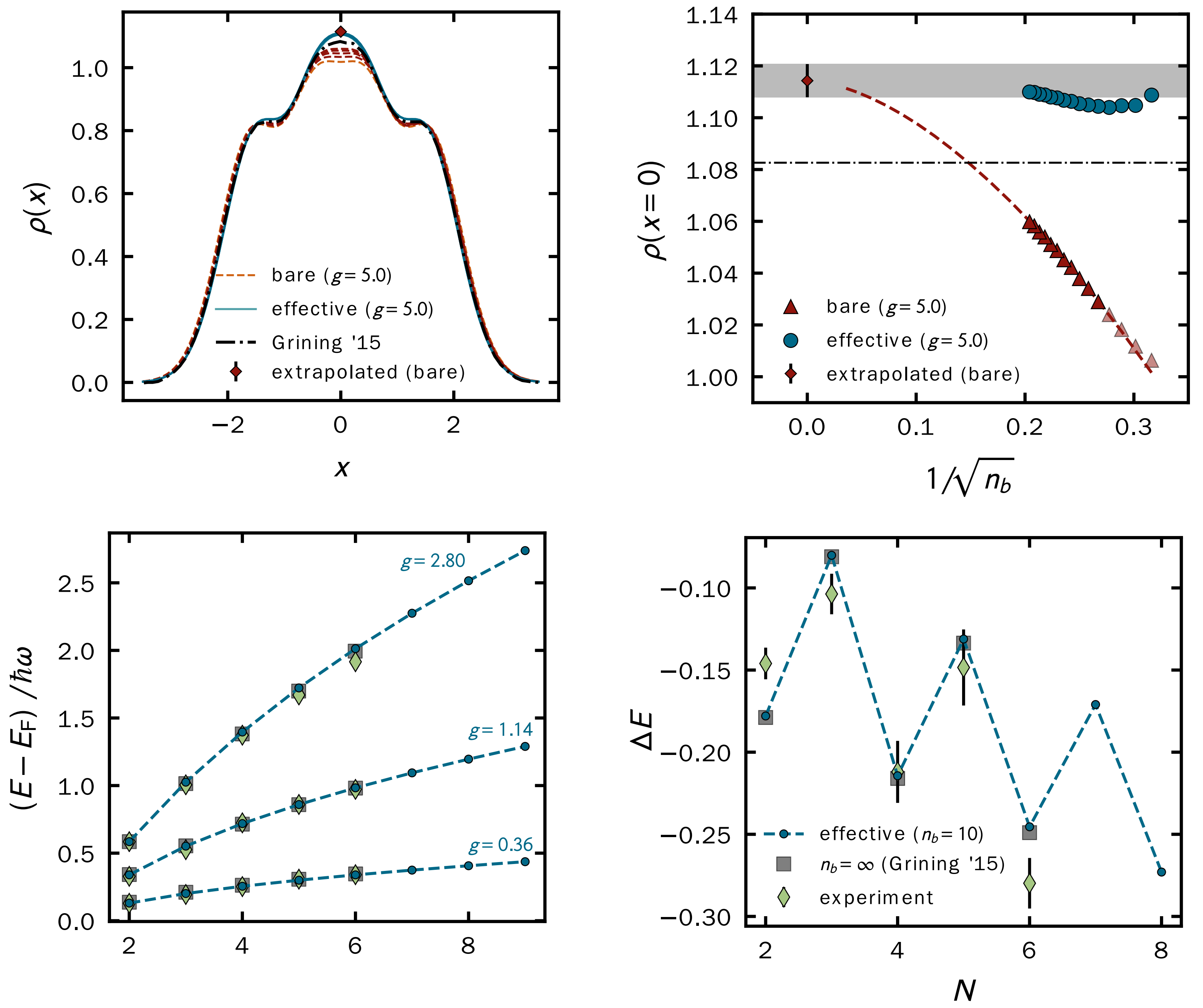


- effective interaction **within ~1% of extrapolated value already at small cutoff**
- low-lying energy states reproduced well up to strong interactions

more benchmarks

[extrapolated FCI: Grining et al. '15; experiment: Wenz et al. '13, Zürn et al. '13]

$N = 3\uparrow + 1\downarrow$



- excellent convergence of density profiles

$$\rho(x) = \langle \psi^\dagger(x)\psi(x) \rangle$$

- experimentally relevant quantities are reproduced reliably

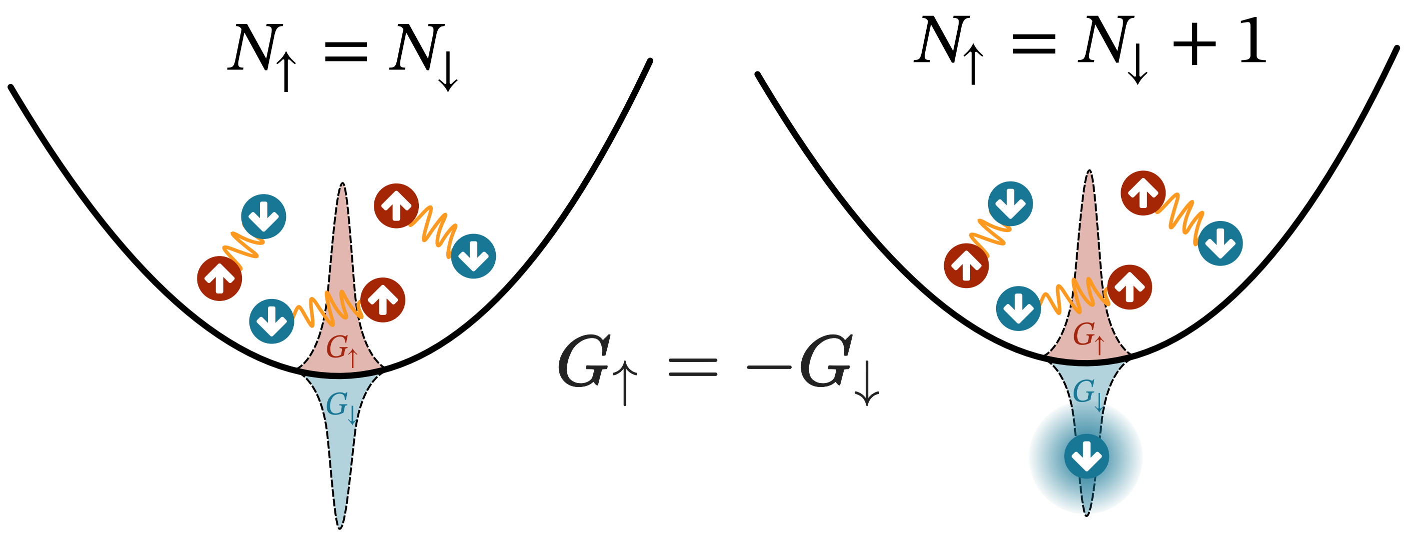
$$\Delta E = \mu(N) - \mu^0(N)$$

$$\mu(N) = E(N) - E(N-1)$$

magnetic impurity in a 1D trap

[Balatsky et al. '06]

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla^2_{\vec{x}_i} + \frac{m\omega^2}{2} x_i^2 \right) + g \sum_{i \neq j} \delta^{(d)}(\vec{x}_i - \vec{x}_j) + \underbrace{\sum_{\sigma} G_\sigma \sum_{i=1}^{N} \delta(x_i)}_{\text{magnetic impurity}}$$

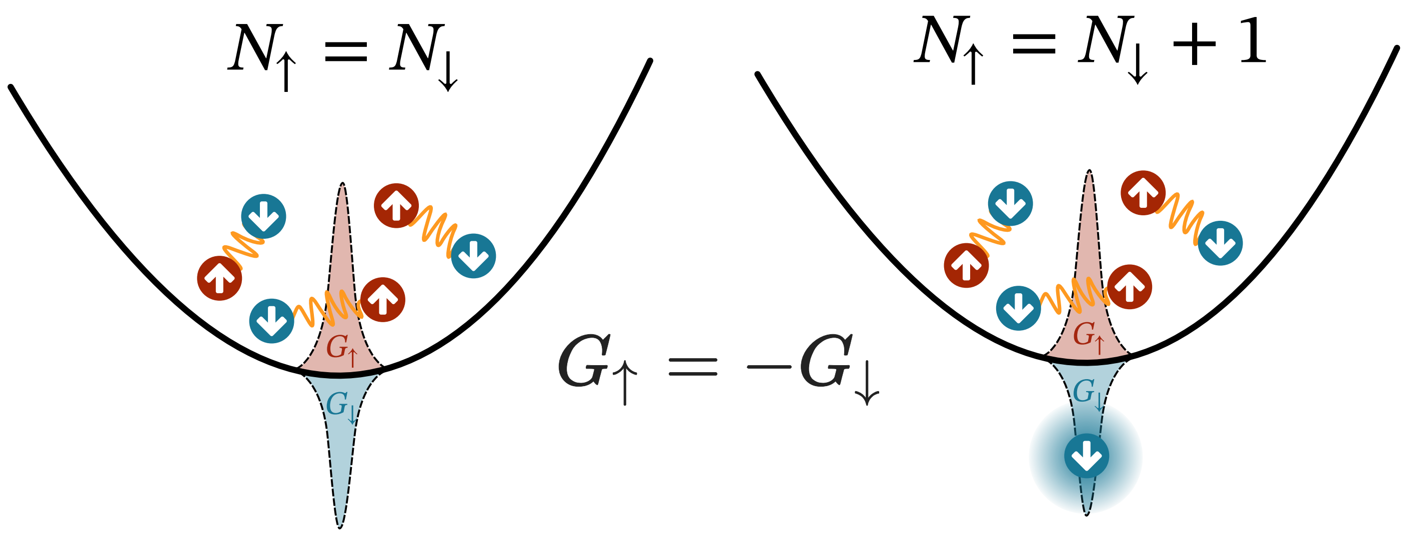


magnetic impurity may form a **bound state** with one of the particles

magnetic impurity in a 1D trap

[Balatsky et al. '06]

$$\hat{H} = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{x}_i} + \frac{m\omega^2}{2}x_i^2\right) + g\sum_{i\neq j}\delta^{(d)}(\vec{x}_i - \vec{x}_j) + \underbrace{\sum_{\sigma} G_\sigma \sum_{i=1}^{N}\delta(x_i)}_{\text{magnetic impurity}}$$



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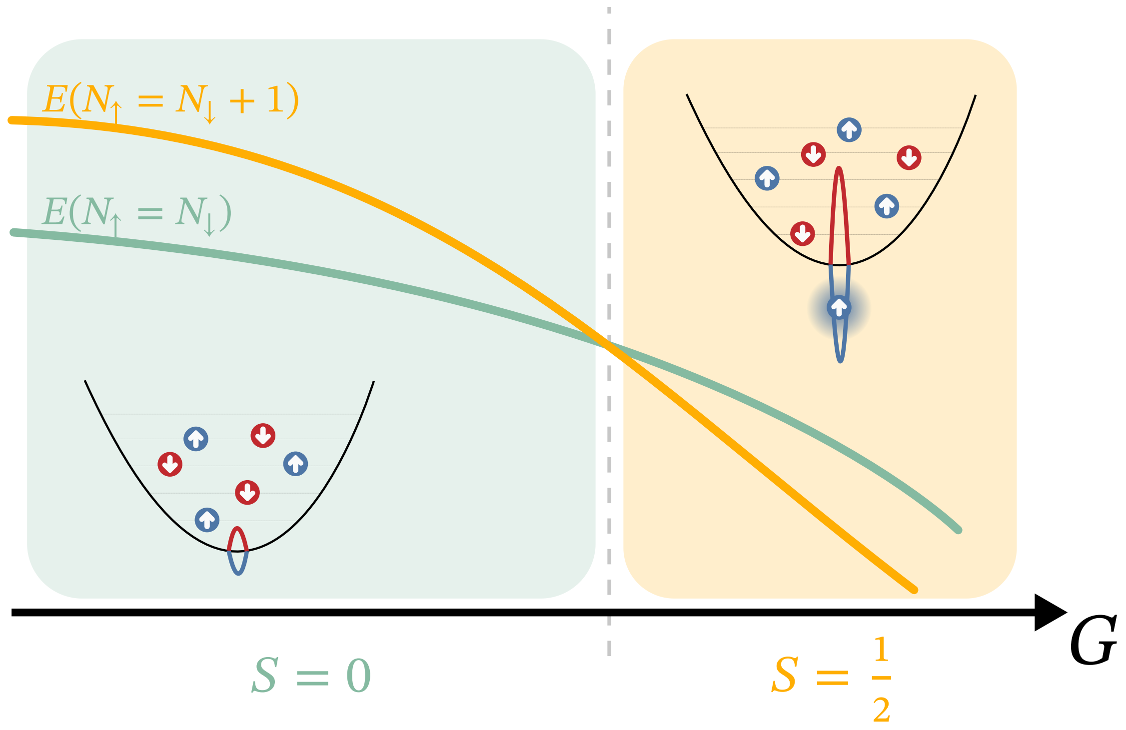
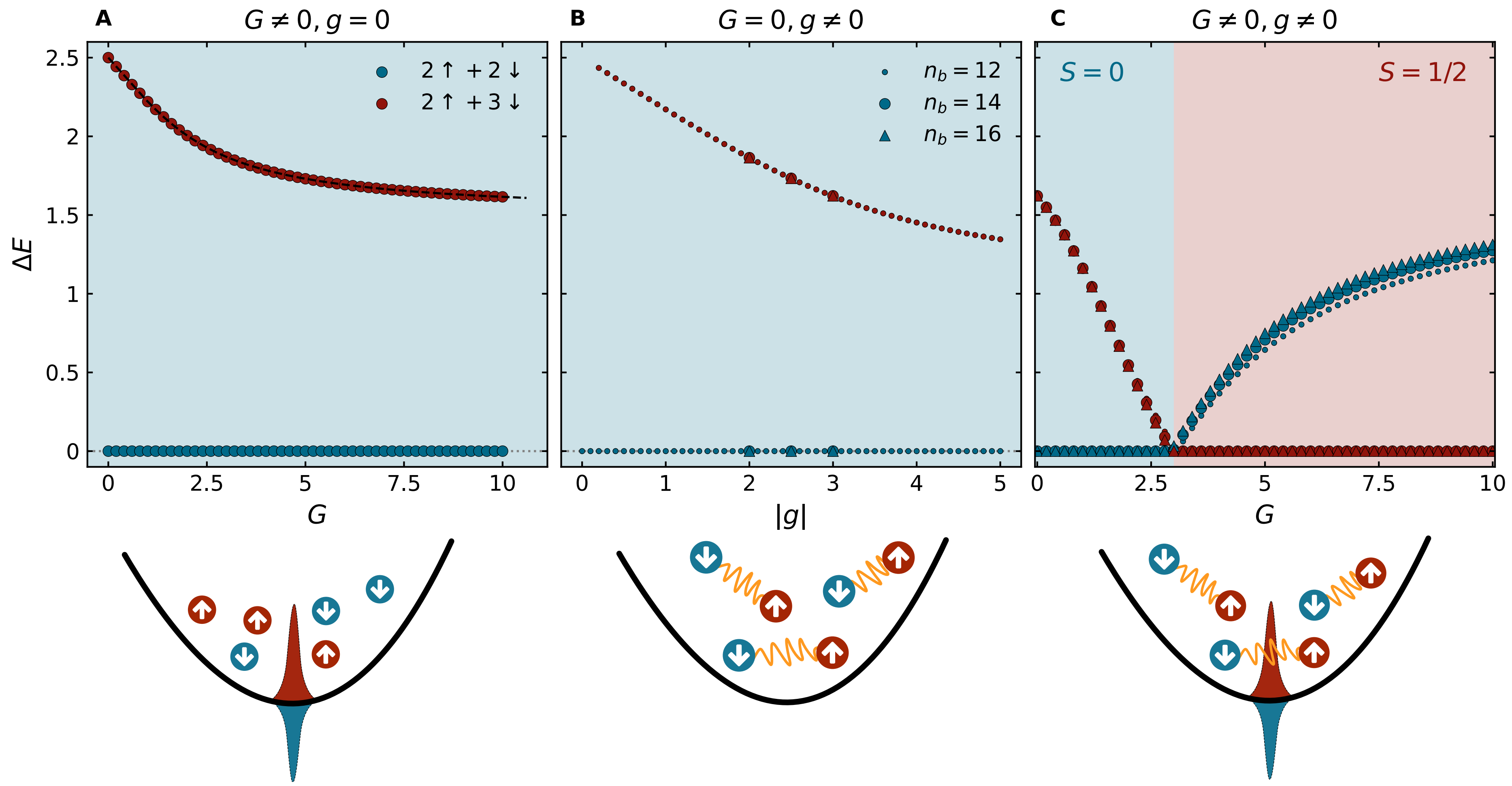


precursor of a one-dimensional QPT **(preliminary)**

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



- no crossover for non-interacting particles ($g = 0$) or no impurity ($G = 0$)
- **ground-state level crossing** between $S = 0$ and $S = \frac{1}{2}$ sectors for $g, G \neq 0$

precursor of a one-dimensional QPT (preliminary)

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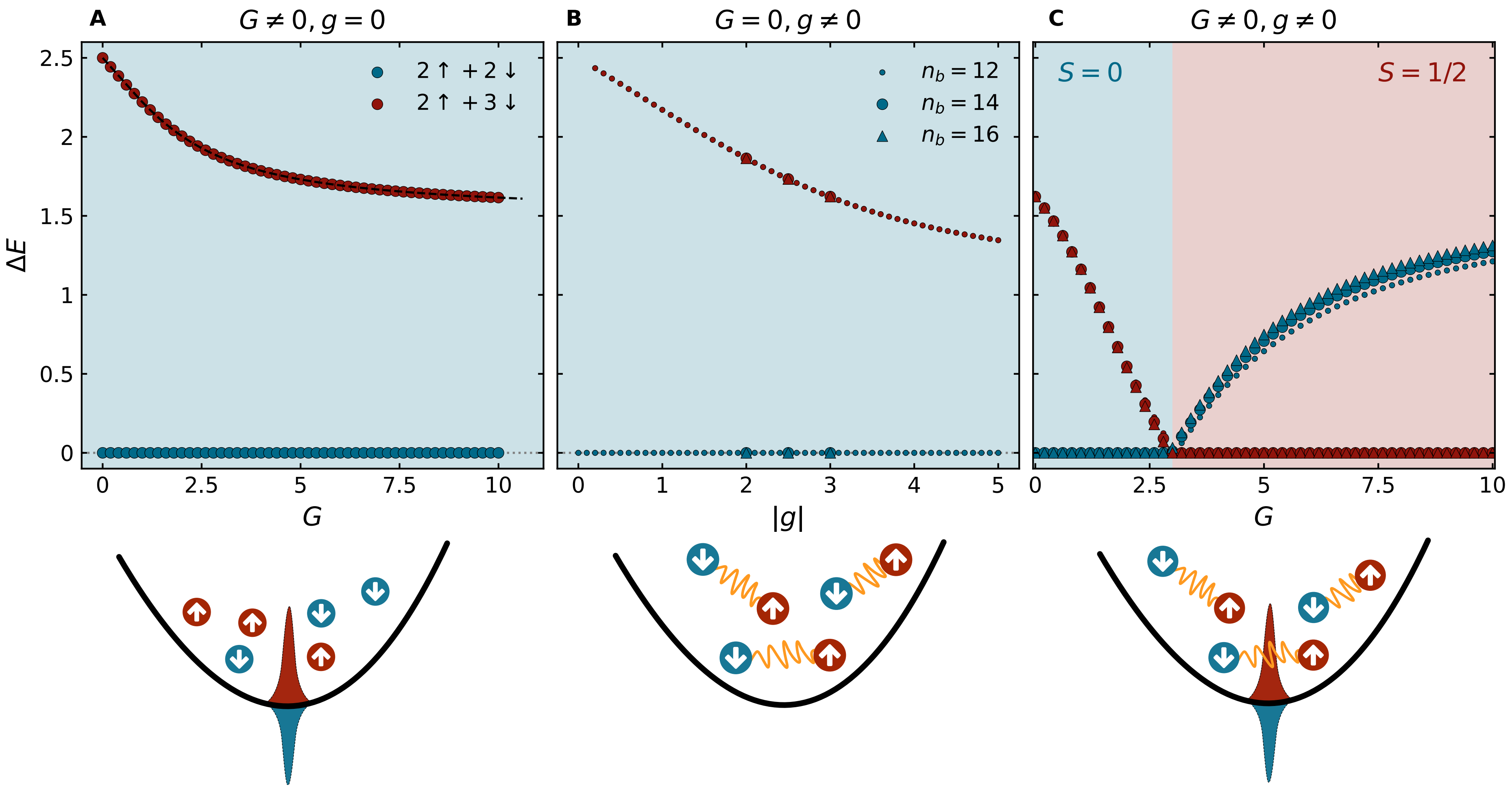
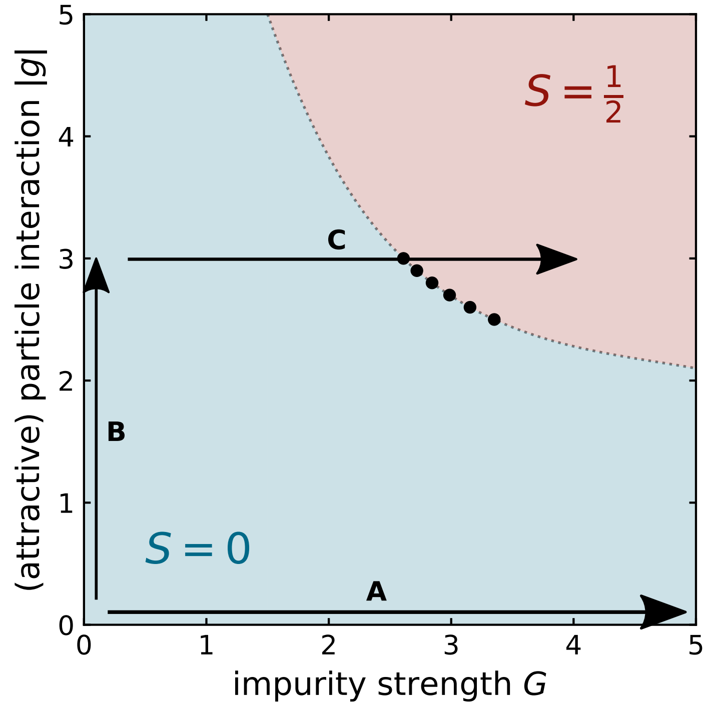


few-body "phase diagram"



transition requires sizeable particle interaction and impurity strength

- no crossover for non-interacting particles ($g = 0$) or no impurity ($G = 0$)
- **ground-state level crossing** between $S = 0$ and $S = \frac{1}{2}$ sectors for $g, G \neq 0$

recap & future directions

an **effective two-body interaction** can help us
to drastically reduce computational burden in FCI calculations

shown to work well for

harmonically trapped fermions with magnetic impurity

(found a few-body precusor of a QPT)

a versatile approach:

not limited to 1D nor harmonic confinement