Density-Matrix Renormalisation Group for Continuous Systems

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SD, Anton Buyskikh, Andrew Daley (Strathclyde), Erich Mueller (Cornell)
arXiv:2108.05366

Open-source code: github.com/Shovan-Physics/cDMRG

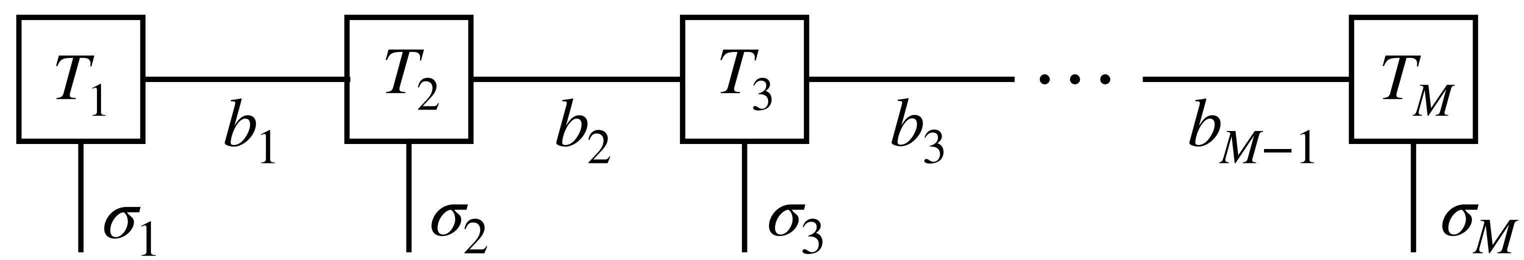
DMRG

U. Schollwöck, Ann. Phys. 326 (2011) 96

State of the art for accurate simulation of discrete 1D systems

- Efficiently truncate Hilbert space based on local entanglement
- Variationally minimise over Matrix Product States

$\Psi_{\sigma_1,\sigma_2,\ldots,\sigma_M} \equiv$



— Bond dimension controls max entanglement

Extension to continuum remains a key challenge

- Discretisation on a grid — poor convergence + can get stuck
- Field-theory (cMPS) — impractical for inhomogeneous systems
- Open problems: shallow lattices, FFLO physics, long-range interactions, prethermalisation, false vacuum decay, …

Main takeaways

Idea

- Divide into segments + use continuous basis functions in each
- Maps onto a discrete Hamiltonian — apply existing DMRG routines

Application: bosons w/ contact interactions + potential

- Reproduces known limits — Bethe Ansatz, Tonks gas, tight-binding
- Fast, tuneable convergence — not achieved by discretisation
- Superfluid-Mott transition in shallow lattice

Generalisations

- Fermions, Mixtures, Long-range interactions, …
- Time evolution with existing techniques (TDVP)

Formalism

Interacting bosons $\hat{H} = \int_0^1 dx \left[-\hat{\psi}^\dagger(x)\, \partial_x^2\, \hat{\psi}(x) + g\, \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x)\right]$

Partition system into M segments

$$\hat{\psi}(x) = \sum_{j=1}^{M} \square_{X_{j-1},X_j}(x)\, \hat{\psi}(x) \quad \text{where} \quad \square_{a,b}(x) = 1 \ \text{ iff } \ a \le x \le b$$

$$\Longrightarrow \ \hat{H} = \sum_j \hat{K}_j + \hat{U}_j + \Lambda\, [\hat{\psi}(X_j^-) - \hat{\psi}(X_j^+)]^\dagger [\hat{\psi}(X_j^-) - \hat{\psi}(X_j^+)] \qquad (\Lambda \to \infty)$$

- Same form as discrete DMRG — increase discontinuity penalty Λ in steps

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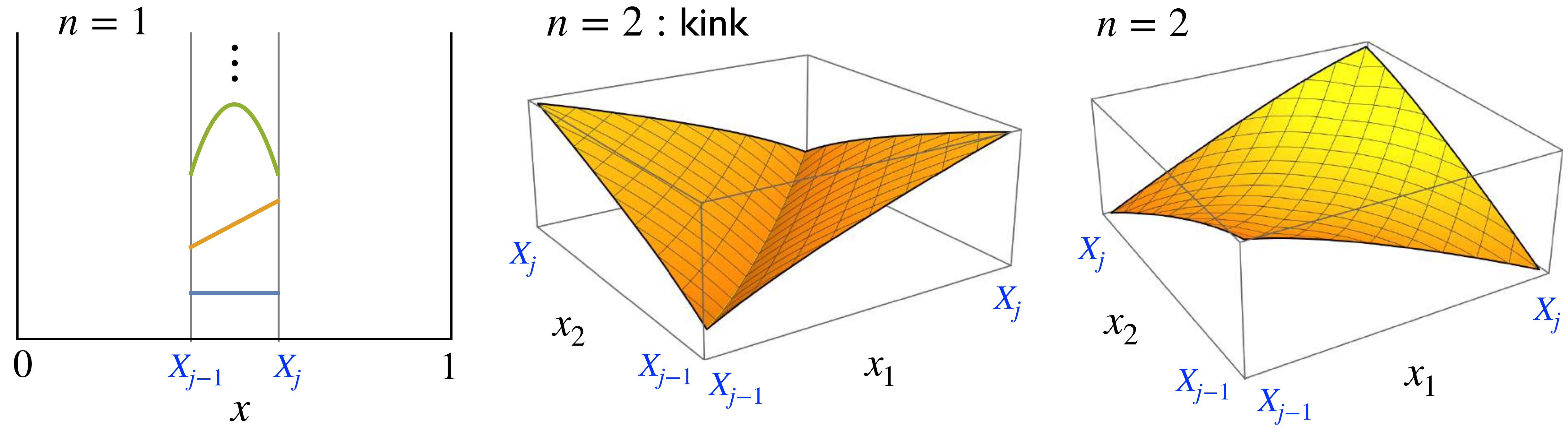
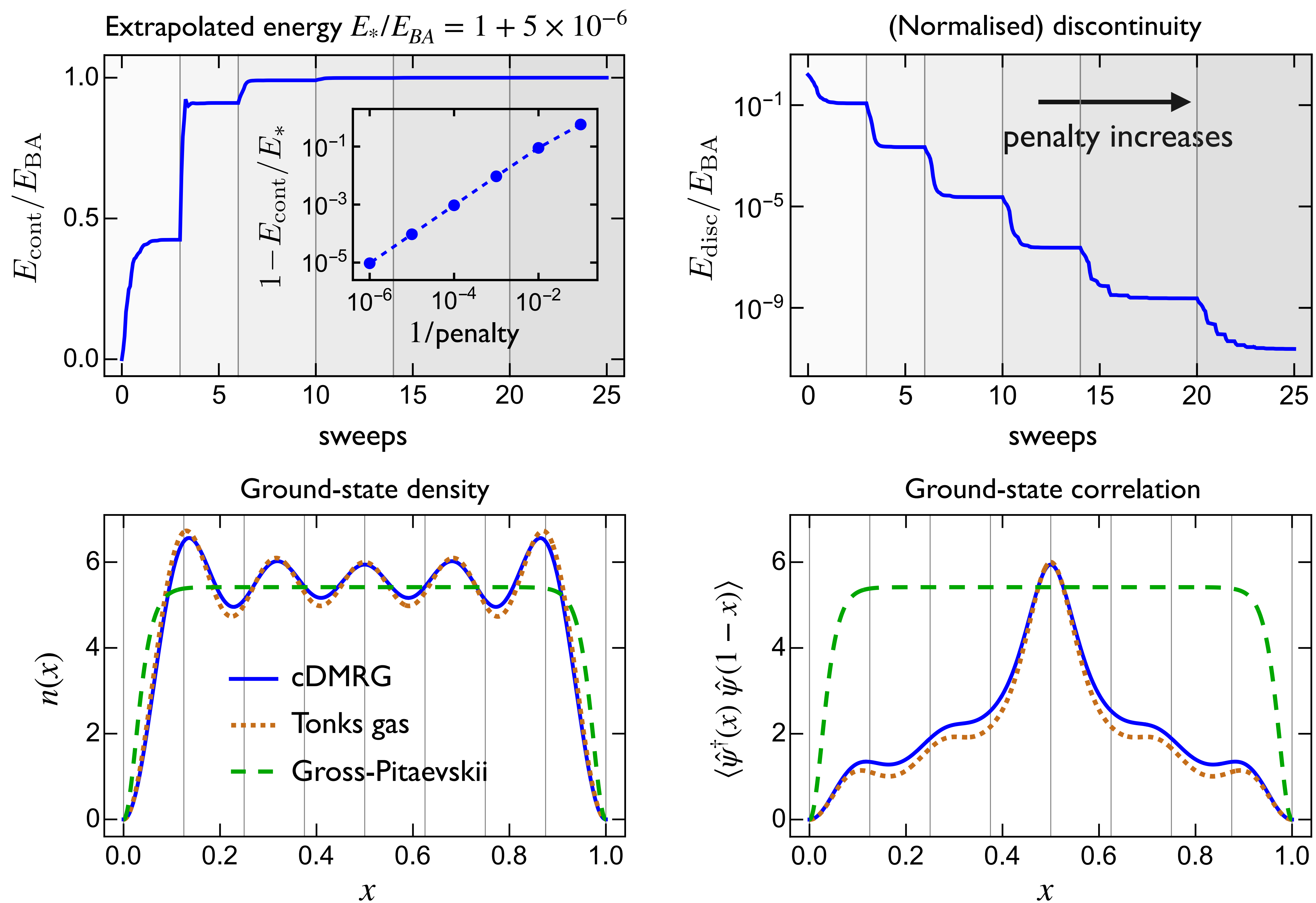
- Same form as discrete DMRG — increase discontinuity penalty Λ in steps
- Choose basis functions $|\phi_{n,k}^{(j)}\rangle$ to encode local (n-body) physics

Not just $|0\rangle_j, |1\rangle_j, |2\rangle_j, \ldots$



Case study

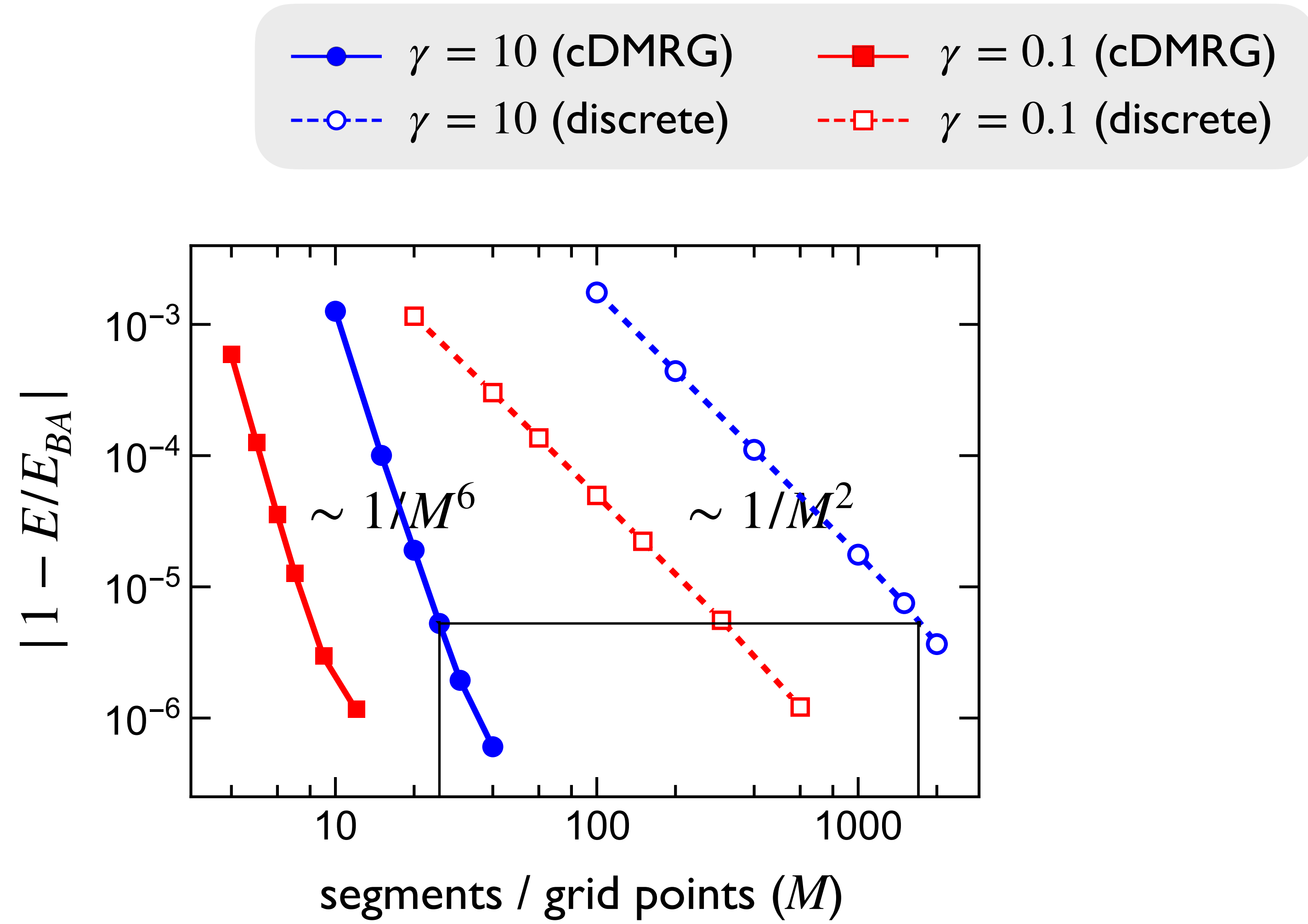
5 particles, 8 segments, strong interactions $\gamma \equiv g/N = 50$



Improvement over discretisation

Fast tuneable convergence relative to discretisation $[\partial_x \hat{\psi} \to (\hat{\psi}_{i+1} - \hat{\psi}_i)/\delta]$

$N = 10$, cubic basis



- Piecewise-polynomial basis with max degree $d_{max} \Longrightarrow$ Error $\propto 1/M^{2d_{max}}$

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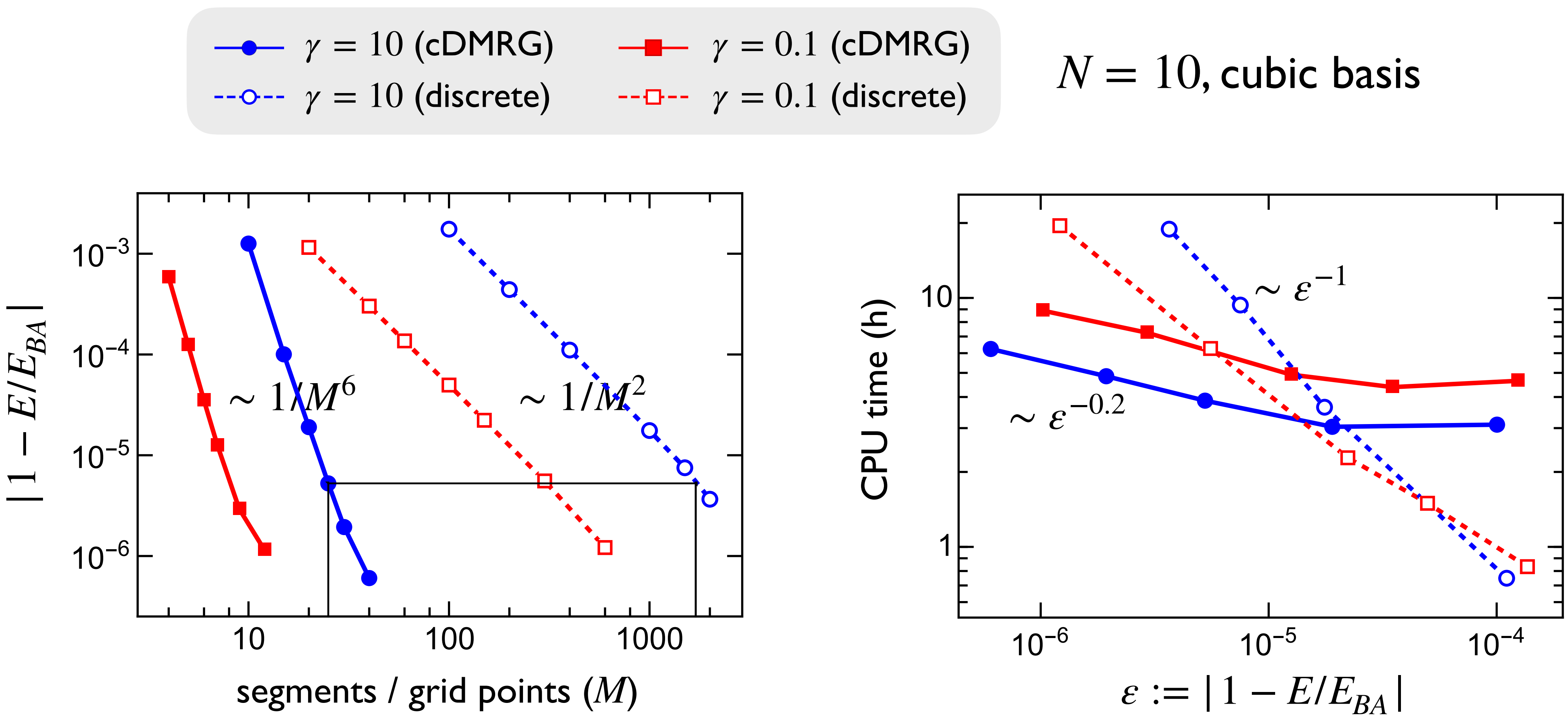
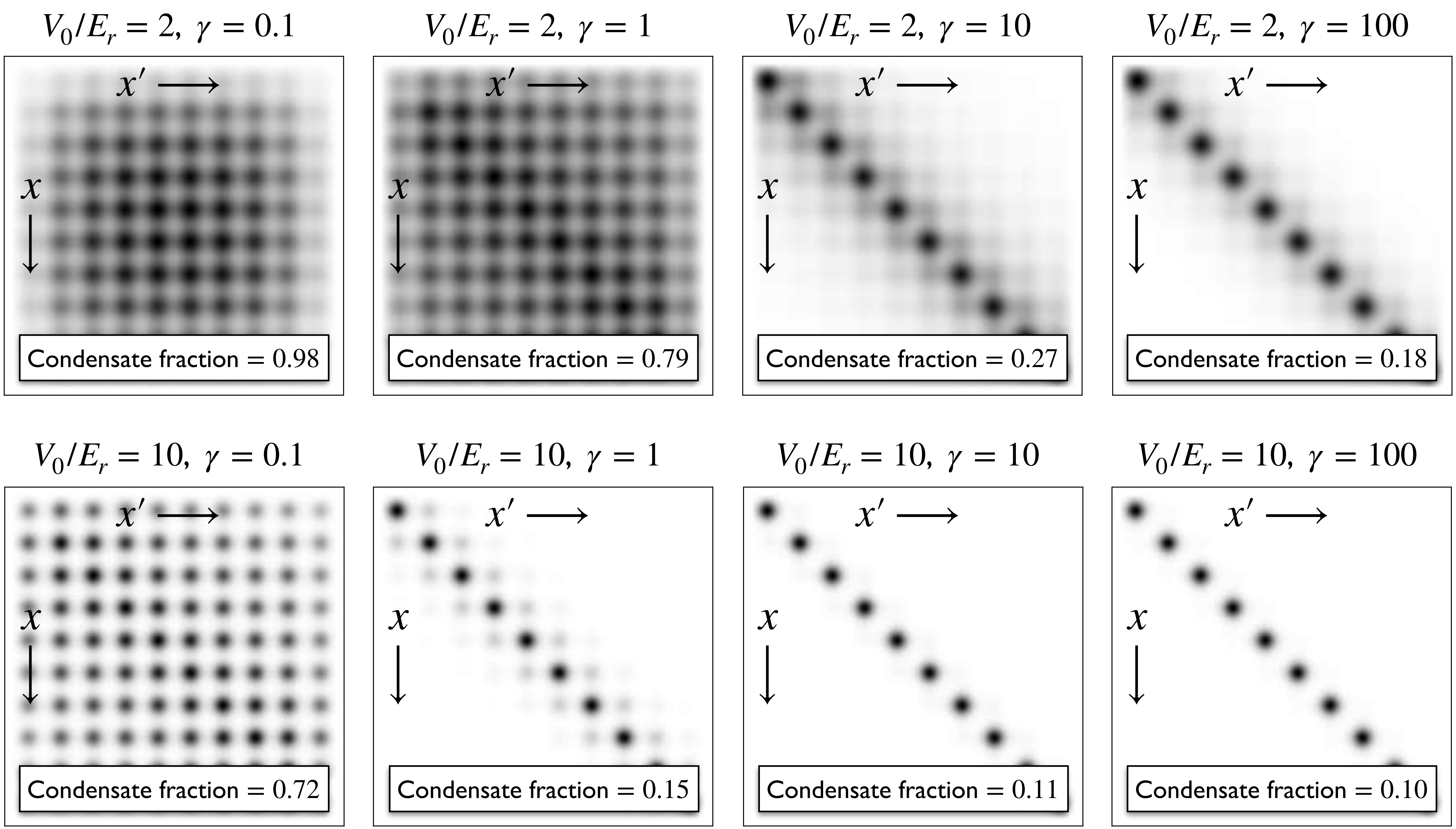


$N = 10$, cubic basis

- Piecewise-polynomial basis with max degree $d_{max} \Longrightarrow$ Error $\propto 1/M^{2d_{max}}$
- More efficient for small errors and stronger interactions

Inhomogeneous: Superfluid-Mott

Lattice potential: 10 particles in 10 wells [20 segments, quartic basis]

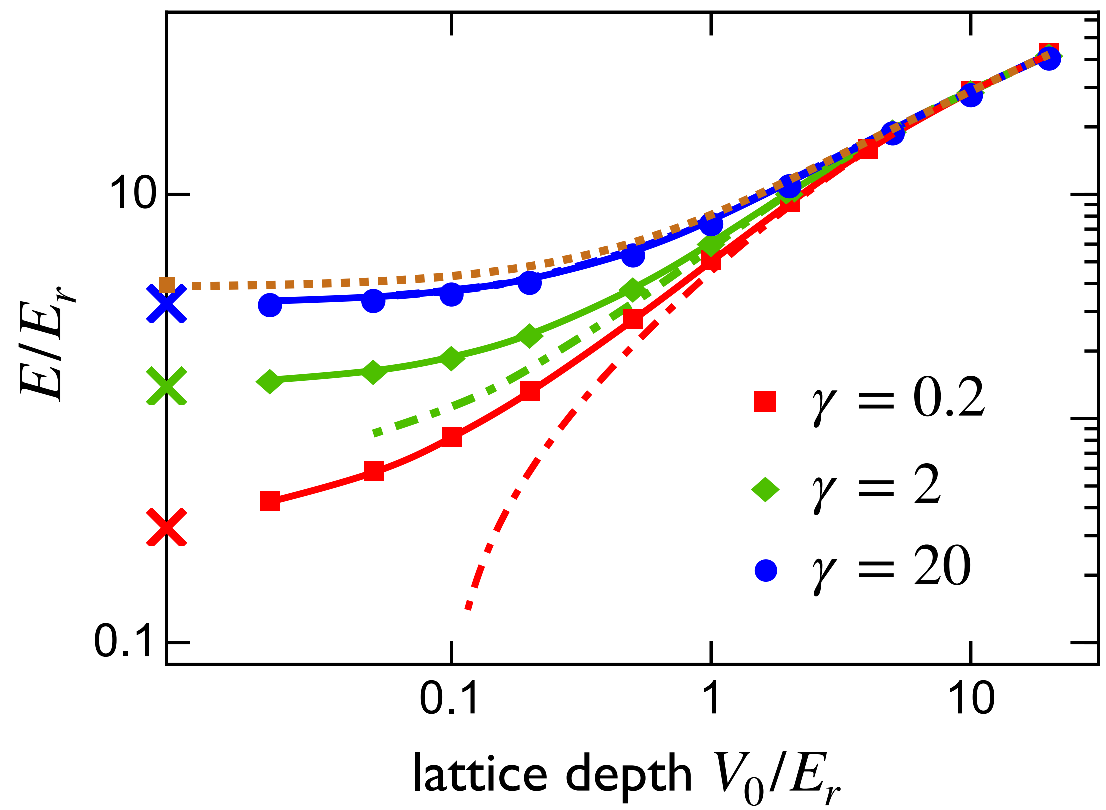


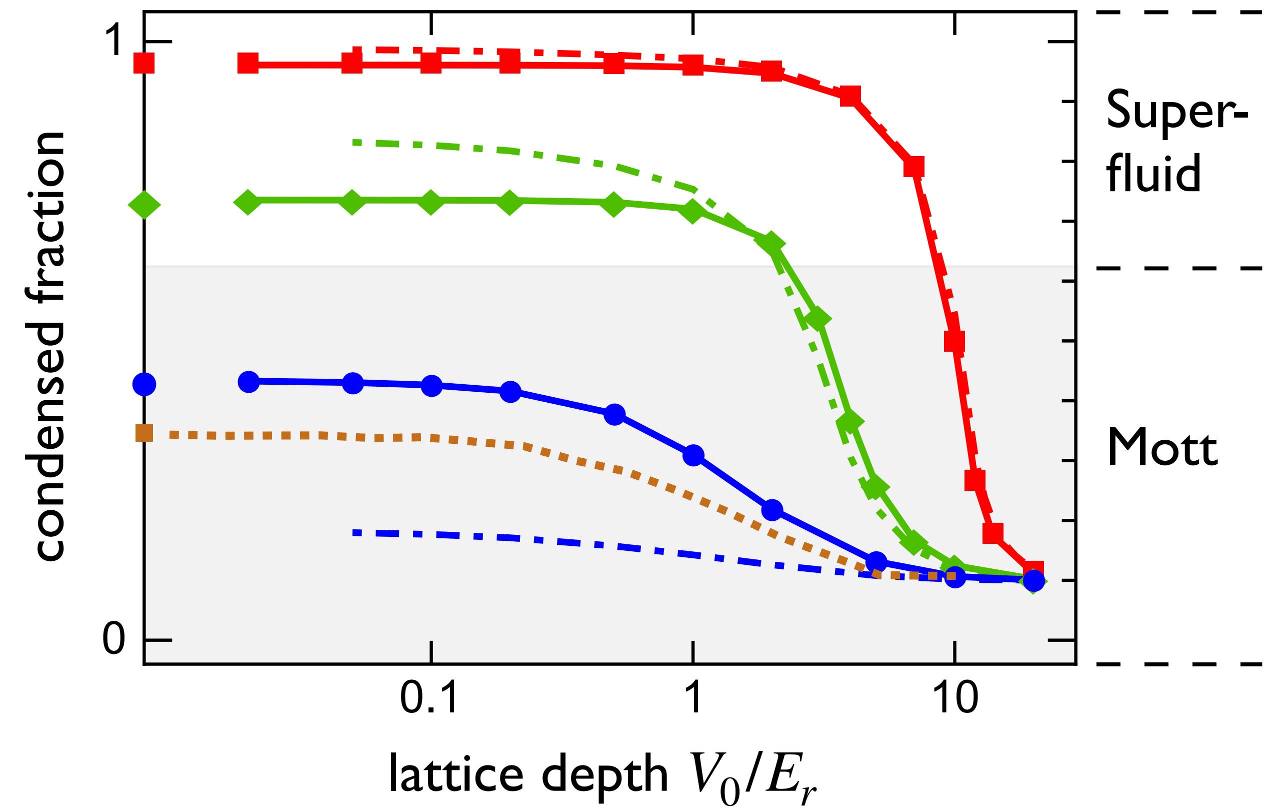
Single-particle density matrix $\langle \hat{\psi}^\dagger(x)\hat{\psi}(x')\rangle$ [V_0/E_r : lattice depth]

Inhomogeneous: Superfluid-Mott

Lattice potential: 10 particles in 10 wells [20 segments, quartic basis]

Solid → cDMRG, × → Bethe Ansatz, Dotted → Tonks, Dash-dotted → tight binding





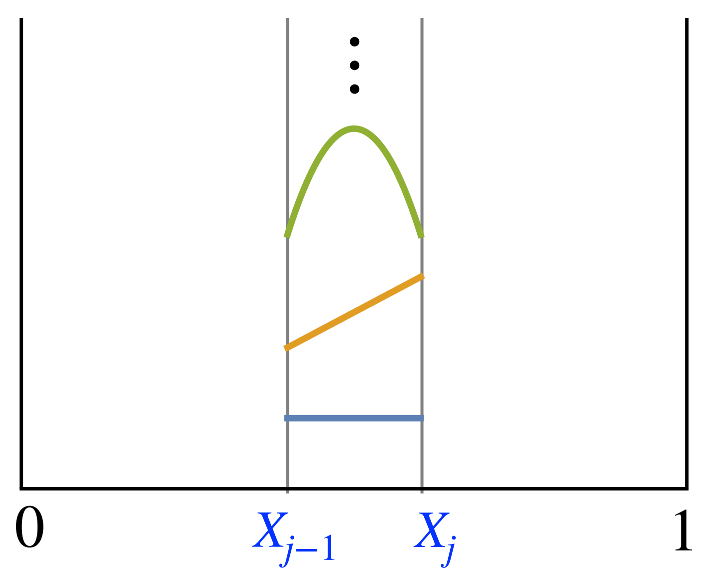
- Matches limits: Bethe Ansatz ($V_0 \to 0$), Tonks ($\gamma \to \infty$), tight binding ($V_0 \to \infty$)
- Evades convergence issues in discretisation on a fine grid

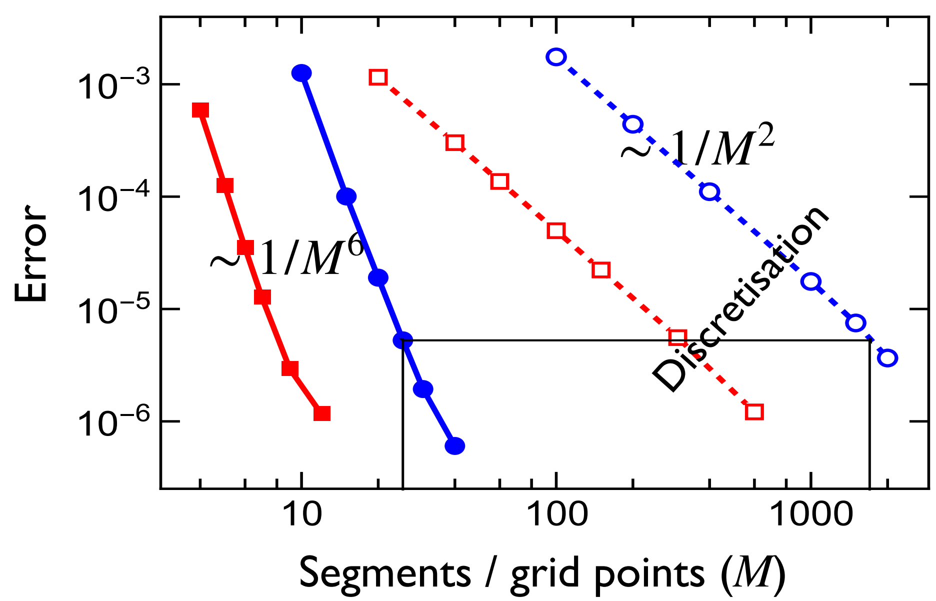
Dolfi *et al.* PRL 109, 020604

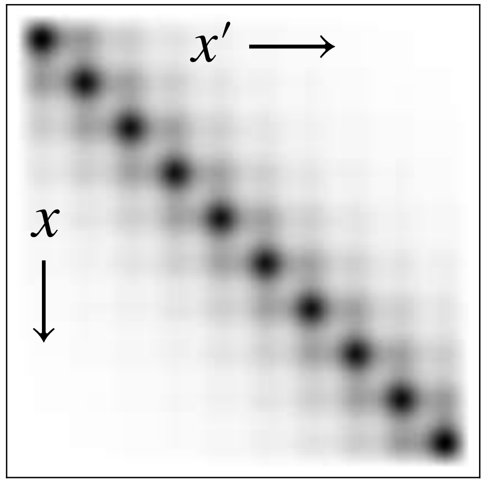
Summary & outlook

SD, A. Buyskikh, A. Daley, & E. Mueller,
arXiv:2108.05366

- Versatile, practical technique to apply DMRG to continuous systems
- Spatial partitioning + existing DMRG routines
  Code: github.com/Shovan-Physics/cDMRG (ITensor + Mathematica)
- Fast convergence w/ small error — controlled by choice of basis







Outlook:

- Apply to topical problems — suggestions welcome
- Extension: fermions, long-range int., time-dependence, dissipation