



Density-Matrix Renormalisation Group for Continuous Systems

Shovan Dutta — University of Cambridge

SD, Anton Buyskikh, Andrew Daley (Strathclyde), Erich Mueller (Cornell)
[arXiv:2108.05366](https://arxiv.org/abs/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

$$\Psi_{\sigma_1, \sigma_2, \dots, \sigma_M} \equiv \begin{array}{ccccccc} \boxed{T_1} & \text{---} & \boxed{T_2} & \text{---} & \boxed{T_3} & \text{---} & \dots & \text{---} & \boxed{T_M} \\ & & b_1 & & b_2 & & b_3 & & b_{M-1} \\ & & | & & | & & | & & | \\ & & \sigma_1 & & \sigma_2 & & \sigma_3 & & \sigma_M \end{array}$$

— Bond dimension controls max entanglement

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Extension to continuum remains a key challenge

- Discretisation on a grid — poor convergence + can get stuck

Dolfi et al. PRL 109, 020604

- Field-theory (cMPS) — impractical for nonuniform — recent progress

Tuybens et al. arXiv:2006.01801

- Open problems: shallow lattices, prethermalisation, false vacuum decay, FFLO physics, long-range interactions, ...

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Extension to continuum remains a

Our approach

- Overcomes these obstacles
- Uses existing DMRG routines
- Widely applicable

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Main takeaways

Idea

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

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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

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

$$\implies \hat{H} = \sum_j \hat{K}_j + \hat{U}_j + \Lambda [\hat{\psi}(X_j^-) - \hat{\psi}(X_j^+)]^\dagger [\hat{\psi}(X_j^-) - \hat{\psi}(X_j^+)] \quad (\Lambda \rightarrow \infty)$$

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

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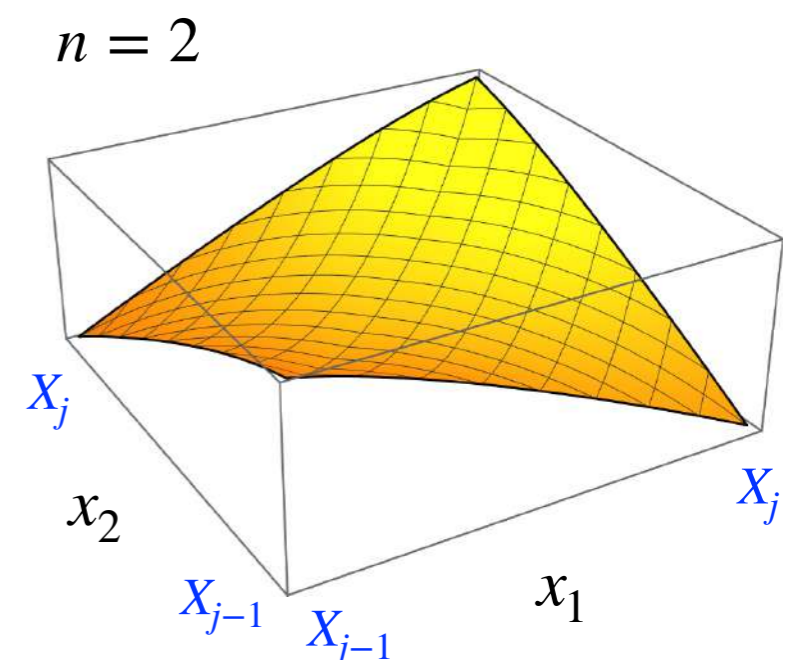
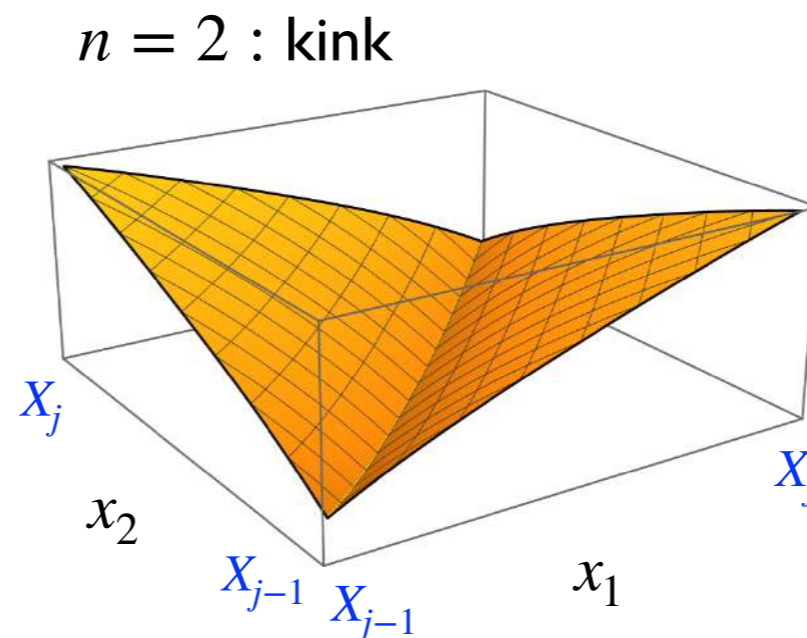
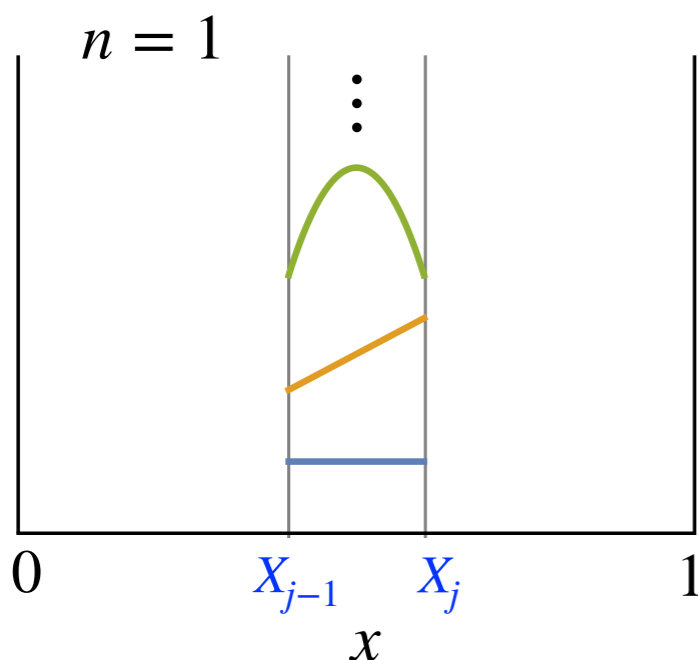
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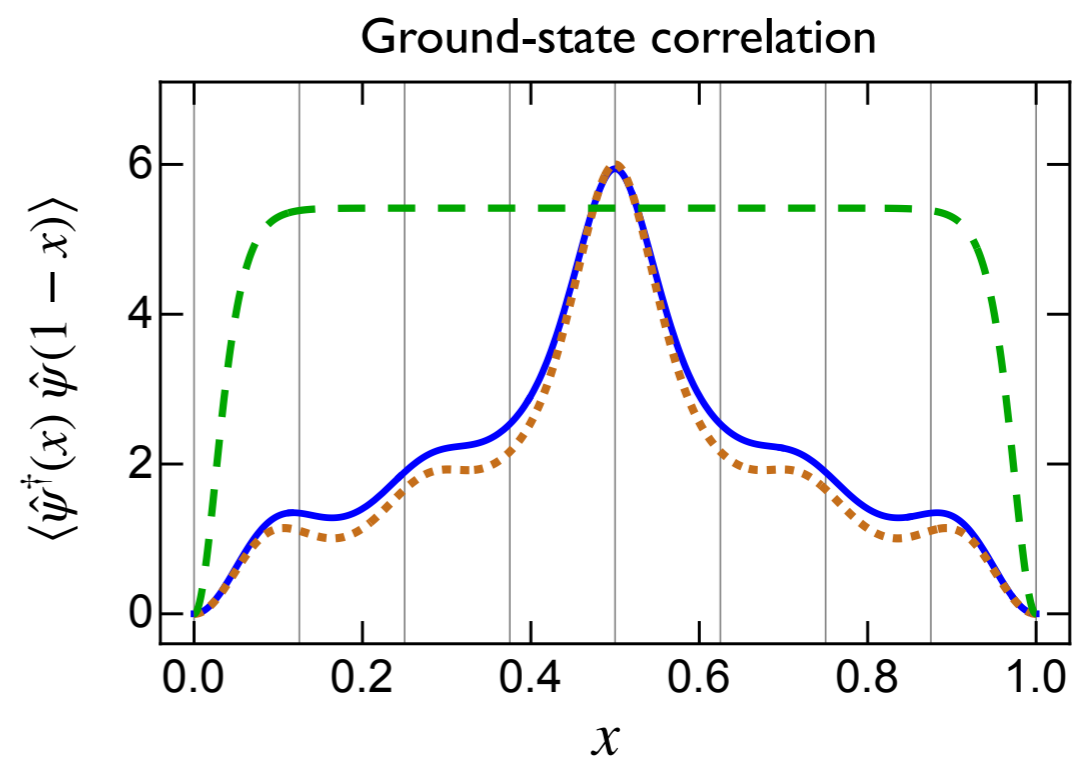
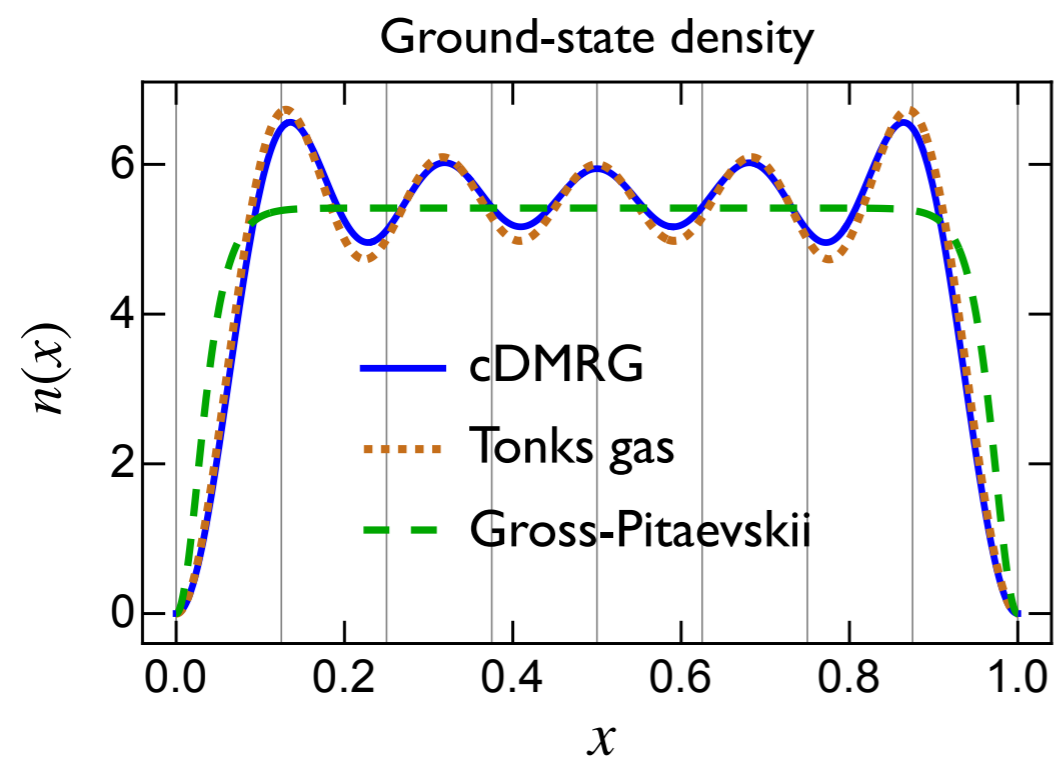
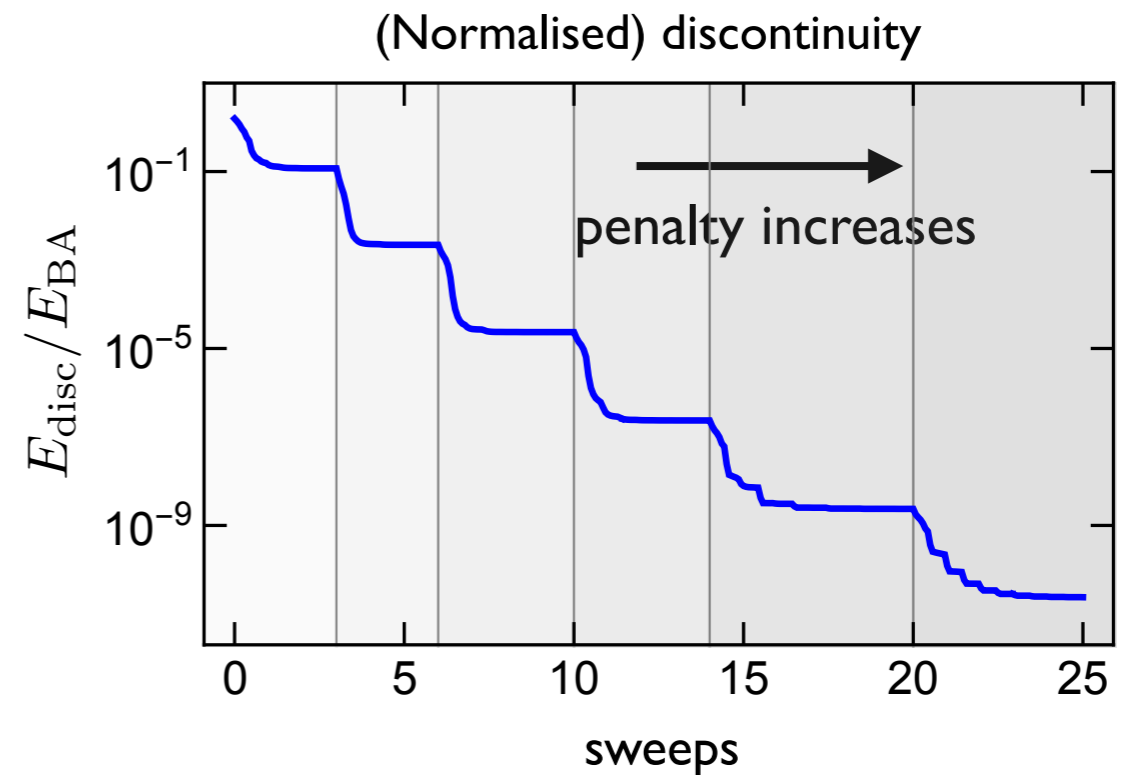
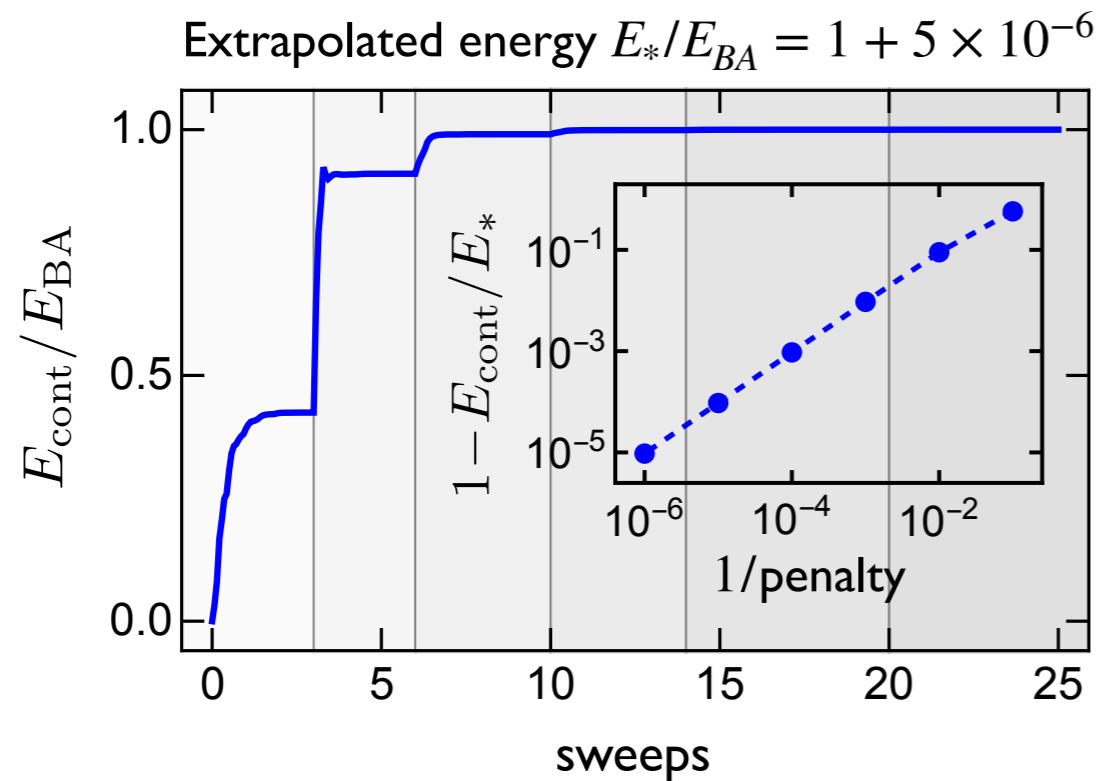
- Same form as discrete DMRG — increase discontinuity penalty Λ in steps

- Choose basis functions $|\phi_{n,k}^{(j)}\rangle$ to encode local (n -body) physics Not just $|0\rangle_j, |1\rangle_j, |2\rangle_j, \dots$



Case study

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

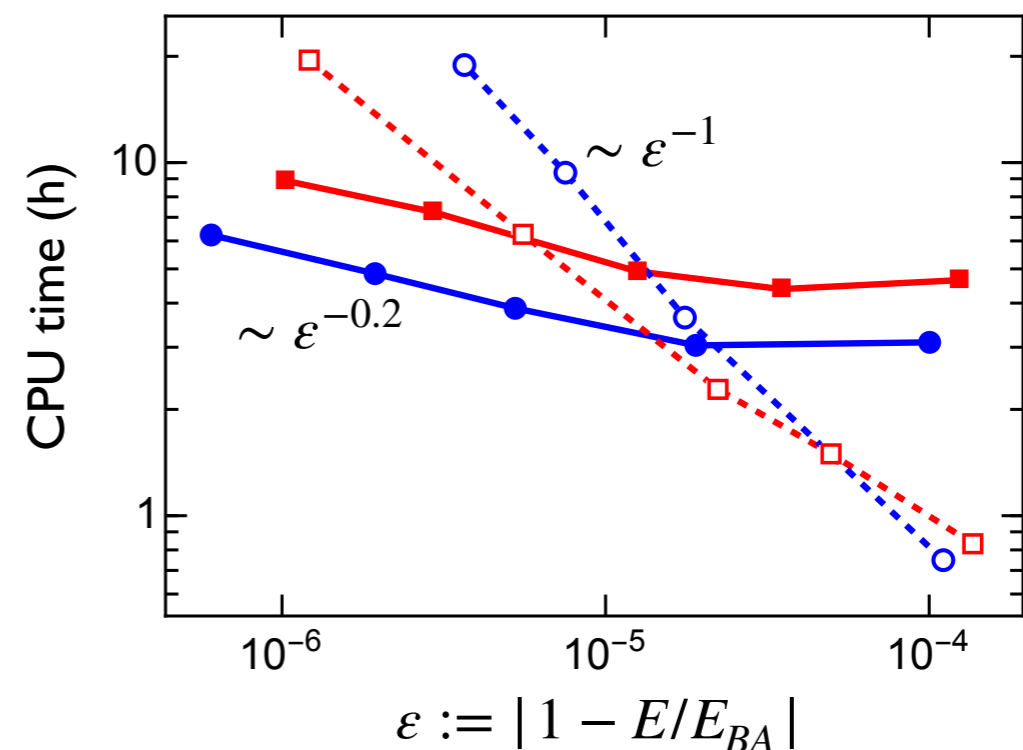
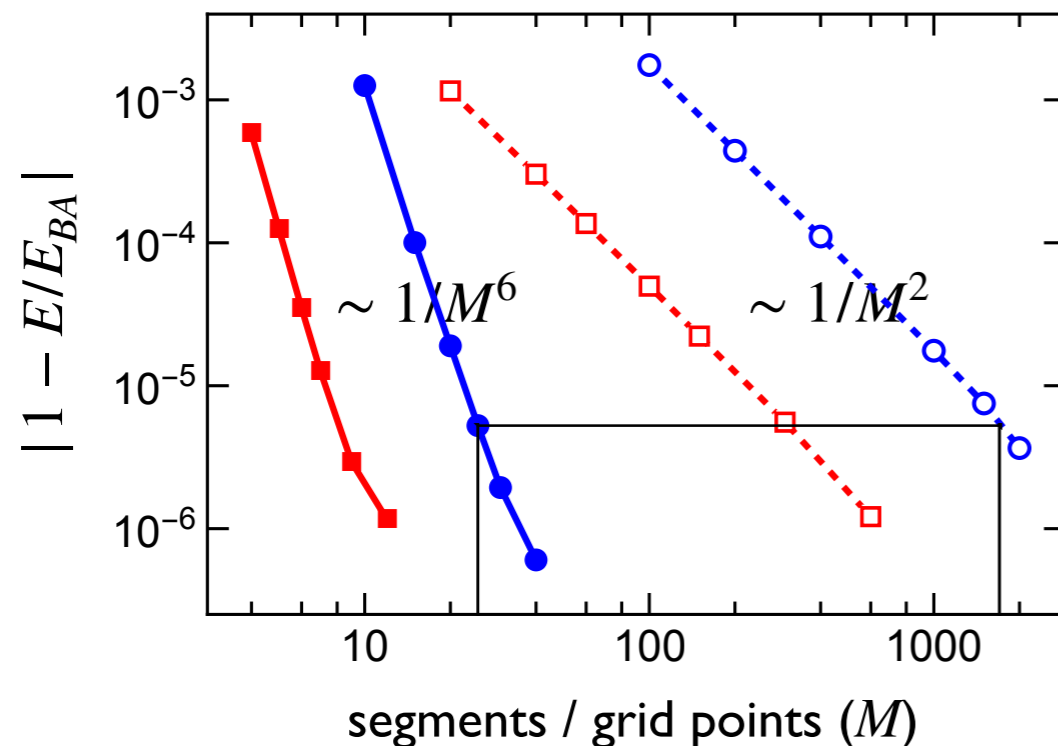


Improvement over discretisation

Faster convergence than discretisation $[\partial_x \hat{\psi} \rightarrow (\hat{\psi}_{i+1} - \hat{\psi}_i)/\delta]$

● $\gamma = 10$ (cDMRG) ■ $\gamma = 0.1$ (cDMRG)
○ $\gamma = 10$ (discrete) □ $\gamma = 0.1$ (discrete)

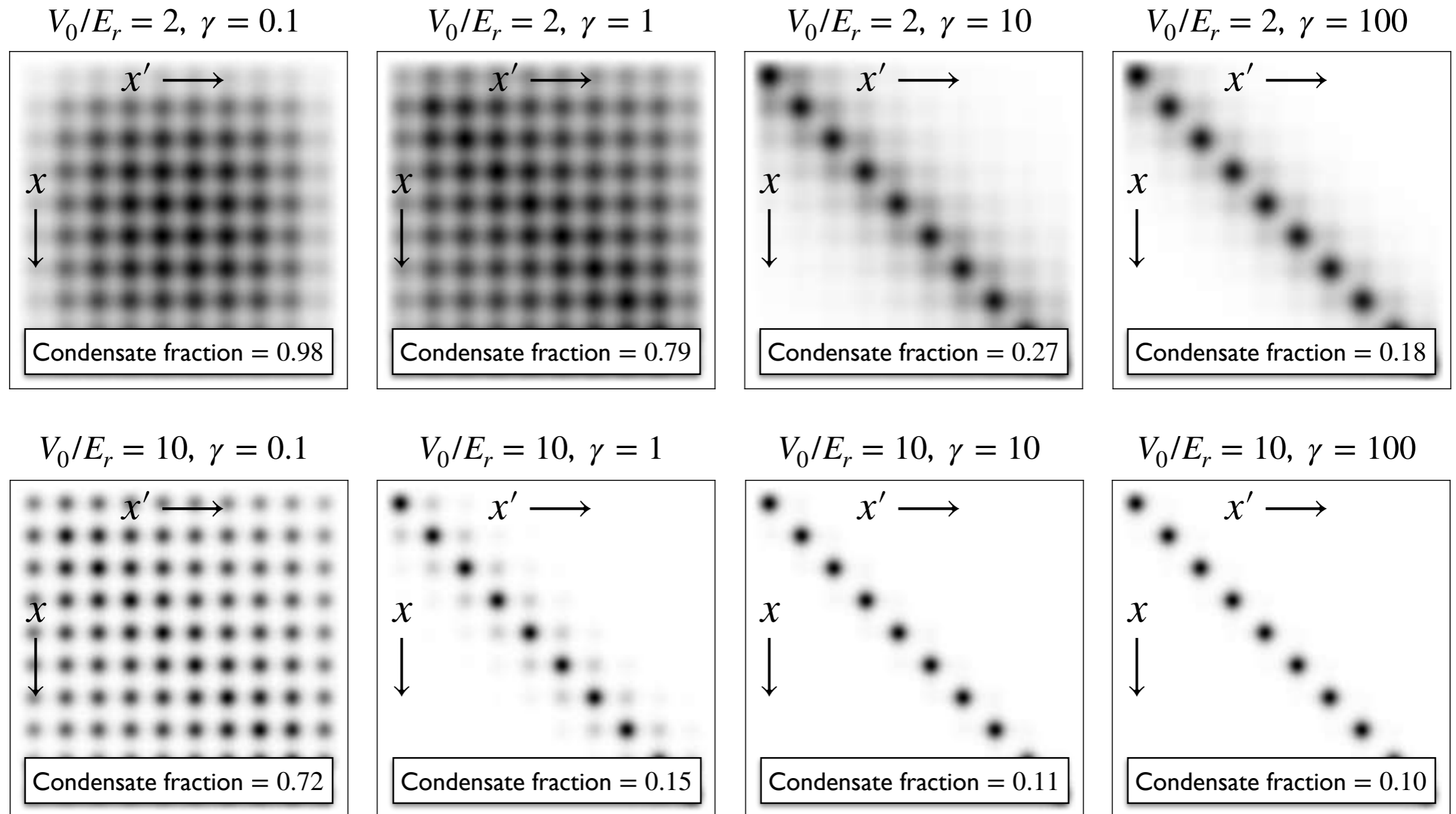
$N = 10$, cubic basis



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

Inhomogeneous: Superfluid-Mott

Lattice potential: 10 particles in 10 wells [20 segments]



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

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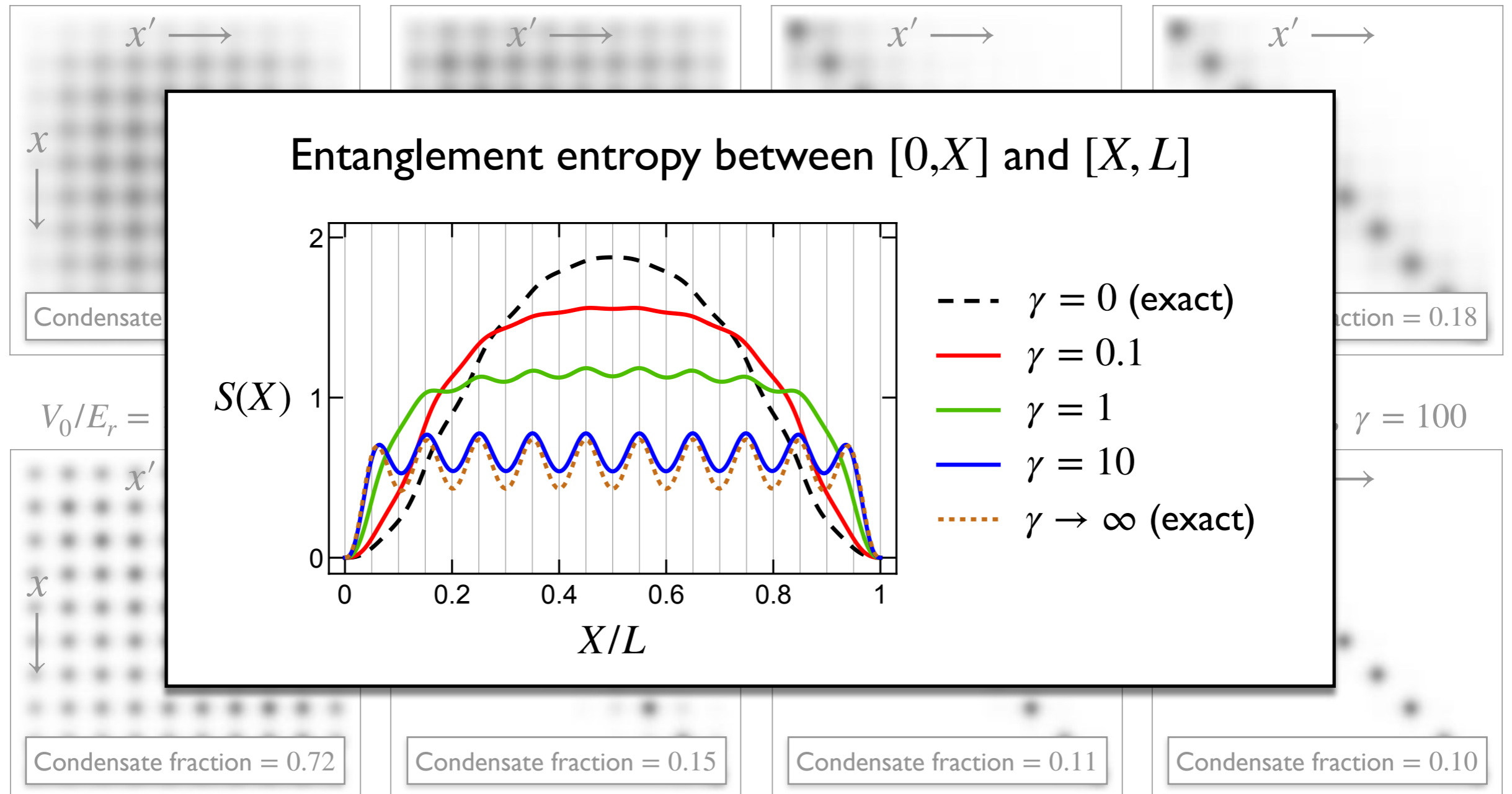
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$V_0/E_r = 2, \gamma = 0.1$

$V_0/E_r = 2, \gamma = 1$

$V_0/E_r = 2, \gamma = 10$

$V_0/E_r = 2, \gamma = 100$

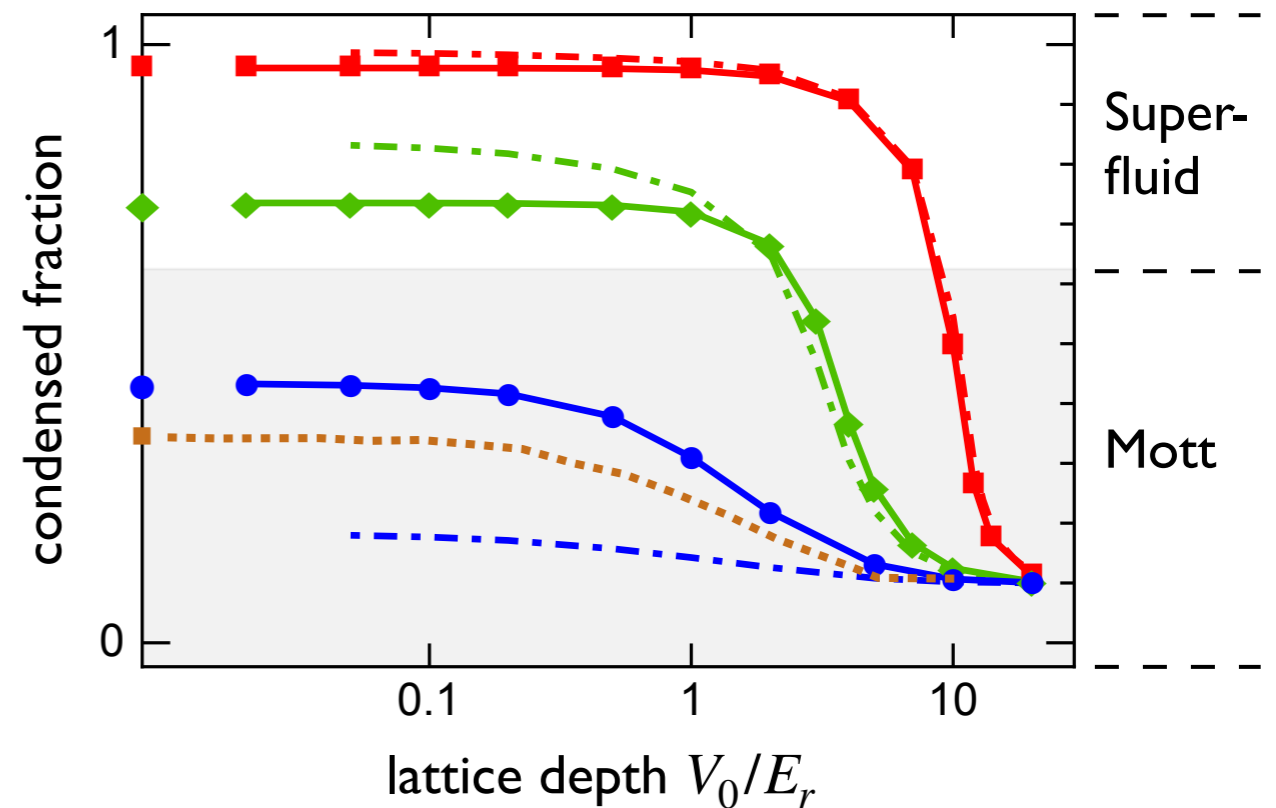
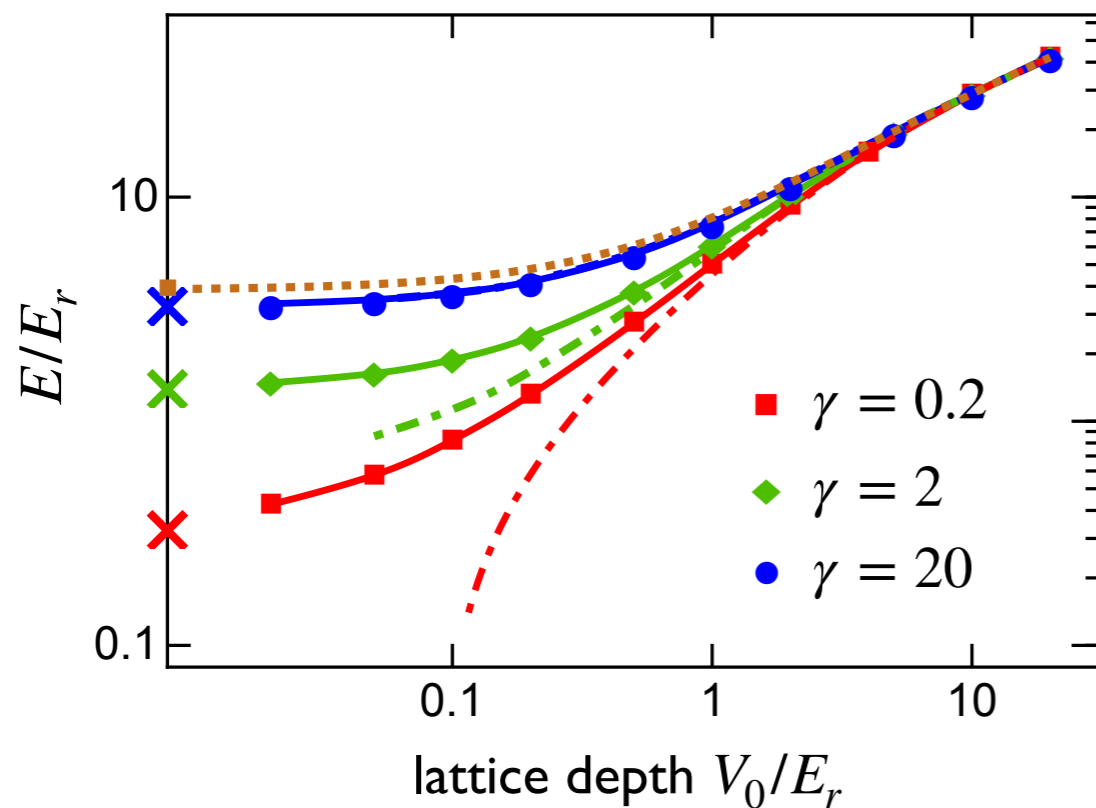


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Inhomogeneous: Superfluid-Mott

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Solid \rightarrow cDMRG, \times \rightarrow Bethe Ansatz, Dotted \rightarrow Tonks, Dash-dotted \rightarrow tight binding



- Matches limits: Bethe Ansatz ($V_0 \rightarrow 0$), Tonks ($\gamma \rightarrow \infty$), tight binding ($V_0 \rightarrow \infty$)
- Evades convergence issues in discretisation on a fine grid Dolfi *et al.* PRL 109, 020604

Extension to other systems

- Multicomponent bosons

- partition each component $\hat{H} = \sum_j [\sum_{\sigma} \hat{K}_j + \Lambda \hat{Y}_{j,j+1}^{\sigma} + \sum_{\sigma,\sigma'} \hat{U}_j^{\sigma,\sigma'}]$

- pairwise interactions determine cusps in basis functions $\phi_{n^{\uparrow},n^{\downarrow},k}^{(j)}$

- Fermions

- basis functions vanish if two fermions of same spin coincide $x_i^{\sigma} = x_{i'}^{\sigma}$

- treated on an equal footing as bosons

- Long-range interactions

- nonlocal coupling $\hat{U}_j \rightarrow \hat{U}_{j,j'} \implies$ larger bond dimension for \hat{H}

- approximate power-law by a sum of exponentials

- Time evolution — TDVP

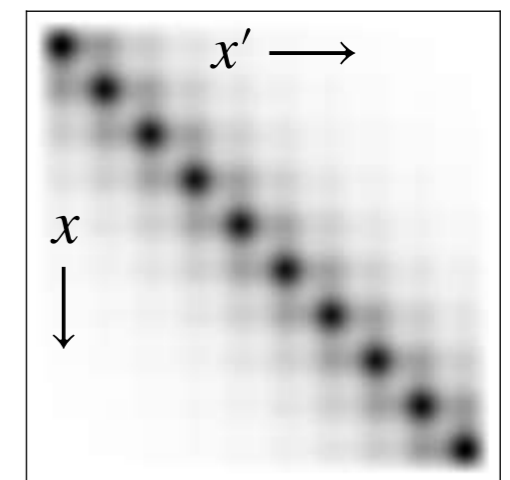
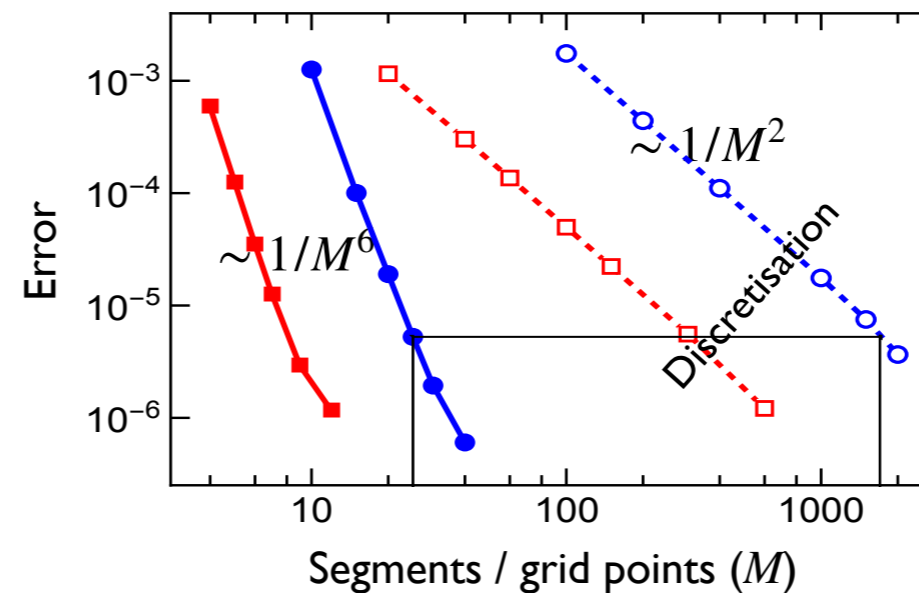
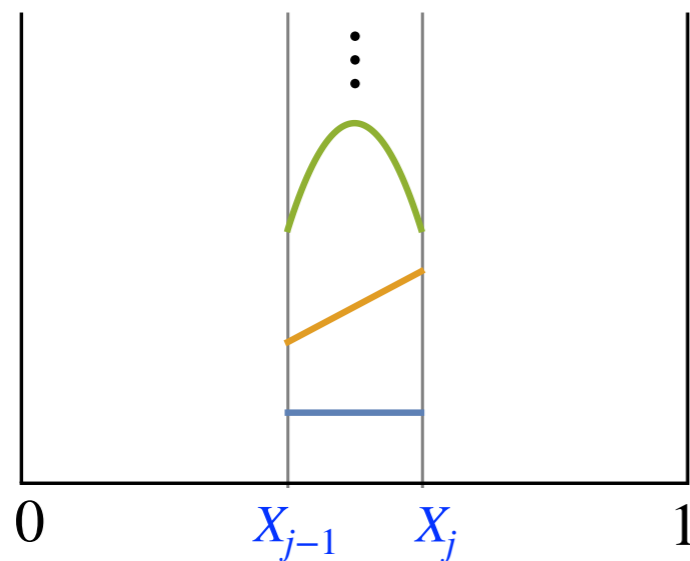
- Relativistic field theory

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Summary & outlook

SD, A. Buyskikh, A. Daley,
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- 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

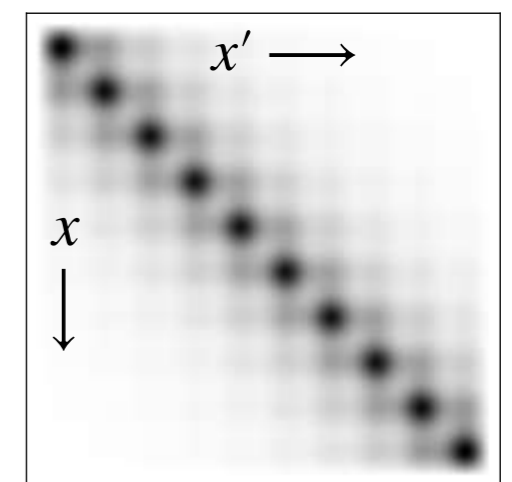
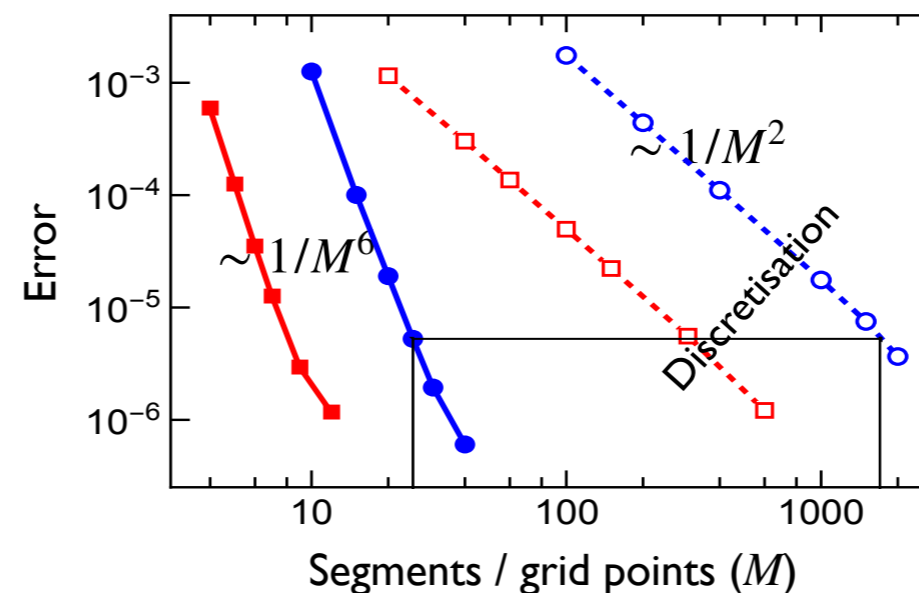
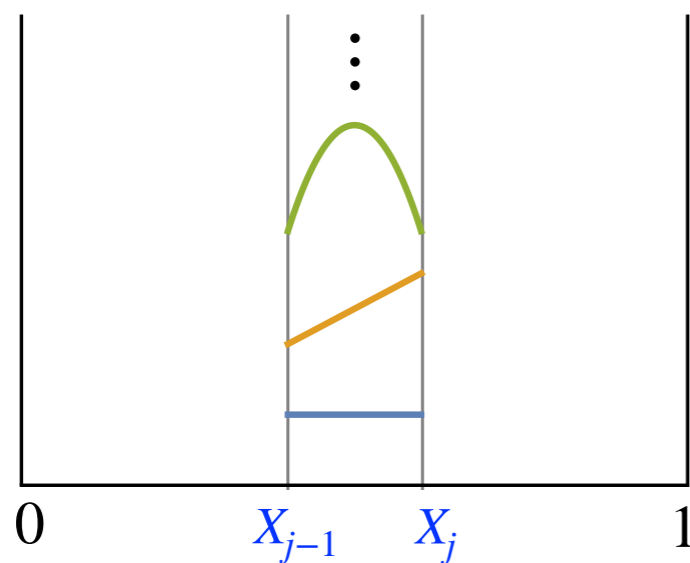


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Outlook:

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