Surrogatising quantum spin systems using reduced basis methods

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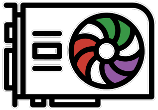
27th July 2023

Quantum effects are everywhere

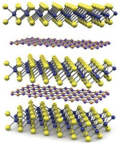
Solar cells

Batteries



Microchips

Quantum computers



Single-layer materials

- Solutions to 21st century challenges:
  - Limited by available materials
- Motivation for research in fundamental physics
  - Focus: Quantum effects
- Quantum effects are expensive to study
  - 50% usage fraction at key supercomputers

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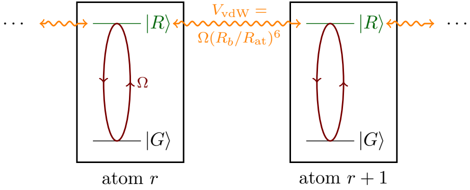
https://upload.wikimedia.org/wikipedia/commons/6/60/IBM_Q_system_(Fraunhofer_2).jpg;
https://www.edfenergy.com/electric-cars/batteries;
J. Evans *Beyond graphene* Chemistry World (2014).

Quantum spin models

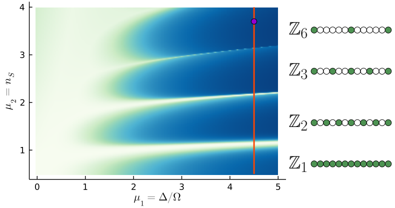
- Real model systems (e.g. regular arrangement of spin-$\frac{1}{2}$ particles)
  - Can be prepared and manipulated experimentally[1]
  - Analytical solutions (sometimes) available
  - Full Schrödinger treatment feasible (contrast to electronic structure)
- Strongly correlated systems: Rich physics
  - Topological order, ordered versus disordered phases[2]
  - Quantum spin liquids[3]
- Analogue quantum simulation:
  - The same equations have the same solutions (Feynman)
  - Spin models can capture dominating physics (e.g. low temperature regime)
  - But: Simpler than real materials

[1] A. Browaeys and T. Lahaye. Nature Physics **16**, 132 (2020).
[2] M. Rader and A. Läuchli. *Floating Phases in One-Dimensional Rydberg Ising Chains* arXiv:1908.02068v1
[3] G. Giudici, M. Lukin, H. Pichler. *Dynamical preparation of quantum spin liquids in Rydberg atom arrays* arXiv:2201.04034v1

Quantum phase diagrams



Rydberg atom chain in detuned laser



Phase diagram for 13 atoms

(green is Rydberg state)

- Rydberg chain Hamiltonian:

$$H(\boldsymbol{\mu}) = \frac{\Omega}{2} \sum_r \hat{\sigma}_r^x - \Delta \sum_r \hat{n}_r + \sum_{r<r'} \left(\frac{\Omega\ R_b}{R_{\mathrm{at}}(r'-r)} \right)^6 \hat{n}_r \hat{n}_{r'}$$

  - Laser: Rabi frequency Ω, detuning Δ
  - System: Blockade radius R_b, atom-atom distance R_{at}

- Parameter studies:
  - Simulate order parameters (e.g. spin patterns, magnetisation, ...)
  - Requires Solution of eigenproblems:

$$H(\boldsymbol{\mu}) \, |\Psi(\boldsymbol{\mu})\rangle = E(\boldsymbol{\mu}) \, |\Psi(\boldsymbol{\mu})\rangle \,, \quad |\Psi(\boldsymbol{\mu})\rangle \in \mathcal{H}$$

Stationary many-body problem

$$H(\boldsymbol{\mu})\,|\Psi(\boldsymbol{\mu})\rangle = E(\boldsymbol{\mu})\,|\Psi(\boldsymbol{\mu})\rangle\,, \quad |\Psi(\boldsymbol{\mu})\rangle \in \mathcal{H}$$

- Many-body setting: $\dim(\mathcal{H}) = \mathcal{O}(\exp(L))$
- Expensive: Need solution for many parameter points $\boldsymbol{\mu} \in \mathbb{P}$

  Computing a $\Psi(\boldsymbol{\mu})$: $\mathcal{O}(\text{hours})$
- Key idea: Exploit linear dependency

$$\langle \Psi(\boldsymbol{\mu}) | \Psi(\boldsymbol{\xi}) \rangle \neq 0 \qquad \text{for} \quad \boldsymbol{\mu}, \boldsymbol{\xi} \in \mathbb{P}$$

⇒ Reduced basis (RB) methods[1]

- This talk discusses:
  - Combination of RB and matrix product states (MPSs)[2]

[1] J. S. Hesthaven, G. Rozza, and B. Stamm, *Certified Reduced Basis Methods for Parametrized Partial Differential Equations* (2016).

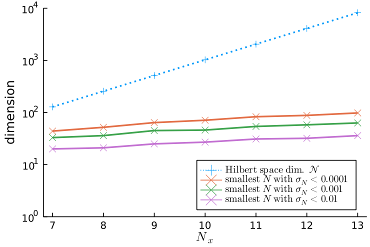
[2] P. Brehmer, M. F. Herbst, M. Rizzi, B. Stamm. Phys. Rev. E (2023).

Potential for reduced basis methods

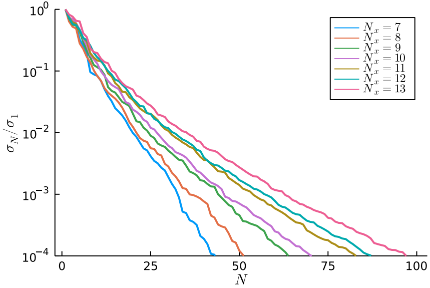
- $|\Psi(\boldsymbol{\mu})\rangle$ within a phase are similar across $\boldsymbol{\mu}$ variation

$\Rightarrow$ RB methods:
  - Approximate $|\Psi\rangle$ for any $\boldsymbol{\mu}$ using N carefully selected $|\Psi(\boldsymbol{\mu}_i)\rangle$
  - Singular value decay: Lower effective dimension feasible

- Successful in computational mathematics / engineering (parametrised PDEs)
- Nuclear physics: Eigenvector continuation[1]



Rydberg chain length N_x



[1] D. Frame et al., *PRL* **121**, 032501 (2018).

Reduced basis method: Overview

- **Offline stage** (Training):
  - Generate *reduced basis space*:

$$\mathbb{V}_n = \mathrm{span}\{\overbrace{|\Psi(\boldsymbol{\mu}_1)\rangle}^{\text{“snapshot”}}, \dots, |\Psi(\boldsymbol{\mu}_n)\rangle\} \subset \mathcal{H}$$

  - Based on training grid $\Xi_{\mathsf{train}} \subset \mathbb{P}$
  - Iterative growth of RB: Add one $|\Psi(\boldsymbol{\mu}_i)\rangle$ at a time
  - Ground truth computation of $|\Psi(\boldsymbol{\mu}_i)\rangle$ at well-selected μ_i

  ⇒ Greedy strategy: Next $\boldsymbol{\mu}_i$ s.t. error of RB method reduces most

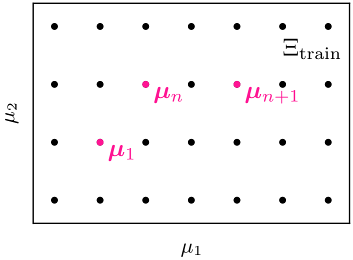
⇒ Yields RB approximation (surrogate ground state)

$$|\Phi_{\mathrm{rb}}(\boldsymbol{\mu})\rangle = \sum_{j=1}^{n} [\varphi_{\mathrm{rb}}(\boldsymbol{\mu})]_j \, |\Psi(\boldsymbol{\mu}_j)\rangle \in \mathbb{V}_n$$

- **Online stage** (employ RB as a surrogate):
  - Evaluate observables independent of $\dim \mathcal{H}$ on any $\boldsymbol{\mu} \in \mathbb{P}$

⇒ $\mathcal{O}(10)$ ground state computations for entire phase diagram (instead of 100–1000)

Offline stage: Greedy basis assembly



- How are the parameter points $\{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_n\}$ selected?
- Given $\mathbb{V}_n = \text{span}\{|\Psi(\boldsymbol{\mu}_1)\rangle, \dots, |\Psi(\boldsymbol{\mu}_n)\rangle\}$ use greedy condition:

$$\boldsymbol{\mu}_{n+1} = \underset{\mu \in \Xi_{\text{train}}}{\arg\max}\, \text{Res}_n(\boldsymbol{\mu})$$

- Eigenproblem residual (error estimate)

$$\text{Res}_n(\boldsymbol{\mu}) = \| H(\boldsymbol{\mu}) |\Phi_{\text{rb}}(\boldsymbol{\mu})\rangle - E_{\text{rb}}(\boldsymbol{\mu}) |\Phi_{\text{rb}}(\boldsymbol{\mu})\rangle \|$$

  (for affine setting can be computed indep. of $\dim \mathcal{H}$)
- Run truth solve to obtain $|\Psi(\boldsymbol{\mu}_{n+1})\rangle$ (expensive step)

Offline stage: Surrogate ground states

- Given $\mathbb{V}_n$, how to determine $|\Phi_{\text{rb}}(\boldsymbol{\mu})\rangle = \sum_{j=1}^{n} [\varphi_{\text{rb}}(\boldsymbol{\mu})]_j \, |\Psi(\boldsymbol{\mu}_j)\rangle$?

1. Compute matrix elements and overlaps (updated iteratively)

$$h_{ij} = \langle \Psi(\boldsymbol{\mu}_i) | H | \Psi(\boldsymbol{\mu}_j) \rangle \,, \quad b_{ij} = \langle \Psi(\boldsymbol{\mu}_i) | \Psi(\boldsymbol{\mu}_j) \rangle$$

2. To get $\varphi_{\text{rb}}(\boldsymbol{\mu})$ use Rayleigh-Ritz ansatz

$$h(\boldsymbol{\mu}) \, \varphi_{\text{rb}}(\boldsymbol{\mu}) = E_{\text{rb}}(\boldsymbol{\mu}) \, b \, \varphi_{\text{rb}}(\boldsymbol{\mu}),$$

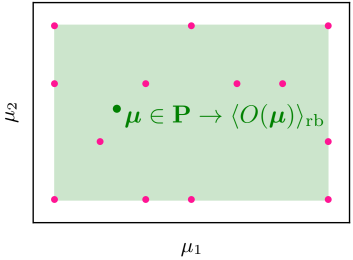
   i.e. we only solve low-dimensional $(\dim \mathbb{V}_n = n)$ eigenproblems

3. Repeat for all $\boldsymbol{\mu} \in \Xi_{\text{train}}$ for each greedy iteration

- Remarks:
  - Conditioning essential, i.e. need $b \simeq I$

  $\Rightarrow$ Explicitly orthogonalise basis: Change $\varphi_{\text{rb}}(\boldsymbol{\mu}) \to V \varphi_{\text{rb}}(\boldsymbol{\mu})$

Observable evaluation in RB framework



- After RB assembly $\mathbb{V}_n$ is known
- Projection of (affinely decomposable) observable into $\mathbb{V}_n$:

$$O(\boldsymbol{\mu}) = \sum_{r=1}^{R} \alpha_r(\boldsymbol{\mu})\, O_r \quad \Rightarrow \quad \langle O(\boldsymbol{\mu})\rangle_{\text{rb}} = \sum_{r=1}^{R} \alpha_r(\boldsymbol{\mu})\, \varphi_{\text{rb}}(\boldsymbol{\mu})^* o_r\, \varphi_{\text{rb}}(\boldsymbol{\mu})$$

- $[o_r]_{ij} = \langle \Psi(\boldsymbol{\mu}_i) | O_r | \Psi(\boldsymbol{\mu}_j) \rangle$ is independent of μ

Compatibility of truth solvers

- Requirements on algorithms for obtaining $|\Psi(\boldsymbol{\mu})\rangle$ from $H(\boldsymbol{\mu})$:

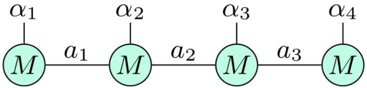
  1. Computation of state overlaps $\langle\Psi(\boldsymbol{\mu}_i)|\Psi(\boldsymbol{\mu}_j)\rangle$
  2. Computation of matrix elements $\langle\Psi(\boldsymbol{\mu}_i)|A|\Psi(\boldsymbol{\mu}_j)\rangle$
  3. Controllable accuracy on overlaps and matrix elements
     (This accuracy limits effectiveness of RB)

- In particular:
  - "Exact" diagonalisation (ED)
  - Matrix product states (MPS) from density matrix renormalisation group (DMRG)

Matrix product states

- MPSs parametrize many-body states as products of matrices

$$|\psi\rangle = \sum_{\alpha_1 \cdots \alpha_L} \sum_{a_1 \cdots a_L} M_{a_1}^{\alpha_1} M_{a_1 a_2}^{\alpha_2} \cdots M_{a_L}^{\alpha_L} |\alpha_1 \cdots \alpha_L\rangle =$$



- Control high-dimensional Hilbert space by low-rank approximating $M_{a_i a_{i+1}}^{\alpha_i}$
  - Ansatz is effective for one-dimensional systems

    (MPSs parametrize the underlying many-body entanglement structure)

  ⇒ Enables study of larger systems and more realistic scenarios

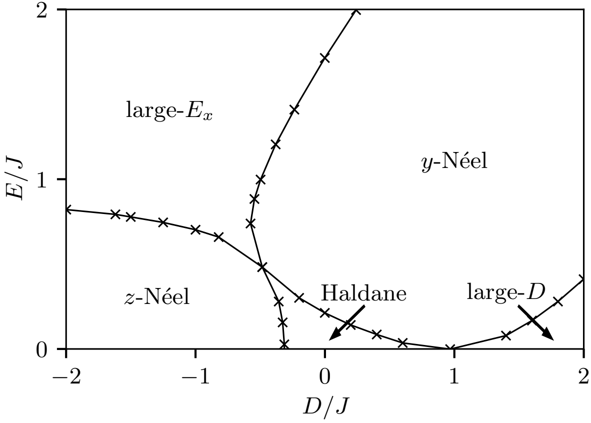
- DMRG algorithm: iteratively optimize $M_{a_i a_{i+1}}^{\alpha_i}$ towards ground state

$$|\Psi_0\rangle = \underset{|\psi\rangle \in \{\mathrm{MPS}\}}{\arg\min} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

Haldane spin-1 chain with single-ion anisotropies

$$H = J\sum_{i=1}^{L-1} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + D\sum_{i=1}^{L}(S_i^z)^2 + E\sum_{i=1}^{L}\left[(S_i^x)^2 - (S_i^y)^2\right]$$

- Phase diagram[1] $\boldsymbol{\mu} = (D/J,\, E/J)$?
- Greedy parameter selection?
  $n \sim 100$ snapshots at $L = 80$
- Residual $\mathrm{Res}(\boldsymbol{\mu})$?



[1] Y.-C. Tzeng et al., *PRB* **96**, 060404, (2017).

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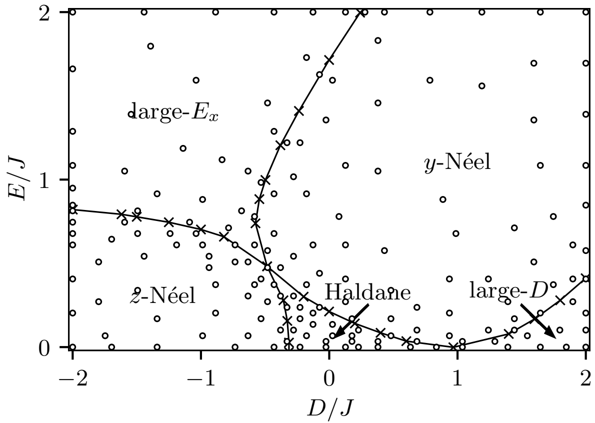

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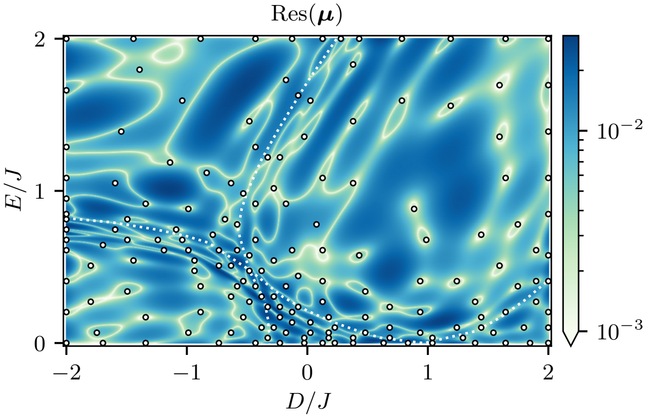
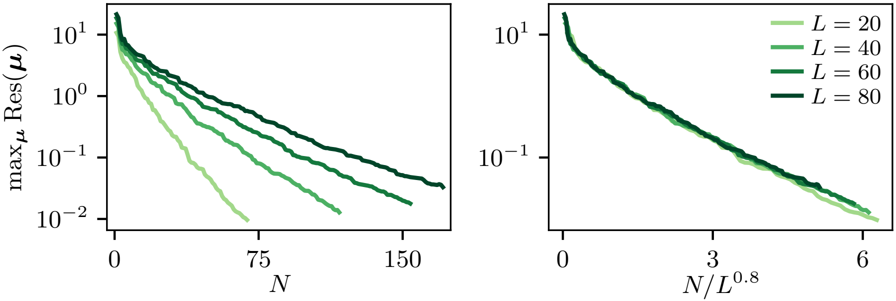


[1] Y.-C. Tzeng et al., *PRB* **96**, 060404, (2017).

Haldane: Growth of RB space with system size

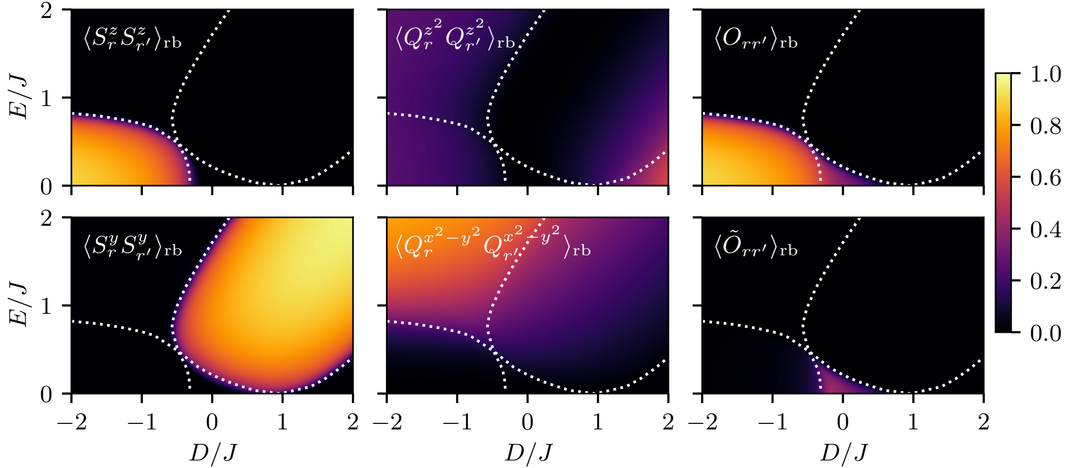
$N = \dim \mathbb{V}_n$ grows sublinearly at fixed residual: $N \sim L^\eta$, $\eta \simeq 0.8$

(As opposed to exponential Hilbert space growth!)



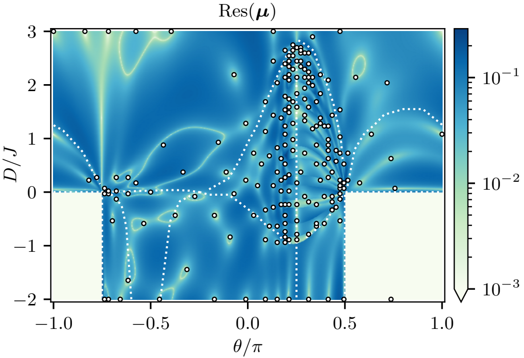
$\implies$ Orthogonality catastrophe as $L \to \infty$, but large L still feasible

Haldane: Correlation functions



Preview: Anisotropic bilinear-biquadratic chain

$$H_{\mathrm{BLBQ}} = J \sum_{i=1}^{L-1} \left[\cos(\theta) \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \sin(\theta)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 \right] + D \sum_{i=1}^{L} (S_i^z)^2$$



$\Longrightarrow$ Greedy RB parameter space exploration is useful for revealing unknown phases

Implementation: `ReducedBasis.jl`

- Written completely in julia
- MPSs and DMRG via `ITensors.jl`[1]
- Implements RB methods for parametrized eigenproblems
  - Customizable solving methods, error estimators, orthonormalization, grid types, assembly strategy, ...
- Open-source implementation:
  `https://github.com/mfherbst/ReducedBasis.jl`

[1] M. Fishman, S. White, and E. Stoudenmire, SciPost Phys. Codebases, 004 (2022).

What julia brings to the table

- Suitable for multidisciplinary research
  (physics – computational mathematics – numerical analysis)
  - Gradual improvements across disciplines
- Fast prototyping of RB-MPS algorithm:
  - first functional version after $\mathcal{O}(\text{weeks})$
  - beginner-friendly
- Generic type system and composability:
  - Customizability made easy
  - Generic mathematical structure translates closely to generic Julia code

Example: Greedy RB assembly

Different solver types call the same greedy `assemble` method:

```
assemble(H, grid_train, greedy, fulldiag, nocomp)
assemble(H, grid_train, greedy, lobpcg, qrcomp)
assemble(H_mpo, grid_train, greedy, dmrg, edcomp)
```

$\Longrightarrow$

Algorithm 1. Overview of the offline step.

Data: Training grid $\Xi_{\text{train}} \subset \mathbb{P}$, $\boldsymbol{\mu}_1 \in \Xi_{\text{train}}$, n_{f} the number of truth eigenvalue computations.

Result: A surrogate reduced basis model $\text{rbm}_{n_{\text{f}}} \equiv \{\mathsf{B}_{n_{\text{f}}}, \mathsf{b}, \mathsf{h}_q, \mathsf{h}_{qq'}\}$ with N basis functions based on n_{f} truth solves.

$\boldsymbol{\Psi}(\boldsymbol{\mu}_1) \leftarrow \text{truth} - \text{solver}_{\mathcal{N}}(\boldsymbol{\mu}_1)$ (2)

$\text{rbm}_1 \leftarrow \text{compress}_{\mathcal{N}}(\boldsymbol{\Psi}(\boldsymbol{\mu}_1))$ (17)

while $\max_{\boldsymbol{\mu}\in\Xi_{\text{train}}} \text{res}_n(\boldsymbol{\mu}) > \texttt{tol}$ **do**

  for $\boldsymbol{\mu} \in \Xi_{\text{train}}$ **do**

    $\boldsymbol{\Phi}^{(n)}_{\text{rb}}(\boldsymbol{\mu}) \leftarrow \text{rb-solver}(\text{rbm}_n)$ (13)

    $\text{res}_n(\boldsymbol{\mu}) \leftarrow \text{residual}(\boldsymbol{\Phi}^{(n)}_{\text{rb}}(\boldsymbol{\mu}), \text{rbm}_n)$ (16)

  $\boldsymbol{\mu}_{n+1} \leftarrow \arg\max_{\boldsymbol{\mu}\in\Xi_{\text{train}}} \text{res}_n(\boldsymbol{\mu})$ (15)

  $\boldsymbol{\Psi}(\boldsymbol{\mu}_{n+1}) \leftarrow \text{truth-solver}_{\mathcal{N}}(\boldsymbol{\mu}_{n+1})$ (2)

  $\mathsf{U}_n \leftarrow \text{compress}_{\mathcal{N}}(\mathsf{B}_n, \boldsymbol{\Psi}(\boldsymbol{\mu}_{n+1}))$ (17)

  $\text{rbm}_{n+1} \equiv \{\mathsf{B}_{n_{\text{f}}+1}, \mathsf{b}, \mathsf{h}_q, \mathsf{h}_{qq'}\} \cdots \leftarrow \text{assemble}_{\mathcal{N}}(\mathsf{B}_n, \mathsf{U}_n)$

precompute $\mathsf{o}_r = \mathsf{B}_N^\dagger \mathsf{O}_r \mathsf{B}_N$

Solver-dependent subroutines call specialized methods via multiple dispatch:

$$h = B^\dagger H B \quad \Longrightarrow \quad \begin{cases} \text{matrix multiplications, if } H \text{ is } \texttt{Matrix\{<:Number\}} \\ \text{MPS-MPO-MPS contractions, if } H \text{ is } \texttt{ITensors.MPO} \end{cases}$$

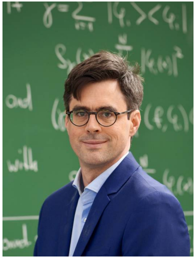
Conclusions

- RB approach efficiently captures phase diagrams of quantum spin systems
- MPSs and DMRG: large systems feasible
- Mathematically justified surrogate models (error estimates)
- Key ingredient for automated parameter space exploration
- Simple integration of additional solvers (PEPSs, GPU, QMC,. . .)
- Code: `github.com/mfherbst/ReducedBasis.jl`
- Preprint: `arXiv:2304.13587`

Acknowledgements

Stefan Wessel

Matteo Rizzi



Benjamin Stamm

EPFL MatMat Institute for Theoretical Solid State Physics | RWTH AACHEN UNIVERSITY

Open PhD & PostDoc positions at MatMat group

Possible topics include:

- Uncertainty quantification for materials models: Error in data-driven first-principle models, pseudopotentials, propagation to properties and interatomic potentials
- Self-adapting numerical methods for high-throughput materials simulations
- See `https://matmat.org/jobs/`

- Interdisciplinary research linking maths and simulation:
  - Become part of maths and materials institutes at EPFL
- Collaboration inside MARVEL national research centre:
  - Reproducible workflows & sustainable software
  - Computational materials discovery
  - Statistical learning methods

Questions?

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https://michael-herbst.com/talks/2023.07.27_juliacon_reducedbasis.pdf

https://github.com/mfherbst/ReducedBasis.jl

P. Brehmer, M. F. Herbst, S. Wessel, M. Rizzi, and B. Stamm, Reduced basis surrogates for quantum spin systems based on tensor networks, arXiv:2304.13587.

Anisotropic bilinear-biquadratic spin-1 chain

$$H_{\mathrm{BLBQ}} = J \sum_{i=1}^{L-1} \left[\cos(\theta) \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \sin(\theta) (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 \right] + D \sum_{i=1}^{L} (S_i^z)^2$$

- Phase diagram $\boldsymbol{\mu} = (\theta, D/J)$?
  [G. De Chiara et al., *PRB* **84**, 054451, (2011)]

- Parameter selection and $\mathrm{Res}(\boldsymbol{\mu})$?
  $n \sim 100$ snapshots at $L = 24$

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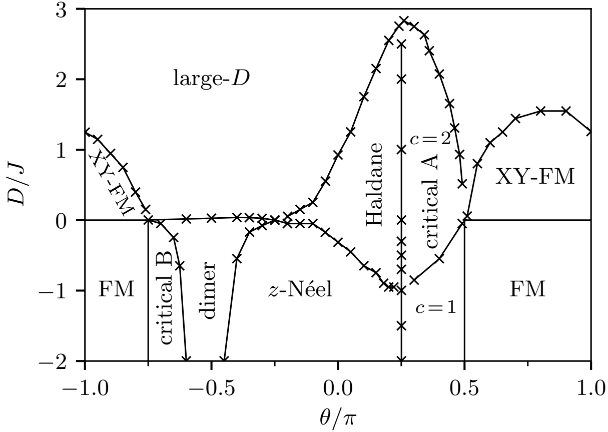

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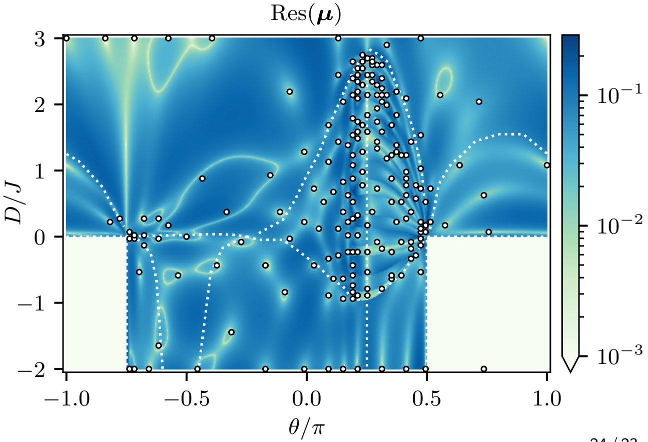
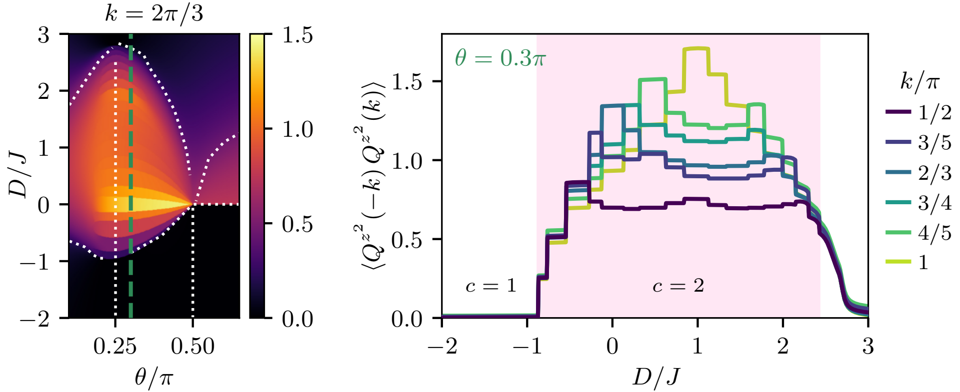


Correlations in critical A phase

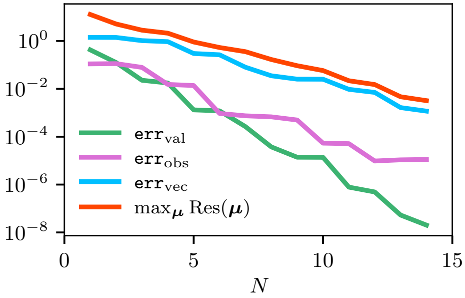
Assemble more accurate RB on 1D cut at $\theta = 0.3\pi$ and measure $\langle Q^{z^2}(-k)\, Q^{z^2}(k)\rangle_{\mathrm{rb}}$:



$\longrightarrow$ incommensurate correlations in $c = 2$ domain of critical A phase!

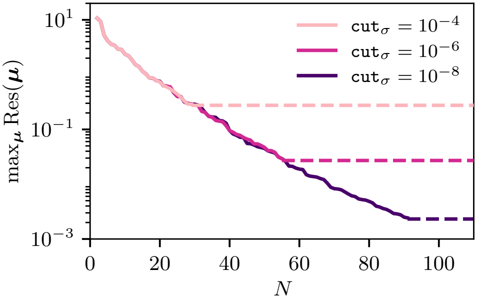
RB accuracy & influence of MPS errors

- Decay of $\max_{\boldsymbol{\mu}\in\Xi_{\text{test}}}$ RB errors:



$\longrightarrow$ Residual serves as upper bound!

- Sensitivity to MPS error cutoff $\texttt{cut}_\sigma$:

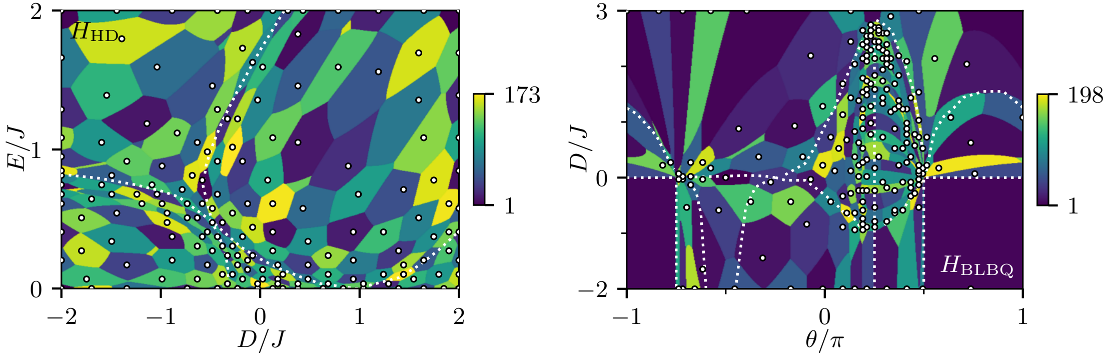


$\longrightarrow$ Sufficient MPS accuracy required!

Structure of basis coefficients

What is the maximal coefficient in $|\Phi_{\mathrm{rb}}(\boldsymbol{\mu})\rangle = \sum_{j=1}^{n} \varphi_{\mathrm{rb},j}(\boldsymbol{\mu})\,|\Psi(\boldsymbol{\mu}_j)\rangle$?

Compute $j_{\max}(\boldsymbol{\mu}) = \arg\max_{j\in\{1,\dots,n\}} |\varphi_{\mathrm{rb},j}(\boldsymbol{\mu})|$ on parameter domain:



$\longrightarrow$ $\varphi_{\mathrm{rb}}(\boldsymbol{\mu})$ contains only a few non-zero components!

Haldane observables

- Quadrupolar correlators $\langle Q_r^{x^2-y^2} Q_{r'}^{x^2-y^2} \rangle_{\rm rb}$ and $\langle Q_r^{z^2} Q_{r'}^{z^2} \rangle_{\rm rb}$ with

$$Q_r^{x^2-y^2} = (S_r^x)^2 - (S_r^y)^2, \quad Q_r^{z^2} = \frac{1}{\sqrt{3}}\left[3(S_r^z)^2 - 2\right]$$

- String order parameters:

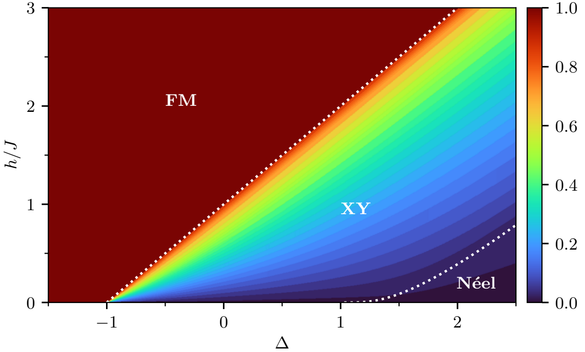
$$\langle O_{rr'} \rangle_{\rm rb} = -\left\langle S_r^z e^{i\pi \sum_{j=r+1}^{r'-1} S_j^z} S_{r'}^z \right\rangle_{\rm rb}$$

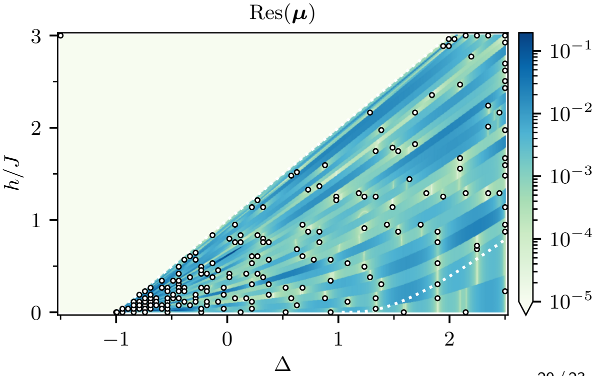
$$\langle \tilde{O}_{rr'} \rangle_{\rm rb} = -\left\langle S_r^z e^{i\pi \sum_{j=r+1}^{r'-1} S_j^z} S_{r'}^z \right\rangle_{\rm rb} - \langle S_r^z S_{r'}^z \rangle_{\rm rb}$$

Spin-1/2 XXZ chain

$$H = J\sum_{i=1}^{L}\left[\frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + \Delta S_i^z S_{i+1}^z\right] - h\sum_{i=1}^{L} S_i^z$$

Magnetization $M = \frac{2}{L}\sum_{i=1}^{L} S_i^z$ and $\mathrm{Res}(\boldsymbol{\mu})$ at $L = 80$:

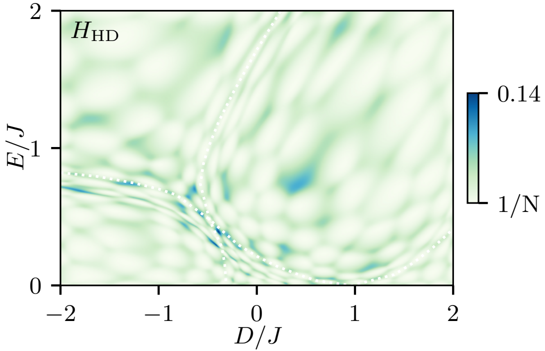


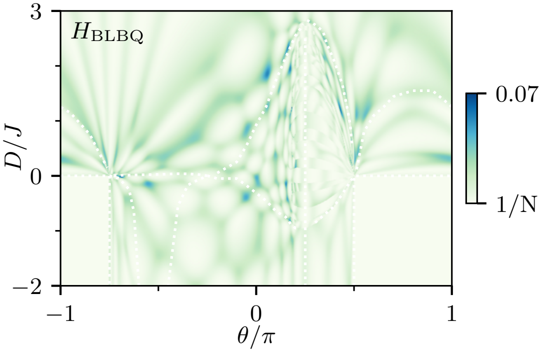


Participation ratio

Defined as the inverse of the *inverse* participation ratio

$$P(\boldsymbol{\mu}) = \frac{1}{N\sum_{j=1}^{N}|p_j(\boldsymbol{\mu})|^4}, \qquad p_j(\boldsymbol{\mu}) = \frac{\tilde{\varphi}_{\mathrm{rb},j}(\boldsymbol{\mu})}{\|\tilde{\varphi}_{\mathrm{rb}}(\boldsymbol{\mu})\|}, \qquad P(\boldsymbol{\mu}) \in [N^{-1}, 1].$$





Fidelity susceptibility approach

Compute fidelity F from RB coefficients

$$F(\boldsymbol{\mu}, \boldsymbol{\mu} + \delta\boldsymbol{\mu}) = |\langle \Phi_{\mathrm{rb}}(\boldsymbol{\mu}) | \Phi_{\mathrm{rb}}(\boldsymbol{\mu} + \delta\boldsymbol{\mu}) \rangle| = |\varphi_{\mathrm{rb}}(\boldsymbol{\mu})^\dagger \, b \, \varphi_{\mathrm{rb}}(\boldsymbol{\mu} + \delta\boldsymbol{\mu})|$$

and average over fidelity susc. in μ_1 and μ_2 directions to obtain total fidelity susc.

$$\chi_F^{\mathrm{tot}}(\boldsymbol{\mu}) = -\frac{1}{2}\left[\frac{2\log F_1(\boldsymbol{\mu})}{\delta\mu_1^2} + \frac{2\log F_2(\boldsymbol{\mu})}{\delta\mu_2^2}\right].$$