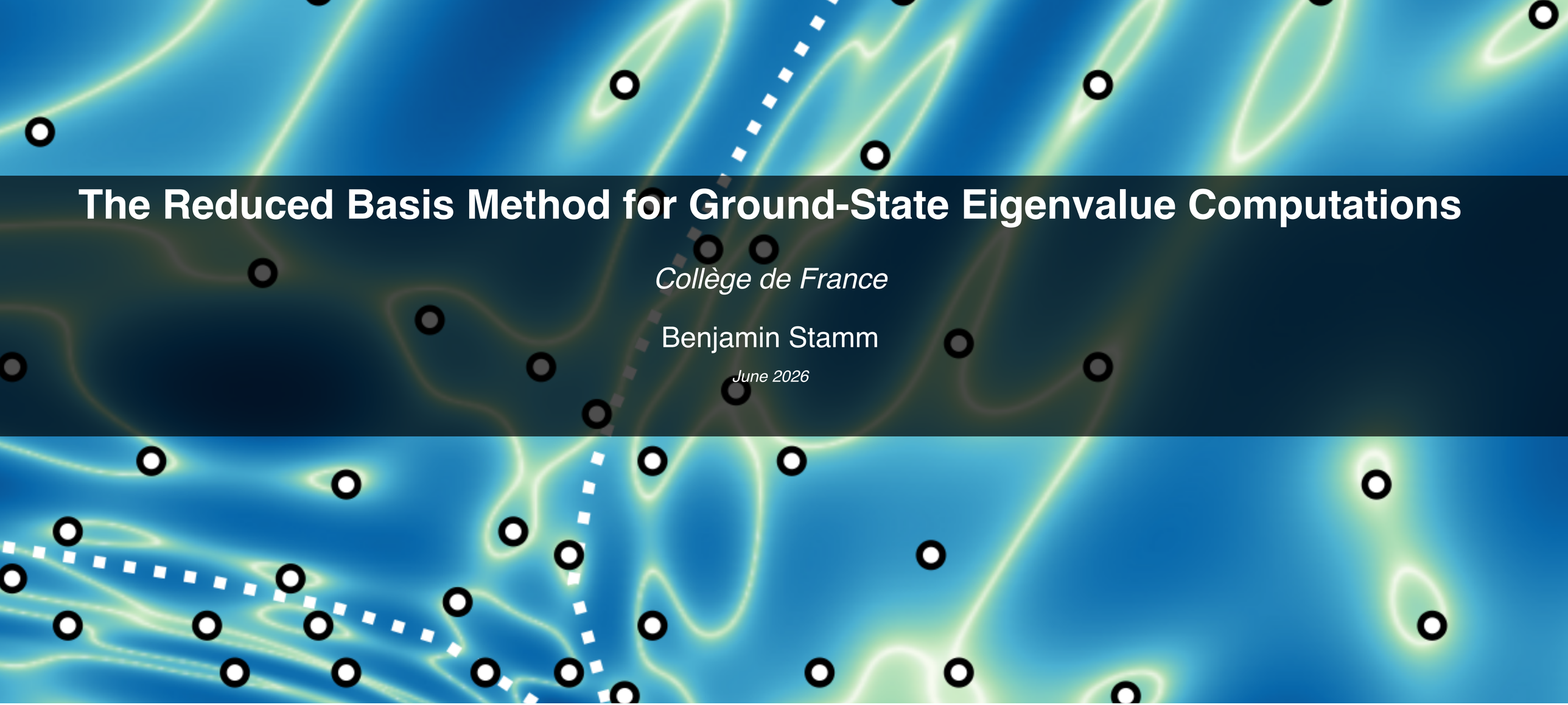

The Reduced Basis Method for Ground-State Eigenvalue Computations

Collège de France

Benjamin Stamm

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Joint-work with Mattia Manucci, Zhuoyao Zeng

following work with L. Garrigue, M. Herbst, M. Rizzi, St. Wessel, P. Brehmer

Universität Stuttgart
Institute of Applied Analysis and Numerical Simulation

Part 1

Motivation: quantum mechanics

Quantum Mechanics is all about eigenvalue problems

Axioms of Quantum Mechanics (Hilbert space formulation):

- State and state space: A state $|\psi\rangle$ is a normalized element in a complex, separable Hilbert space $\mathcal{H}$ (very high-dimensional or infinite-dimensional)
- Observables: Every physical property $\mathcal{O}$ (energy, position, momentum, …) corresponds to an associated linear, self-adjoint but possibly unbounded operator $\mathbf{O}$ acting on $\mathcal{H}$. *Spectral theorem (finite-dimensional case):*

$$\mathbf{O} = \sum_i \omega_i \mathbf{P}_i \qquad \mathbf{P}_i \text{ : Spectral projector onto eigenspace.}$$

  Key-message: only eigenspaces are relevant, not individual eigenvectors (the phase of a state is not an observable)!

- Born rule: The probability of measuring an eigenvalue ω_i with a state $|\psi\rangle$ is $\|\mathbf{P}_i|\psi\rangle\|^2 = \langle\psi|\mathbf{P}_i|\psi\rangle$. Thus, the expectation value of the observable $\mathbf{O}$ with state $|\psi\rangle$ is

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$$|\psi\rangle \quad \xrightarrow{\text{meas. } \mathcal{O}=\mu_i} \quad |\psi'\rangle = \frac{\mathbf{P}_i|\psi\rangle}{\|\mathbf{P}_i|\psi\rangle\|}.$$

- Time evolution: The state of an isolated system (when not being measured) is given by $|\psi(t)\rangle = \mathbf{U}(t)|\psi(0)\rangle$ where the unitary time evolution is given by $\mathbf{U}(t) = \exp\{-it\mathbf{H}/\hbar\}$ where $\mathbf{H}$ is the hermitian energy operator (Hamiltonian).
- Composition of subsystems: The state of a combined system consisting of the two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ belongs to the tensor product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$.

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Moral of the story:

- Eigenvalues of Hermitian matrices are important;
- Eigenspaces are the correct notion, not eigenvectors;
- The energetically interesting eigenvalue is the the smallest one of the Hamiltonian (energy operator).

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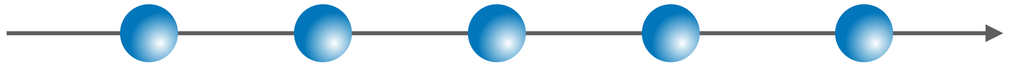
Example: A so-called spin-1 system has $d = 3$ states per particle. The size of the Hilbert space grows exponentially $\mathcal{H}_L = \mathbb{C}^n$ with $n = 3^L$: the dimension triples with each new particle.

Example of spin-1/2 XXZ chain (well-studied toy model)

Hamiltonian: Chain of L particles with $d = 2$ states and Hamiltonian

$$\mathbf{A}(\Delta, \tfrac{h}{J}) := \sum_{i=1}^{L-1} (\mathbf{S}_i^x \mathbf{S}_{i+1}^x + \mathbf{S}_i^y \mathbf{S}_{i+1}^y) + \sum_{i=1}^{L-1} \Delta\, \mathbf{S}_i^z \mathbf{S}_{i+1}^z - \tfrac{h}{J} \sum_{i=1}^{L} \mathbf{S}_i^z \quad \in \quad \mathbb{C}^{2^L \times 2^L},$$

where



- $\mathbf{A}_i := \left(\otimes^{i-1} \mathbf{I}_2\right) \otimes \mathbf{A} \otimes \left(\otimes^{L-i} \mathbf{I}_2\right)$;
- $\mathbf{S}^x = \frac{1}{2}\sigma^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\mathbf{S}^y = \frac{1}{2}\sigma^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\mathbf{S}^z = \frac{1}{2}\sigma^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$: single-particle Pauli operators;
- Parameters Δ (next-neighbour coupling), J (bilinear coupling) and h (external magnetic field strength)

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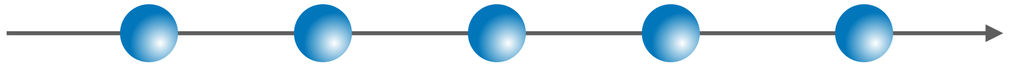
$$\mathbf{A}(\boldsymbol{\mu}) := \theta_1(\boldsymbol{\mu})\,\mathbf{A}_1 + \theta_2(\boldsymbol{\mu})\,\mathbf{A}_2 + \theta_3(\boldsymbol{\mu})\,\mathbf{A}_3 \qquad\qquad \boldsymbol{\mu} = (\Delta, \tfrac{h}{J})$$

where θ_q are real-analytic functions in $\boldsymbol{\mu}$ and $\mathbf{A}_q \in \mathbb{C}^{2^L \times 2^L}$ fixed matrices.



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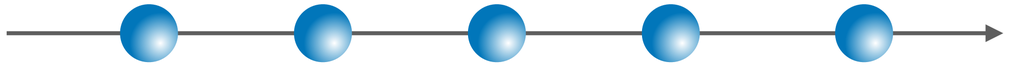
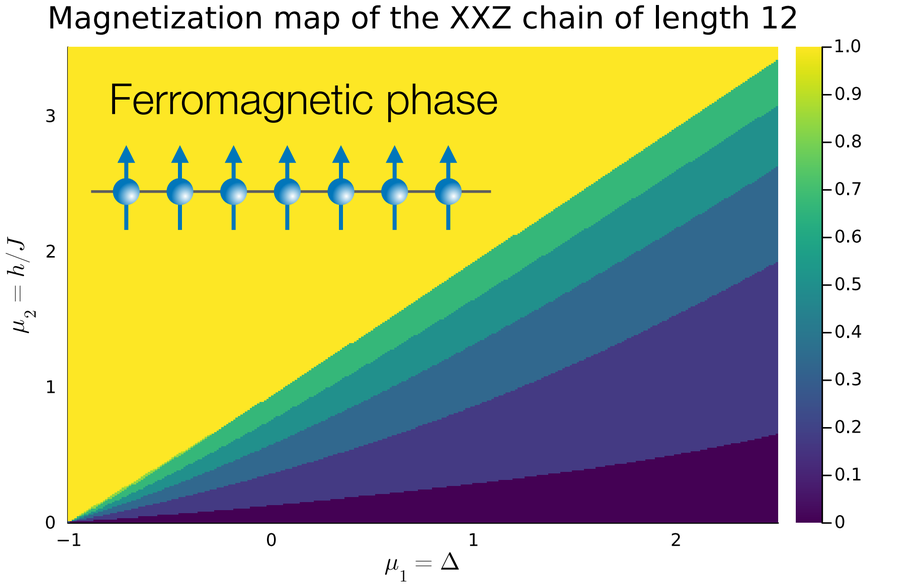


Observable: Magnetization

$$\mathbf{M} = \frac{2}{L}\sum_{i=1}^{L} \mathbf{S}_i^z$$

Since **M** commutes with **H**, they share the same the eigenstates $|\psi_m\rangle$ and there holds

$$\mathbf{M}|\psi_m\rangle = \frac{2m}{L}|\psi_m\rangle$$



Ground-state eigenvalue (truth) problems

- Given a compact parameter domain $\mathcal{P} \subset \mathbb{R}^p$, analytic functions $\theta_1, \ldots, \theta_Q : \mathcal{P} \to \mathbb{R}$, and Hermitian matrices $\mathbf{A}_1, \ldots, \mathbf{A}_Q \in \mathbb{C}^{n \times n}$,

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- **How:** Solve the parametrized eigenvalue problem: find eigenvalue $\lambda_1(\boldsymbol{\mu})$ and eigenvectors $\mathbf{W}(\boldsymbol{\mu}) \in \mathbb{C}^{n \times m_1(\boldsymbol{\mu})}$ such that

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- Build the eigenspace projector $\mathbf{P}_1(\boldsymbol{\mu}) = \mathbf{W}(\boldsymbol{\mu})\mathbf{W}(\boldsymbol{\mu})^*$ and the observable is computed as

$$\langle \mathbf{O} \rangle(\boldsymbol{\mu}) = \tfrac{1}{m_1(\boldsymbol{\mu})} \mathrm{Tr}\big(\mathbf{O}\, \mathbf{P}_1(\boldsymbol{\mu})\big).$$

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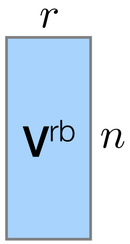

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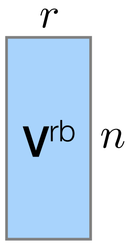

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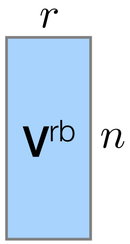

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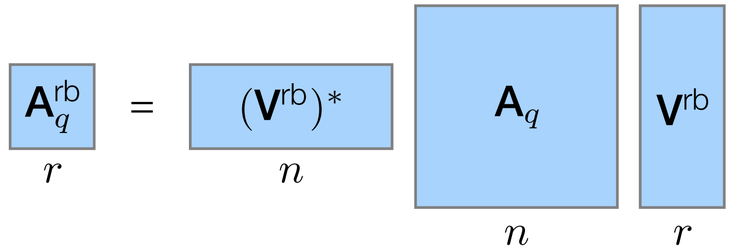

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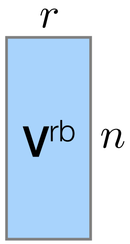

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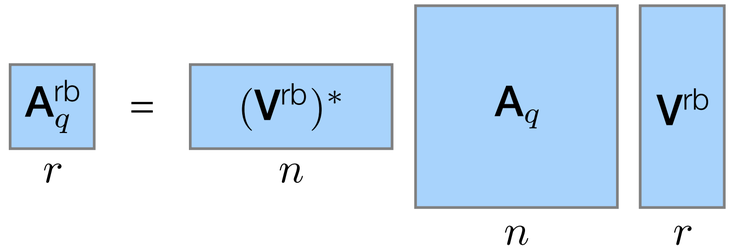

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$$\mathbf{A}^{\text{rb}}(\boldsymbol{\mu}) \, \mathbf{z}(\boldsymbol{\mu}) = \lambda_1^{\text{rb}}(\boldsymbol{\mu}) \, \mathbf{z}(\boldsymbol{\mu}), \qquad \mathbf{W}^{\text{rb}}(\boldsymbol{\mu}) = \mathbf{V}^{\text{rb}} \, \mathbf{z}(\boldsymbol{\mu}),$$

where $m_1^{\text{rb}}(\boldsymbol{\mu})$ denotes the multiplicity of the eigenvalue $\mathbf{V}^{\text{rb}}$ of $\mathbf{A}^{\text{rb}}(\boldsymbol{\mu})$.

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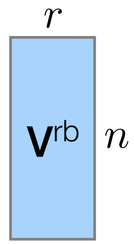

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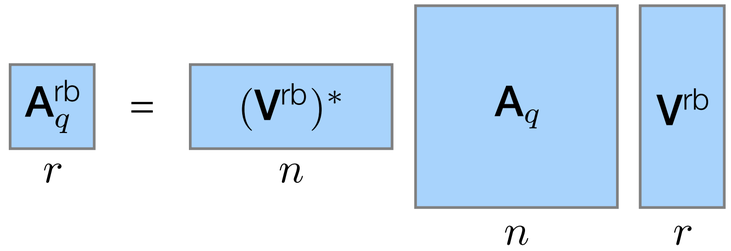

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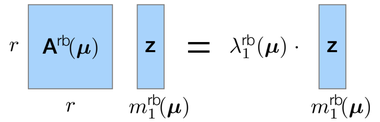
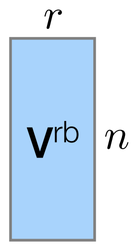


where $m_1^{\text{rb}}(\boldsymbol{\mu})$ denotes the multiplicity of the eigenvalue $\mathbf{V}^{\text{rb}}$ of $\mathbf{A}^{\text{rb}}(\boldsymbol{\mu})$.

RBM for ground-state eigenvalue problems

Offline phase:

- Find suitable $\mathbf{W}(\boldsymbol{\mu}_1), \ldots, \mathbf{W}(\boldsymbol{\mu}_J)$ (and other vectors...) $\xrightarrow{\text{spans}}$ Orthonormal basis: $\mathbf{V}^{\text{rb}} \in \mathbb{C}^{n \times r}$.



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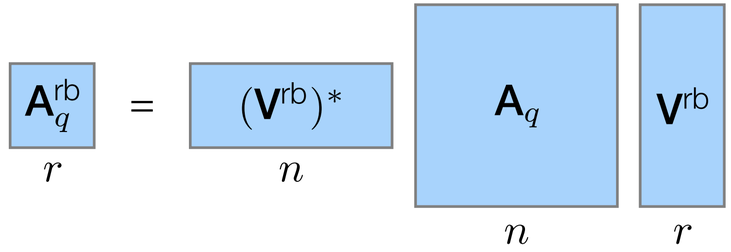

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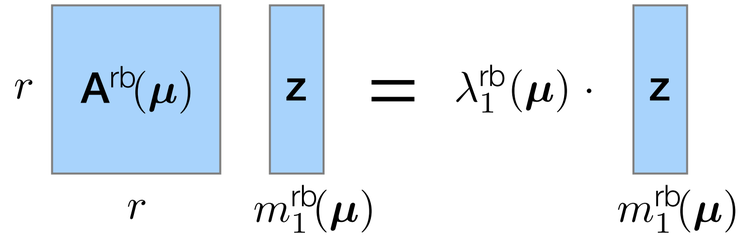

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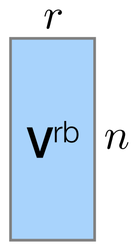

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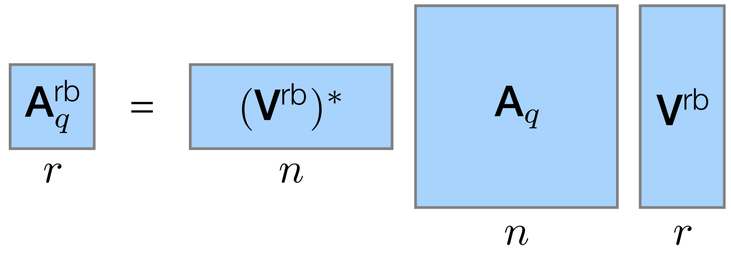

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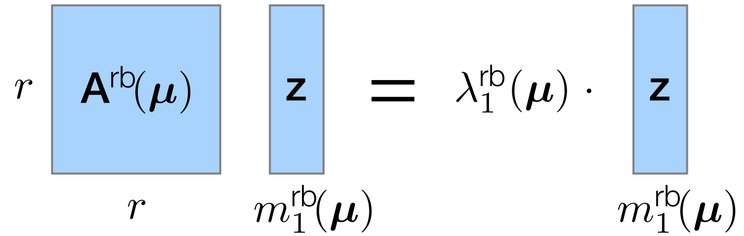

where $m_1^{\text{rb}}(\boldsymbol{\mu})$ denotes the multiplicity of the eigenvalue $\mathbf{V}^{\text{rb}}$ of $\mathbf{A}^{\text{rb}}(\boldsymbol{\mu})$.

- Build the approximate RB-eigenspace projector $\mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu}) = \mathbf{W}_1^{\text{rb}}(\boldsymbol{\mu}) \, \mathbf{W}_1^{\text{rb}}(\boldsymbol{\mu})^*$ and the observable is computed as

$$\langle \mathbf{O} \rangle_{\text{rb}}(\boldsymbol{\mu}) := \tfrac{1}{m_1^{\text{rb}}(\boldsymbol{\mu})} \text{Tr}\big(\mathbf{O} \, \mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\big).$$

RBM for eigenvalue problems

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Eigenvalue-problems are also at the origin of the RBM:

E. Aktas and F. Moses, Reduced Basis Eigenvalue Solutions for Damaged Structures, Mech. Struct. Mach. 26, 63 (1998).

P. B. Nair, A. J. Keane, and R. S. Langley, Improved First-Order Approximation of Eigenvalues and Eigenvectors, AIAA J. 36, 1721 (1998)

L. Machiels, Y. Maday, I. B. Oliveira, A. T. Patera, and D. V. Rovas, Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems, Comptes Rendus de l'Académie des Sciences - Séries I - Mathematics 331, 153 (2000)

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Only a few contributions (probably not complete) after these seminal works:

I. Fumagalli, A. Manzoni, N. Parolini, M. Verani, Reduced basis approximation and a posteriori error estimates for parametrized elliptic eigenvalue problems, ESAIM: Math. Model. Numer. Anal. 50, 1857 (2016).

Th. Horger, B. Wohlmuth, and Th. Dickopf, Simultaneous reduced basis approximation of parameterized elliptic eigenvalue problems, ESAIM: Math. Model. Numer. Anal. 51, 443 (2017).

F. Pla and H. Herrero, Reduced basis method applied to eigenvalue problems from convection, Int. J. Bifurc. Chaos Appl. Sci. Eng. 29, 1950028 (2019).

F. Pichi, A. Quaini, and G. Rozza, A Reduced Order Modeling Technique to Study Bifurcating Phenomena: Application to the Gross–Pitaevskii Equation, SIAM J. Sci. Comp. 42, B1115 (2020).

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   - local analytic spectral projector viewpoint,
   - Taylor-type reduced spaces,
   - (Local) convergence theory for parametric EVPs from a eigenspace-projector viewpoint.

Part 2

Eigenproblem-specific obstacles

Local regularity of eigenspaces

Assume the smallest m-dimensional eigenspace $\mathcal{W}_1(\boldsymbol{\mu}_0)$ is well-separated from the rest of the spectrum near $\boldsymbol{\mu}_0$:

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$$\mathbf{P}_1(\boldsymbol{\mu}) = \frac{1}{2\pi i} \int_\Gamma (z\mathbf{I} - \mathbf{A}(\boldsymbol{\mu}))^{-1}\, dz,$$

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In consequence:

- separation gives a locally well-defined projector $\mathbf{P}_1(\boldsymbol{\mu})$;
- $\mathbf{P}_1(\boldsymbol{\mu})$ is the regular object (analytic), not the individual eigenvector labels;
- local regularity implies approximability by Taylor-series.

Measuring approximation error of eigenspaces in the RBM-context

Specific notation for eigenspaces:

- Each subspace $\mathcal{W}$ is uniquely associated with and represented by an orthogonal projector $\mathbf{P}_{\mathcal{W}}$.
- Thus $\mathcal{W} = \operatorname{range} \mathbf{P}_{\mathcal{W}}$.
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Exact and approximate (RB) eigenspaces:

- $\lambda_k(\boldsymbol{\mu})$ and $\lambda_k^{\text{rb}}(\boldsymbol{\mu})$ denote the exact and RB eigenvalues without counting multiplicities, e.g. $\lambda_i(\boldsymbol{\mu}) < \lambda_{i+1}(\boldsymbol{\mu})$.
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Error between eigenspaces:

- Distance between $\mathcal{W}_1(\boldsymbol{\mu})$ and $\mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})$: Define $\operatorname{dist}\big(\mathcal{W}_1(\boldsymbol{\mu}), \mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})\big) := \|\mathbf{P}_1(\boldsymbol{\mu}) - \mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\|$. (Frobenius norm)
- There holds

$$\|\mathbf{P}_1(\boldsymbol{\mu}) - \mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\| = \begin{cases} 1 & \text{if } \dim \mathcal{W}_1(\boldsymbol{\mu}) < \dim \mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu}), \\ \|\mathbf{P}_1^{\perp}(\boldsymbol{\mu})\,\mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\| & \text{if } \dim \mathcal{W}_1(\boldsymbol{\mu}) = \dim \mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu}), \\ 1 & \text{if } \dim \mathcal{W}_1(\boldsymbol{\mu}) > \dim \mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu}), \end{cases}$$

  where $\mathbf{P}_1^{\perp}(\boldsymbol{\mu}) = \mathbf{I} - \mathbf{P}_1(\boldsymbol{\mu})$.

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- For $\mu \in [0, 2\pi]$, consider

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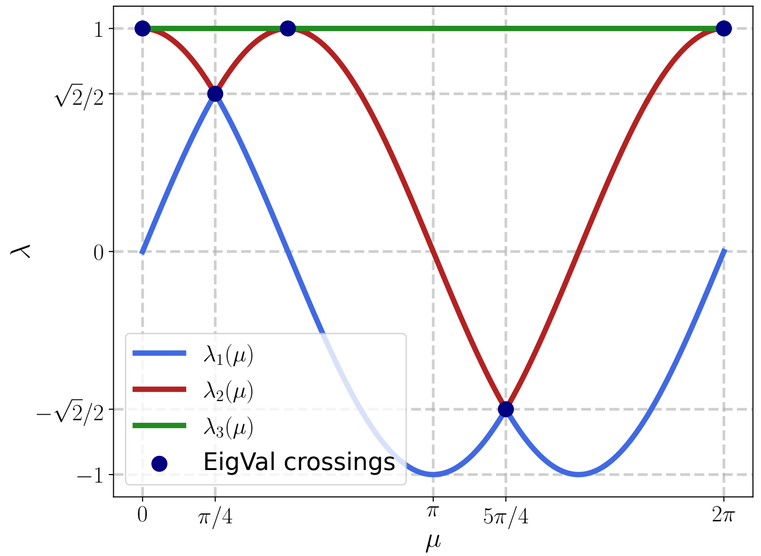

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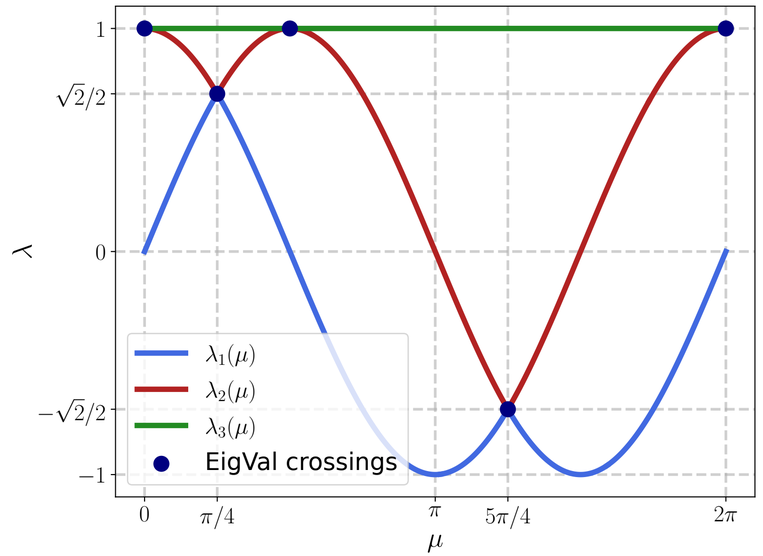

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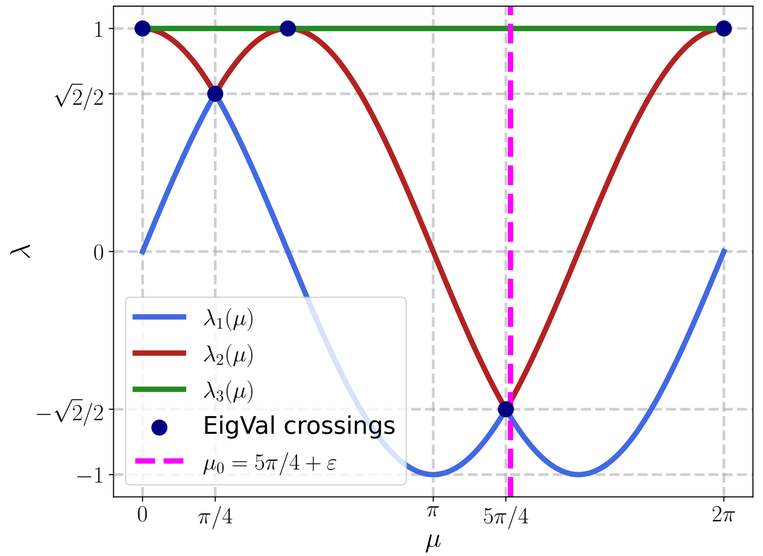

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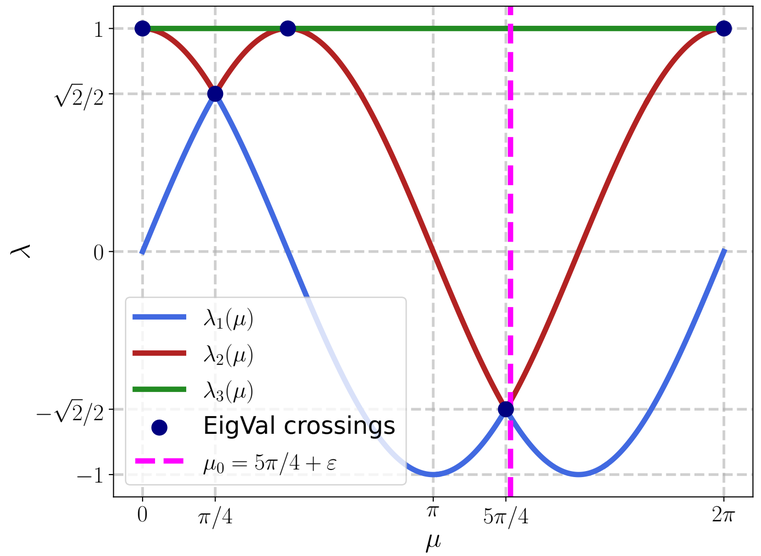

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- Before / at / after the crossing:

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Residual: For the reduced basis approximation $\mathbf{W}^{\mathrm{rb}}(\boldsymbol{\mu}) = \mathbf{V}^{\mathrm{rb}}\mathbf{z}(\boldsymbol{\mu})$ of the smallest eigenspace, write the (block-) residual as

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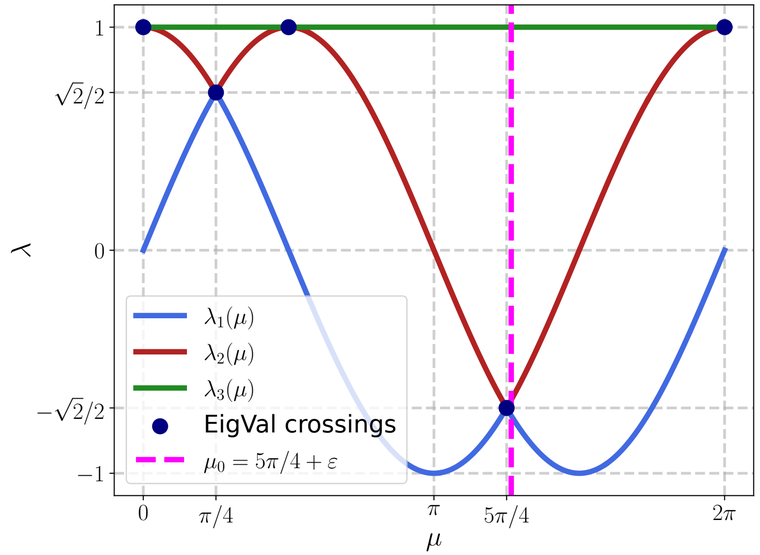
Remarks:

- A zero residual confirms invariance of the subspace, i.e. $[\mathbf{A}(\boldsymbol{\mu}), \mathbf{P}^{\text{rb}}(\boldsymbol{\mu})] = \mathbf{A}(\boldsymbol{\mu})\,\mathbf{P}^{\text{rb}}(\boldsymbol{\mu}) - \mathbf{A}(\boldsymbol{\mu})\,\mathbf{P}^{\text{rb}}(\boldsymbol{\mu}) = \mathbf{0}$.
- It does not identify which true eigenspace has been approximated. It could contain a (proper) subspace (dimension mismatch) of the true eigenspace and/or higher eigenspaces (or parts of it).
- To certify the smallest eigenspace, additional spectral information is needed.



What changes from source problems to eigenproblems?

Coercive source problems	Eigenproblems
target: solution $u(\mu)$	target: eigenspace $\mathcal{W}_1(\mu)$
analytic data often gives analytic solution map	analytic matrix entries do **not** imply globally analytic labeled eigenvectors/eigenspaces
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Central issues:

- Eigenvalue crossings: $\mathcal{W}_1(\boldsymbol{\mu})$ resp. $\mathbf{P}_1(\boldsymbol{\mu})$ (changes discontinuously with $\boldsymbol{\mu}$).
- Residual not reliable quantity to estimate error: A zero residual does not identify the sought eigenspace (related to "non-uniqueness")

Part 3

Certified RBM assembly for the smallest eigenspace

(Global perspective)

Certified greedy assembly on a finite parameter set

Greedy method:
Iterative subspace enlargement based on an efficient error estimator $\Delta(\boldsymbol{\mu}, \mathcal{V})$ & a (discrete) training set $\Xi \subseteq \mathcal{P}$:

- Initialise: Select $\boldsymbol{\mu}_1$ randomly, compute $\big(\lambda_1(\boldsymbol{\mu}_1), \mathcal{W}_1(\boldsymbol{\mu}_1)\big)$, set $\mathcal{V}_1 := \mathcal{W}_1(\boldsymbol{\mu}_1)$.
- Loop:
  i) Suppose $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_J \in \Xi$ selected, and $\mathcal{V}_J$ constructed.
  ii) Then $\boldsymbol{\mu}_{J+1} := \arg\max_{\boldsymbol{\mu} \in \Xi} \Delta(\boldsymbol{\mu}, \mathcal{V}_J)$, and $\mathcal{V}_{J+1} := \operatorname{span}\{\mathcal{V}_J, \mathcal{W}_1(\boldsymbol{\mu}_{J+1})\}$.
  iii) Terminate when $\max_{\boldsymbol{\mu} \in \Xi} \Delta(\boldsymbol{\mu}, \mathcal{V}_{J+1}) < \varepsilon$.

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We should find a good error indicator $\Delta(\boldsymbol{\mu}, \mathcal{V})$!

Certified greedy assembly on a finite parameter set

Greedy method:
Iterative subspace enlargement based on an efficient error estimator $\Delta(\boldsymbol{\mu}, \mathcal{V})$ & a (discrete) training set $\Xi \subseteq \mathcal{P}$:

- Initialise: Select $\boldsymbol{\mu}_1$ randomly, compute $\big(\lambda_1(\boldsymbol{\mu}_1), \mathcal{W}_1(\boldsymbol{\mu}_1)\big)$, set $\mathcal{V}_1 := \mathcal{W}_1(\boldsymbol{\mu}_1)$.
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Recall:

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Strategy: Ensure that

- the projection error $\|\mathbf{P}_1^{\perp}(\boldsymbol{\mu})\mathbf{W}_1^{\mathrm{rb}}(\boldsymbol{\mu})\|$ is small,
- $\dim \mathcal{W}_1(\boldsymbol{\mu}) = \dim \mathcal{W}_1^{\mathrm{rb}}(\boldsymbol{\mu})$.

Projection-error estimate for the true bottom eigenspace

A simple result we weren't able to find in the literature:

Theorem: If $\mathbf{A}(\boldsymbol{\mu}) \neq c\,\mathbf{I}$, then

$$\|\mathbf{P}_1^{\perp}(\boldsymbol{\mu})\mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\| \;\leq\; \frac{1}{\gamma(\boldsymbol{\mu})}\Big(\|\mathbf{R}(\boldsymbol{\mu})\| + \lambda_1^{\text{rb}}(\boldsymbol{\mu}) - \lambda_1(\boldsymbol{\mu})\Big),$$

where

- $\mathbf{W}_1^{\text{rb}}(\boldsymbol{\mu})$ is an ONB matrix of the approximated EigSpace $\mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})$,
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$$\text{projection error} \;\leq\; \frac{\text{residual term} + \text{eigenvalue error term}}{\text{spectral gap}}$$

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How to make this error bound practically useful?

- Replace $\lambda_1(\boldsymbol{\mu})$ by an efficiently computable lower bound $\lambda_1^{\text{LB}}(\boldsymbol{\mu}, \mathcal{V})$ following Širković–Kressner (2016).
- Construct a separate reduced basis subspace $\mathcal{V}_\gamma$ for the approximation of $\gamma(\boldsymbol{\mu})$.

Efficiently computable error bounds for eigenvalues

- Notation: We now (have to) consider eigenvalues counting multiplicities

$$\tilde{\lambda}_k(\boldsymbol{\mu}), \quad \tilde{\lambda}_k^{\mathrm{rb}}(\boldsymbol{\mu}), \qquad k = 1, \ldots, n.$$

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- A general and efficiently computable lower bound $\tilde{\lambda}_k^{\text{LB}}(\boldsymbol{\mu})$ has been derived:
  - Key idea is perturbation theory + SCM method, extending $\tilde{\lambda}_1^{\text{LB}}(\boldsymbol{\mu})$ from Širković–Kressner.
  - The bound has the form

$$\tilde{\lambda}_k^{\text{LB}}(\boldsymbol{\mu}) \;=\; \min\{\tilde{\lambda}_k^{\text{rb}}(\boldsymbol{\mu}), \eta_*(\boldsymbol{\mu})\} \;-\; \varepsilon_k(\boldsymbol{\mu})$$

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- A nice and important property of $\lambda_1^{\mathrm{LB}}(\boldsymbol{\mu})$:
  - If $\eta_*(\boldsymbol{\mu}) > \lambda_1^{\mathrm{rb}}(\boldsymbol{\mu}) + \varepsilon_1(\boldsymbol{\mu})$, then it holds that $\dim \mathcal{W}_1(\boldsymbol{\mu}) = \dim \mathcal{W}_1^{\mathrm{rb}}(\boldsymbol{\mu})$.

  $\rightsquigarrow$ Sufficient condition for dimension recovery!

Tools we now have at hand

- **Efficiently computable eigenspace-dimension condition:**

  If $\eta_*(\boldsymbol{\mu}) > \lambda_1^{\text{rb}}(\boldsymbol{\mu}) + \varepsilon_1(\boldsymbol{\mu})$, then it holds that $\dim\left(\mathcal{W}_1(\boldsymbol{\mu})\right) = \dim\left(\mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})\right)$.

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▷ **Efficiently computable upper and lower bounds of eigenvalues and spectral gaps:**

$$\tilde{\lambda}_k^{\text{LB}}(\boldsymbol{\mu}) \leq \tilde{\lambda}_k(\boldsymbol{\mu}) \leq \tilde{\lambda}_k^{\text{rb}}(\boldsymbol{\mu}) \;=\; \tilde{\lambda}_k^{\text{UB}}(\boldsymbol{\mu}) \qquad \text{(counting multiplicities)}$$

$$\max\big(\lambda_2^{\text{LB}}(\boldsymbol{\mu}) - \lambda_1^{\text{UB}}(\boldsymbol{\mu}), 0\big) \;=:\; \gamma^{\text{LB}}(\boldsymbol{\mu}) \leq \gamma(\boldsymbol{\mu}) \leq \gamma^{\text{UB}}(\boldsymbol{\mu}) \;:=\; \lambda_2^{\text{UB}}(\boldsymbol{\mu}) - \lambda_1^{\text{LB}}(\boldsymbol{\mu}) \qquad \text{if } \dim\big(\mathcal{W}_1(\boldsymbol{\mu})\big) = \dim\big(\mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})\big)$$

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▷ **Estimation:**

$$\begin{aligned}
\|\mathbf{P}_1(\boldsymbol{\mu}) - \mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\| \;&\leq\; \frac{1}{\gamma(\boldsymbol{\mu})}\Big(\|\mathbf{R}(\boldsymbol{\mu})\| + \lambda_1^{\text{rb}}(\boldsymbol{\mu}) - \lambda_1(\boldsymbol{\mu})\Big), && \text{if } \dim\big(\mathcal{W}_1(\boldsymbol{\mu})\big) = \dim\big(\mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})\big) \\
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2-stage greedy algorithm:

- Stage 1: Assemble reduced basis $\mathbf{V}_\gamma^{\text{rb}}$ to approximate the first and second eigenspaces to get a certified gap estimation.
- Stage 2: Assemble another reduced basis $\mathbf{V}^{\text{rb}}$ to approximate only the first eigenspaces using the gap-estimator from Stage 1.

Stage 1: Spectral gap approximation

- **Goal:** Construct a subspace $\mathcal{V}_\gamma$ to approximate the spectral gap $\gamma(\boldsymbol{\mu})$ by the subspace spectral gap of $\mathbf{V}_\gamma^* \mathbf{A}(\boldsymbol{\mu}) \mathbf{V}_\gamma$ via

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- **Result:** $\mathcal{V}_\gamma$ provides a reliable and certified approximation of $\gamma(\boldsymbol{\mu})$ with

$$\gamma(\boldsymbol{\mu}) > (1-\varepsilon_\gamma)\gamma^{\text{rb}}(\boldsymbol{\mu}) \qquad \text{for all } \boldsymbol{\mu} \in \Xi.$$

$$\gamma(\boldsymbol{\mu}) \geq \gamma^{\text{LB}}(\boldsymbol{\mu}) \qquad \text{if } \underbrace{\eta_*(\boldsymbol{\mu}) > \lambda_1^{\text{rb}}(\boldsymbol{\mu}) + \varepsilon_1(\boldsymbol{\mu})}_{\Rightarrow \dim\left(\mathcal{W}_1(\boldsymbol{\mu})\right) = \dim\left(\mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})\right)} \qquad \text{for all } \boldsymbol{\mu} \in \mathcal{P}\backslash\Xi,$$

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- **How:** Again via the greedy method with error indicator

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- **Result:** Reduced basis space $\mathcal{V}_{\text{rb}}$ satisfying

$$\|\mathbf{P}_1(\boldsymbol{\mu}) - \mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\| \le \Delta(\boldsymbol{\mu}) < \varepsilon \quad \text{for all } \boldsymbol{\mu} \in \Xi,$$

$$\|\mathbf{P}_1(\boldsymbol{\mu}) - \mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\| \le \tilde{\Delta}(\boldsymbol{\mu}) \quad \text{if } \underbrace{\eta_*(\boldsymbol{\mu}) > \lambda_1^{\text{rb}}(\boldsymbol{\mu}) + \varepsilon_1(\boldsymbol{\mu})}_{\Rightarrow \dim\left(\mathcal{W}_1(\boldsymbol{\mu})\right) = \dim\left(\mathcal{W}_1^{\text{rb}}(\boldsymbol{\mu})\right)} \quad \text{for all } \boldsymbol{\mu} \in \mathcal{P}\backslash\Xi,$$

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Numerical results for the the XXZ model: stage 1

- Recall $\boldsymbol{\mu} = (\mu_1, \mu_2) \in [-1, 2.5] \times [0, 3.5]$ and $\mathbf{A}(\boldsymbol{\mu}) = \mathbf{A}_1 + \mu_1 \mathbf{A}_2 - \mu_2 \mathbf{A}_3 \in \mathbb{C}^{2^L \times 2^L}$.
- $L = 14$, i.e., $N = 2^L = 16384$, Ξ consisting of $35 \times 35 = 1225$ Chebyshev nodes, $\varepsilon_\gamma = 10^{-8}$.
- Stage 1 yields $\mathcal{V}_\gamma$ of dimension 265.

Numerical results for the the XXZ model: stage 1

- Recall $\boldsymbol{\mu} = (\mu_1, \mu_2) \in [-1, 2.5] \times [0, 3.5]$ and $\mathbf{A}(\boldsymbol{\mu}) = \mathbf{A}_1 + \mu_1 \mathbf{A}_2 - \mu_2 \mathbf{A}_3 \in \mathbb{C}^{2^L \times 2^L}$.
- $L = 14$, i.e., $N = 2^L = 16384$, Ξ consisting of $35 \times 35 = 1225$ Chebyshev nodes, $\varepsilon_\gamma = 10^{-8}$.
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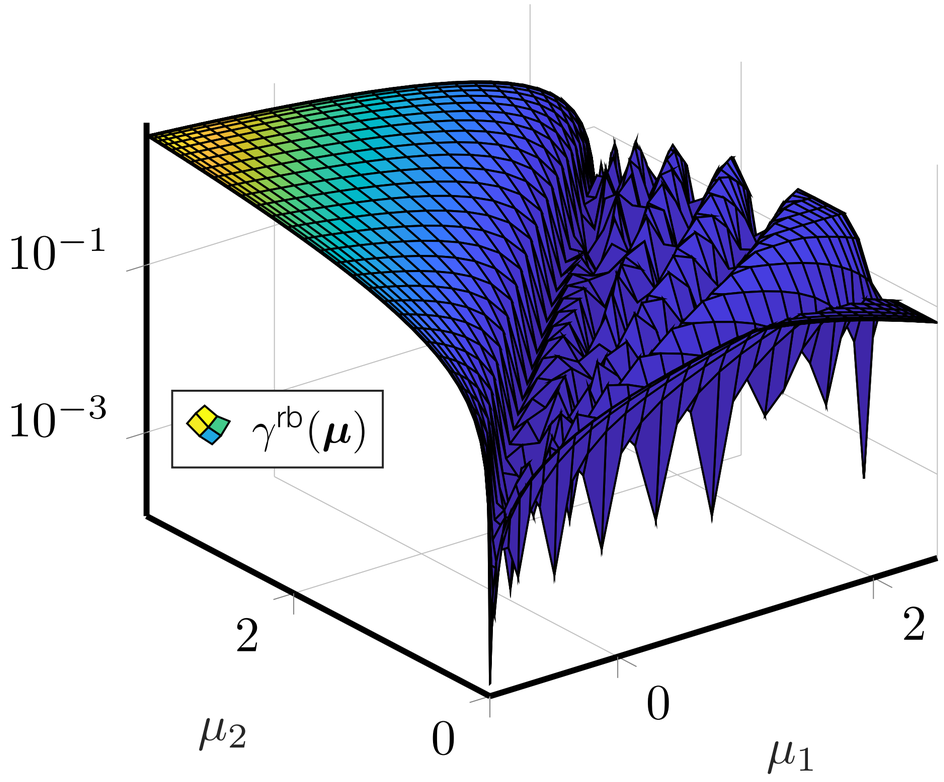

Spectral gap $\gamma^{\mathrm{rb}}(\boldsymbol{\mu})$

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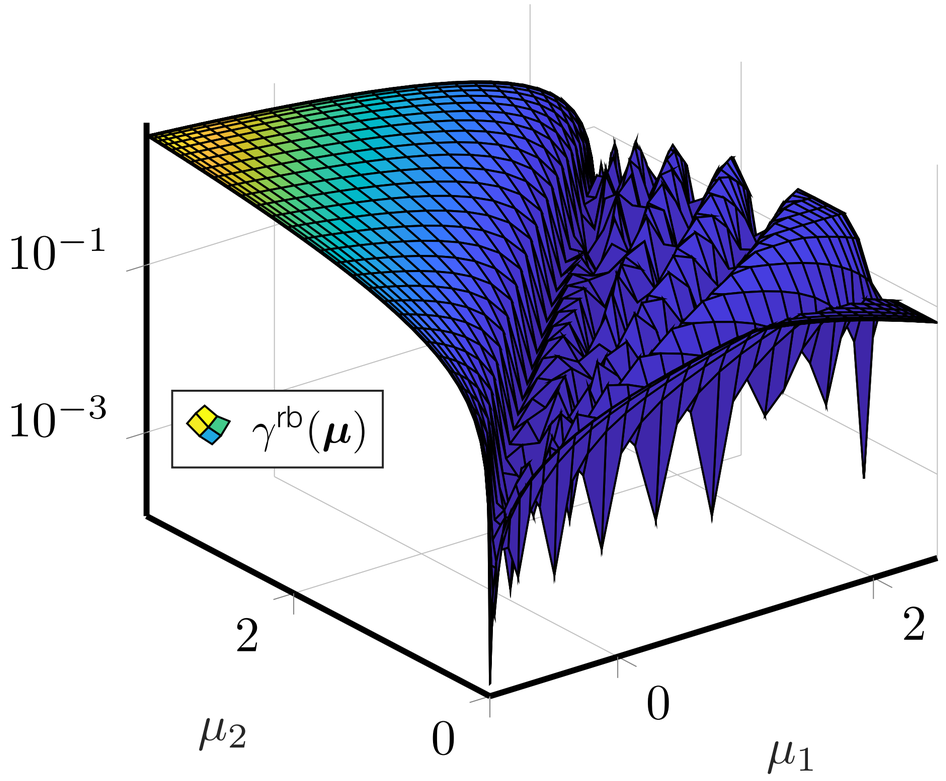

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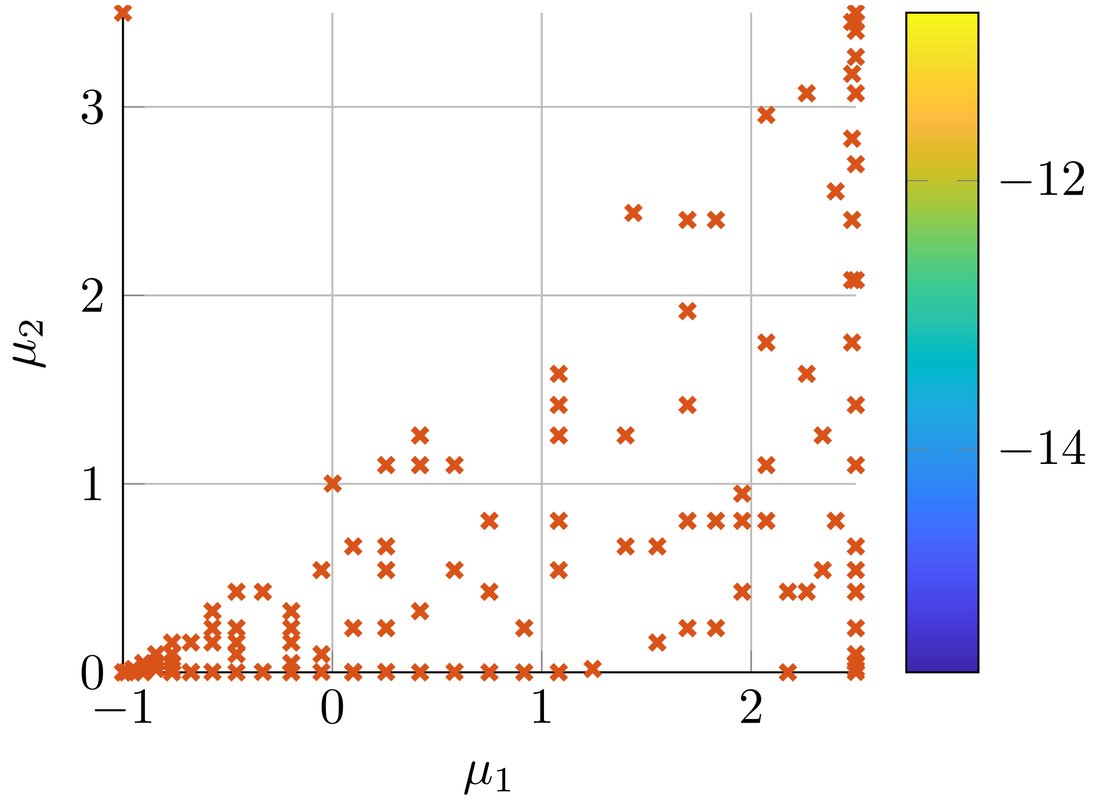

Spectral gap approximation error $\frac{|\gamma^{\text{rb}}(\boldsymbol{\mu}) - \gamma(\boldsymbol{\mu})|}{\gamma^{\text{rb}}(\boldsymbol{\mu})}$ in $\log_{10}$ scale

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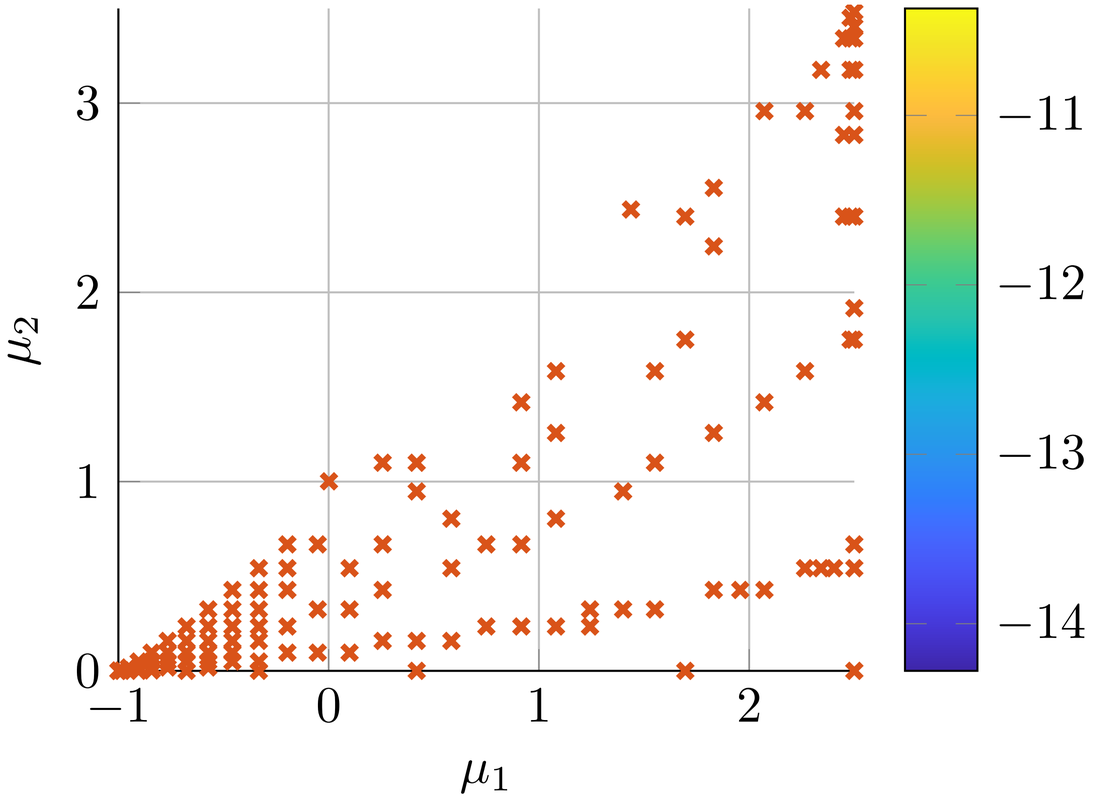

Approximation error $\|\mathbf{P}_1(\boldsymbol{\mu}) - \mathbf{P}_1^{\text{rb}}(\boldsymbol{\mu})\|$ over Ξ in $\log_{10}$ scale.
Red crosses are the selected interpolation points by the greedy.

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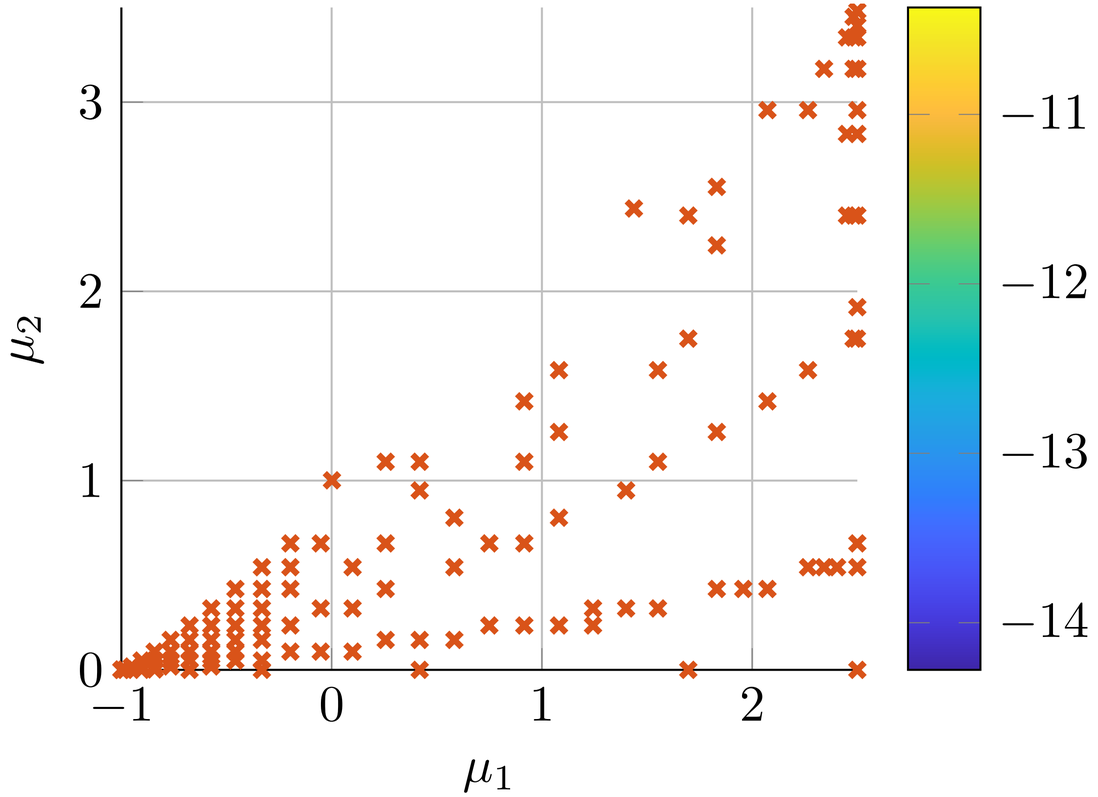

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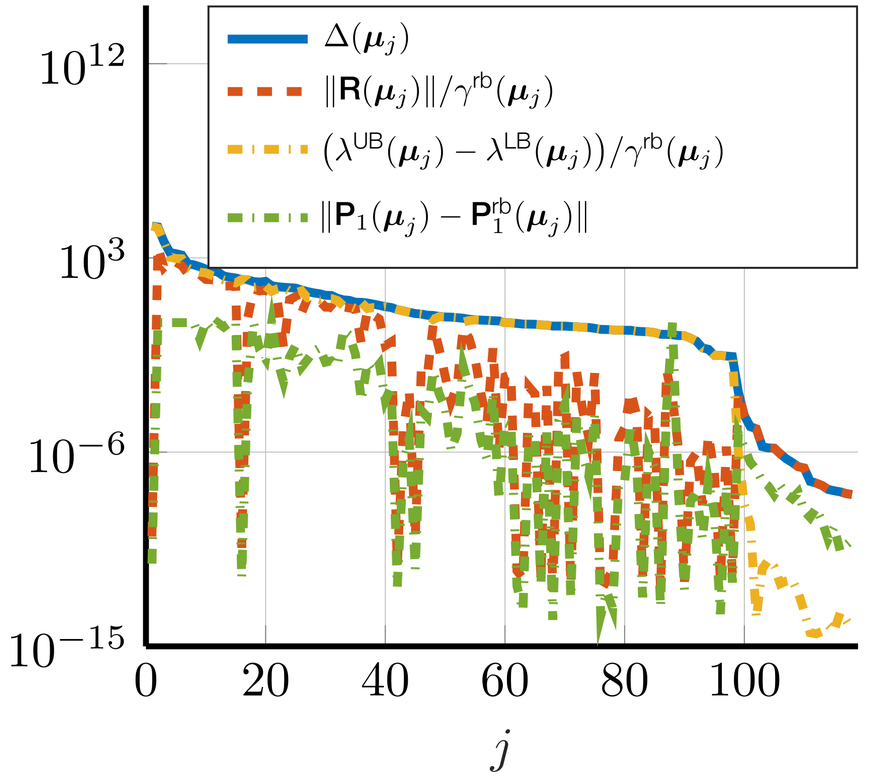

Decay of the estimator $\Delta(\boldsymbol{\mu})$ with its residual and eigenvalue error components along the iterations

Part 4

Local Taylor RBM / eigenvector continuation

(Local perspective)

Problem setting and idea

- Let $\mathbf{P}(\boldsymbol{\mu}_0)$ has rank $m := m_1 + \cdots + m_K$ and project onto the direct sum of eigenspaces $\mathcal{W}_1 \oplus \cdots \oplus \mathcal{W}_K$ asscociated to the (distinct) eigenvalues $\lambda_1 < \cdots < \lambda_K$ of $\mathbf{A}(\boldsymbol{\mu}_0)$.

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$\rightsquigarrow$ Efficient assembly possible?!

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Efficient assembly of Taylor RB-space

Main idea:

- Let $\mathbf{P}(\boldsymbol{\mu}_0) = \mathbf{U}_0\mathbf{U}_0^*$ with $\mathbf{U}_0 \in \mathbb{C}^{n\times m}$ ONB so that

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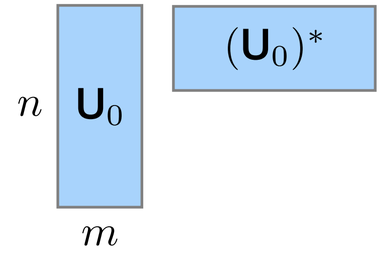

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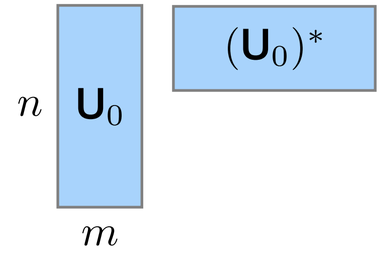

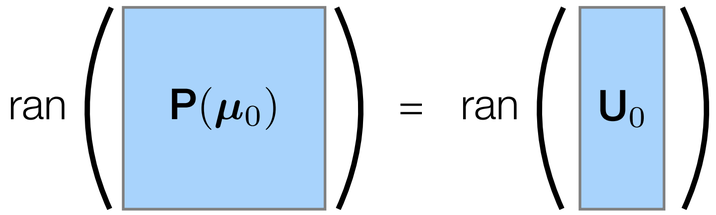

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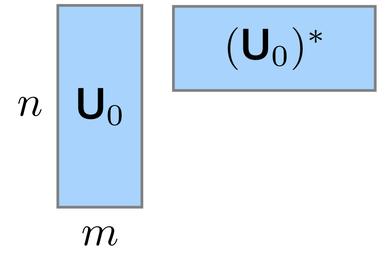

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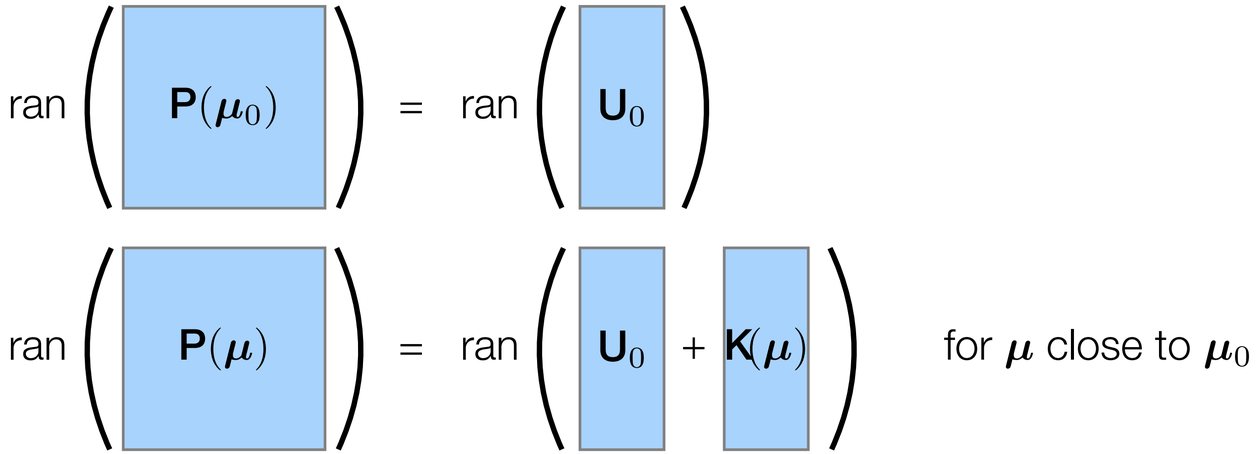

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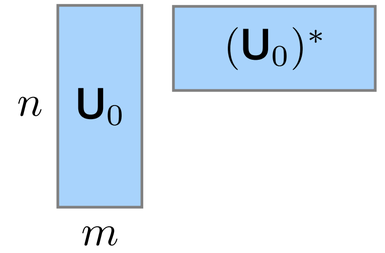

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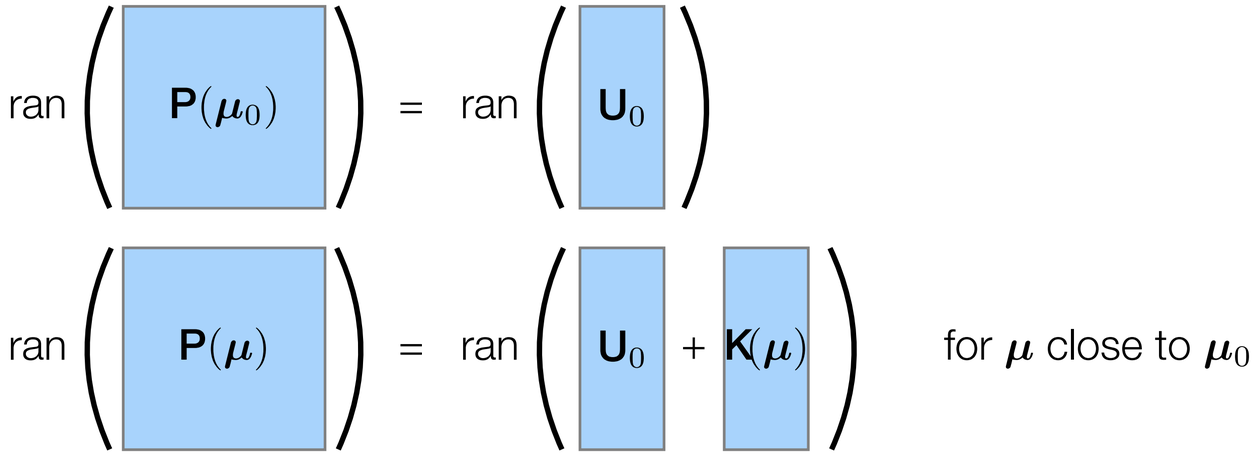
- Then $\big\{\operatorname{ran}(\mathbf{U}_0), \operatorname{ran}(\mathbf{K}^{(\boldsymbol{\beta})}) : |\boldsymbol{\beta}| \leq \ell\big\}$ spans the Taylor-RB space w.r.t. $\boldsymbol{\mu}_0$ of order ℓ.

$\rightsquigarrow$ It suffices to compute thin $\{\mathbf{K}^{(\boldsymbol{\beta})}\}_{|\boldsymbol{\beta}|\leq\ell}$, which can be efficiently done recursively.



Eigenspace approximation: Local error estimate for the Taylor-RBM

Theorem: (Bounding eigenspace approximation error by eigenspace projection error)

Let
- **A** be Hermitian.
- **P** be a projector with $m := \text{rank}(\mathbf{P})$ and $\mathbf{PA} = \mathbf{AP}$. (Exact eigen-projector)
- $\mathbf{\Pi}$ be an arbitrary projector with $\text{rank}(\mathbf{\Pi}) \geq m$. (Projector on RB-subspace)
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Suppose the eigenvalues of $\mathbf{PA}|_{\mathbf{P}}$ and $(\mathbf{P}^{\text{rb}})^{\perp}\mathbf{\Pi}\mathbf{A}|_{(\mathbf{P}^{\text{rb}})^{\perp}\mathbf{\Pi}}$ do not share the same eigenvalue, i.e.,

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Then, it holds that

$$\|\mathbf{P}^{\text{rb}} - \mathbf{P}\|^2 \;\leq\; \left(1 + \frac{\operatorname{Res}^2(\mathbf{A}, \mathbf{\Pi})}{\gamma^2}\right)\|\mathbf{\Pi}^{\perp}\mathbf{P}\|^2,$$

where $\operatorname{Res}^2(\mathbf{A}, \mathbf{\Pi}) := \|\mathbf{\Pi}\mathbf{A}\mathbf{\Pi}^{\perp}\|^2$ is the squared residual of $\operatorname{ran}\mathbf{\Pi}$ w.r.t. $\mathbf{A}$.

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Remark: Note similarity with Cea's lemma:

- Main driver for approximability $\|\mathbf{\Pi}^{\perp}\mathbf{P}\|$: How well is the exact subspace represented in the RB-subspace.
- Stability is provided by the gap γ and Res

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- $\mathbf{P}^{\text{rb}}$ a projector onto an m-dimensional subspace of $\operatorname{ran}\mathbf{\Pi}$. (RB-projector on eigenspace)

Suppose the eigenvalues of $\mathbf{PA}|_{\mathbf{P}}$ and $(\mathbf{P}^{\text{rb}})^{\perp}\mathbf{\Pi}\mathbf{A}|_{(\mathbf{P}^{\text{rb}})^{\perp}\mathbf{\Pi}}$ do not share the same eigenvalue, i.e.,

$$\gamma := \min\left\{|\lambda - \hat{\lambda}| : \lambda \in \sigma(\mathbf{PA}|_{\mathbf{P}}), \hat{\lambda} \in \sigma((\mathbf{P}^{\text{rb}})^{\perp}\mathbf{\Pi}\mathbf{A}|_{(\mathbf{P}^{\text{rb}})^{\perp}\mathbf{\Pi}})\right\} > 0.$$

Then, it holds that

$$\|\mathbf{P}^{\text{rb}} - \mathbf{P}\|^2 \;\leq\; \left(1 + \frac{\text{Res}^2(\mathbf{A}, \mathbf{\Pi})}{\gamma^2}\right)\|\mathbf{\Pi}^{\perp}\mathbf{P}\|^2,$$

where $\text{Res}^2(\mathbf{A}, \mathbf{\Pi}) := \|\mathbf{\Pi}\mathbf{A}\mathbf{\Pi}^{\perp}\|^2$ is the squared residual of $\operatorname{ran}\mathbf{\Pi}$ w.r.t. $\mathbf{A}$.

Remark: Note similarity with Cea's lemma:

- Main driver for approximability $\|\mathbf{\Pi}^{\perp}\mathbf{P}\|$: How well is the exact subspace represented in the RB-subspace.
- Stability is provided by the gap γ and Res

Remark: Similar results reported in literature (Ovtchinnikov, 2006).

Squaring effect from a projector viewpoint

Lemma: (Squaring effect of Ritz-value difference)

Let
- $\mathbf{A}$ be Hermitian.
- $\mathbf{P}$ be a projector with $\mathbf{PA} = \mathbf{AP}$. (Exact eigen-projector)
- $\mathbf{P}^{\mathrm{rb}}$ be a projector of the same rank as $\mathbf{P}$. (RB-projector on eigenspace)

Then, there holds that

$$\mathrm{Tr}\big(\mathbf{AP}\big) - \mathrm{Tr}\big(\mathbf{AP}^{\mathrm{rb}}\big) \;=\; \mathrm{Tr}\big(\mathbf{A}(\mathbf{I} - 2\mathbf{P})(\mathbf{P} - \mathbf{P}^{\mathrm{rb}})^2\big).$$

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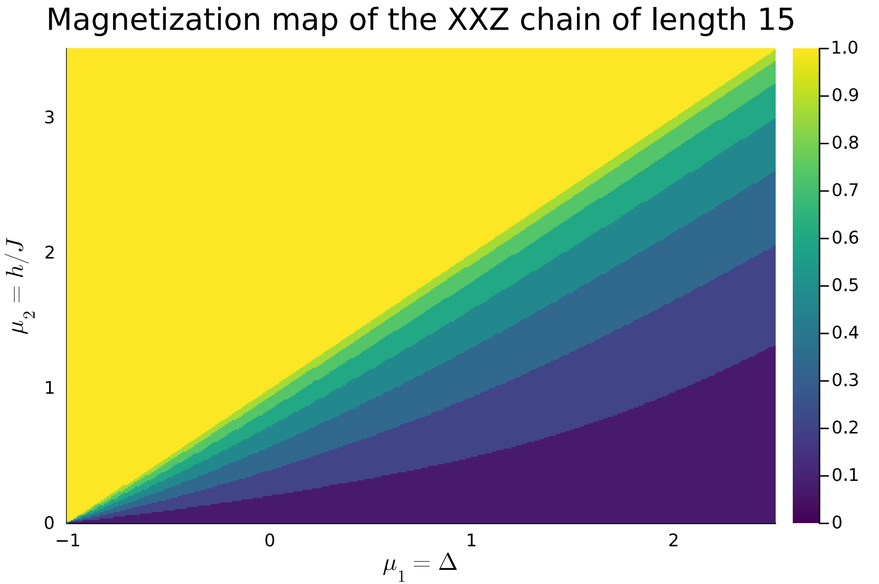
Remark:

- Related but not similar results found in (Sun, 1991) and (Garrigue/BS, 2024) involving far more advanced concepts.

Numerical results for the the XXZ model

- Recall $\boldsymbol{\mu} = (\mu_1, \mu_2) \in [-1, 2.5] \times [0, 3.5]$ and $\mathbf{A}(\boldsymbol{\mu}) = \mathbf{A}_1 + \mu_1 \mathbf{A}_2 - \mu_2 \mathbf{A}_3 \in \mathbb{C}^{2^L \times 2^L}$.
- $L = 15$, i.e., $n = 2^L = 33768$



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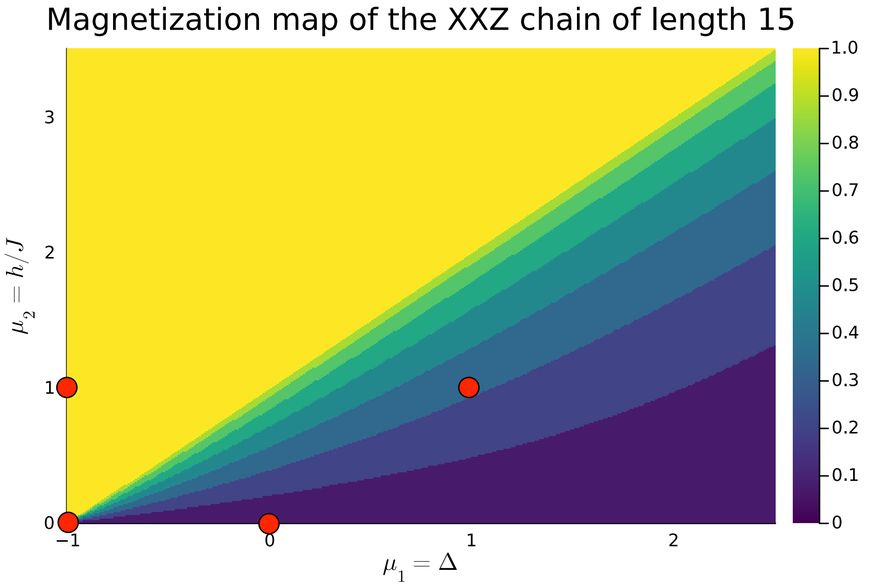
Very rich behaviors of the Taylor-RB spaces at different parameter points:

	$\boldsymbol{\mu}_0 = (-1, 0)^\top$		$\boldsymbol{\mu}_0 = (0, 0)^\top$		$\boldsymbol{\mu}_0 = (1, 1)^\top$		$\boldsymbol{\mu}_0 = (-1, 1)^\top$	
ℓ	r	UB	r	UB	r	UB	r	UB
0	16	16	2	2	1	1	1	1
1	48	48	4	6	3	3	1	3
2	96	96	6	12	6	6	1	6
3	160	160	8	20	8	10	1	10



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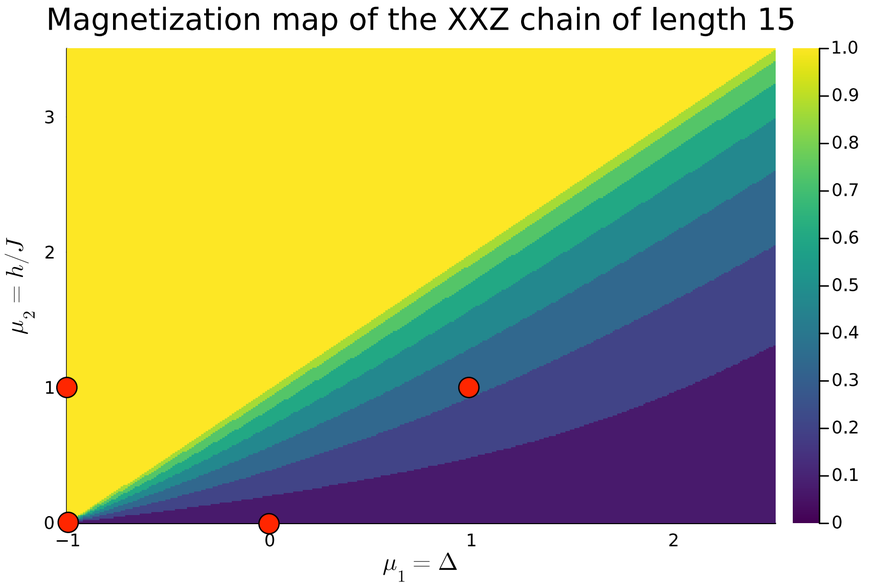
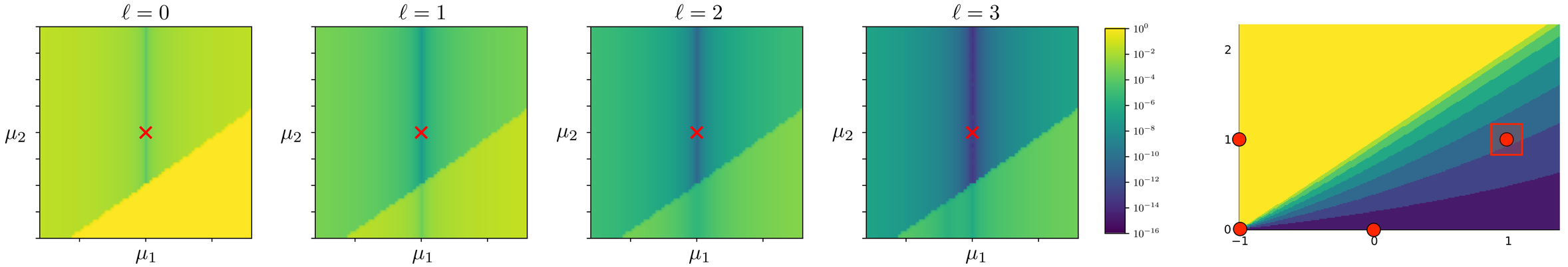
- Targeting the smallest eigenvalue (not counting multiplicities)
- RB-space dimension r depending on truncation order ℓ
- UB: theoretical upper bound dimension $m_1 \cdot \binom{\ell+2}{2}$, where $m_1 = r|_{\ell=0}$.



Numerical results for the the XXZ model around $\mu_0 = (1,1)$



Eigenprojector error $\|\mathbf{P}^{\mathrm{rb}}(\boldsymbol{\mu}) - \mathbf{P}(\boldsymbol{\mu})\|$ for $(\boldsymbol{\mu} - \boldsymbol{\mu}_0) \in [-0.08, 0.08]^2$

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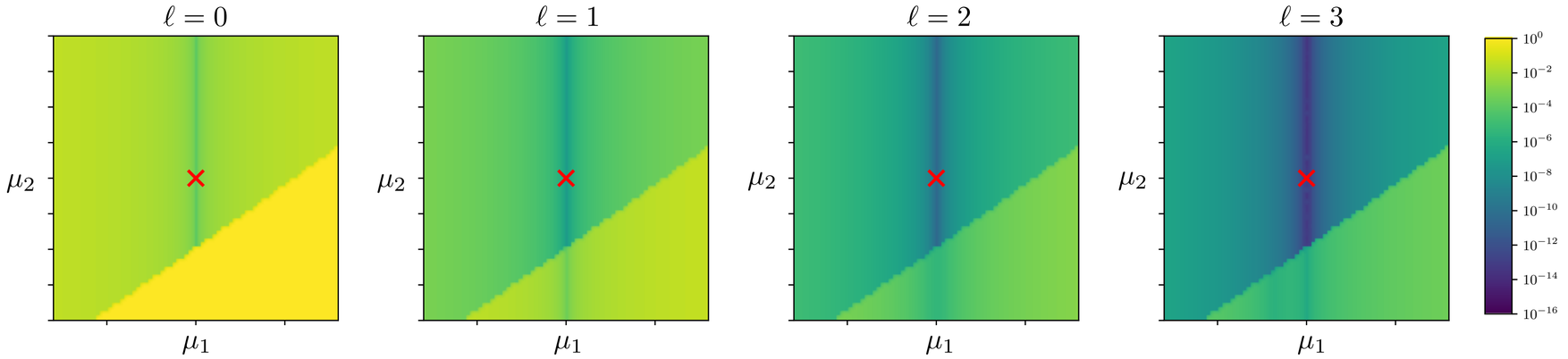

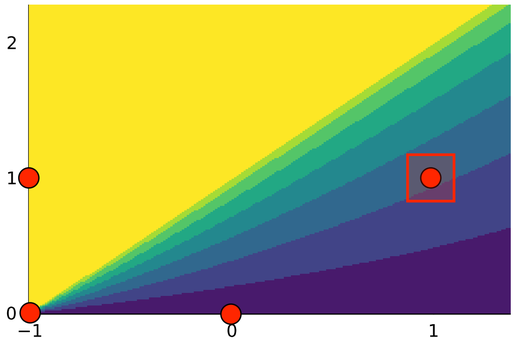

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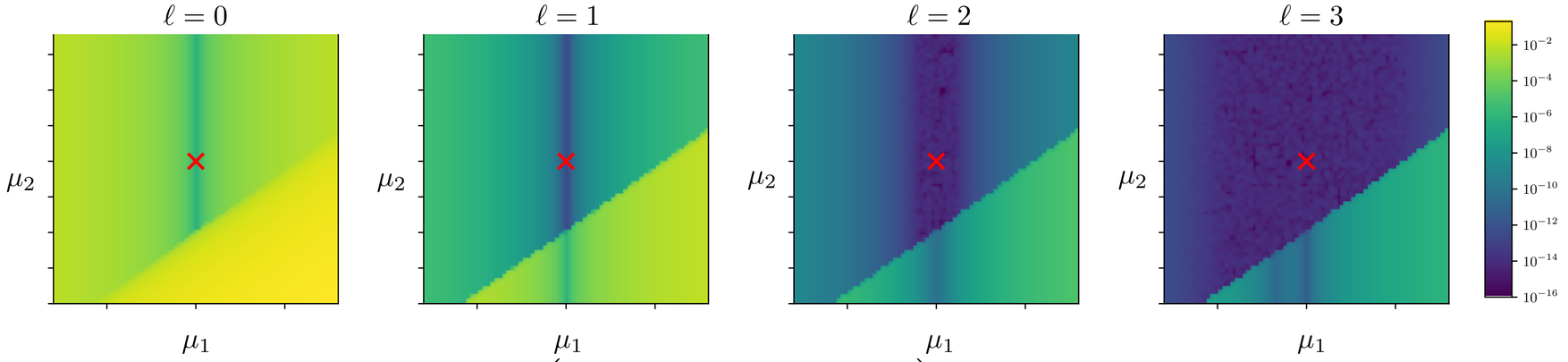

Ritz-value sum error $\text{Tr}\left(\mathbf{A}(\boldsymbol{\mu})\left(\mathbf{P}^{\text{rb}}(\boldsymbol{\mu}) - \mathbf{P}(\boldsymbol{\mu})\right)\right)$ for $(\boldsymbol{\mu} - \boldsymbol{\mu}_0) \in [-0.08, 0.08]^2$

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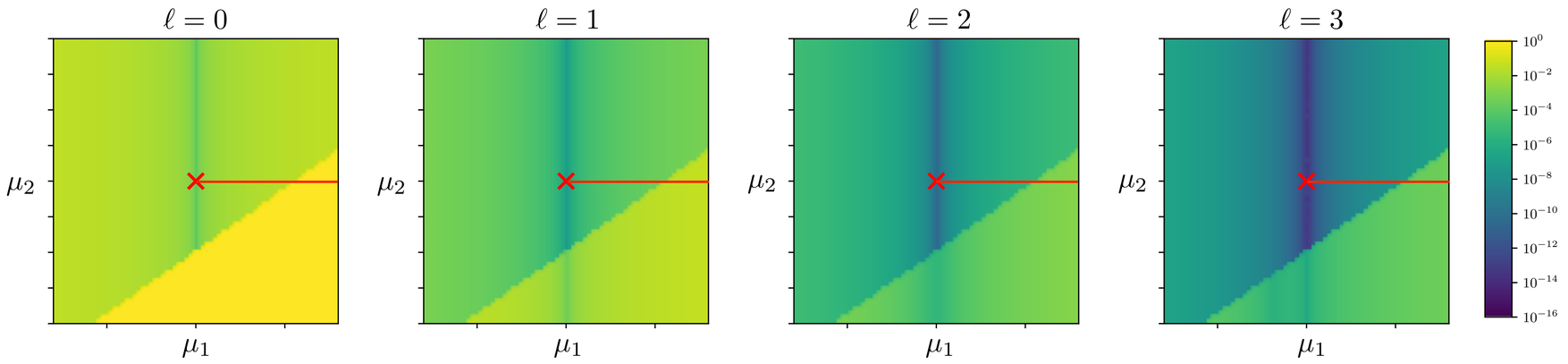

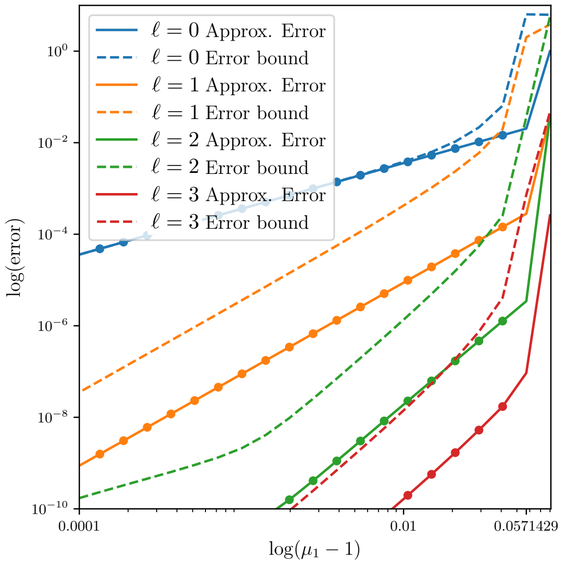

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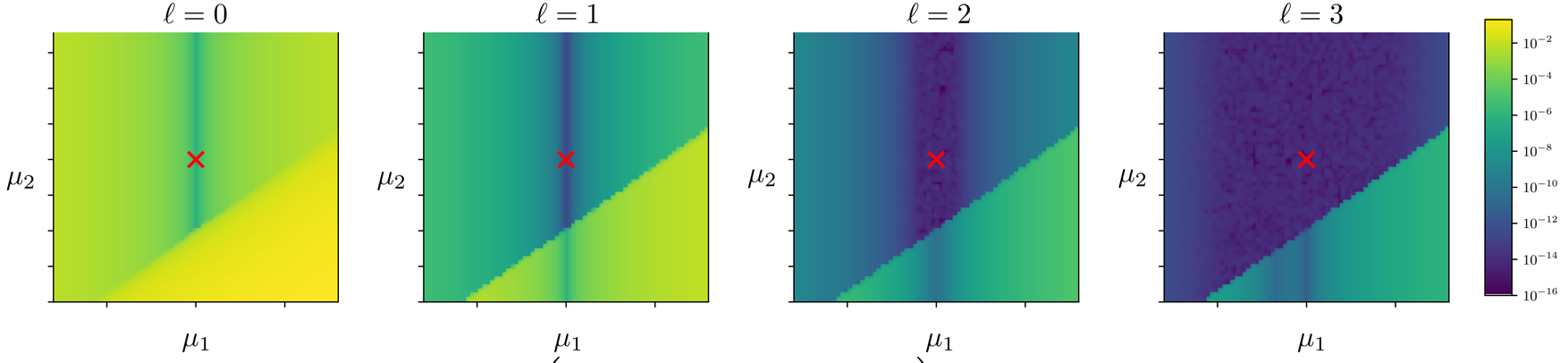

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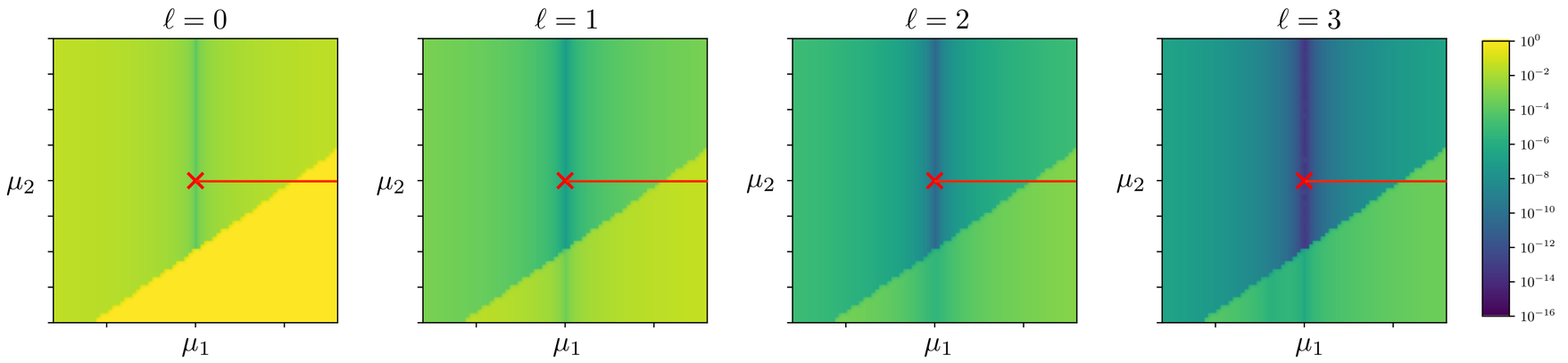

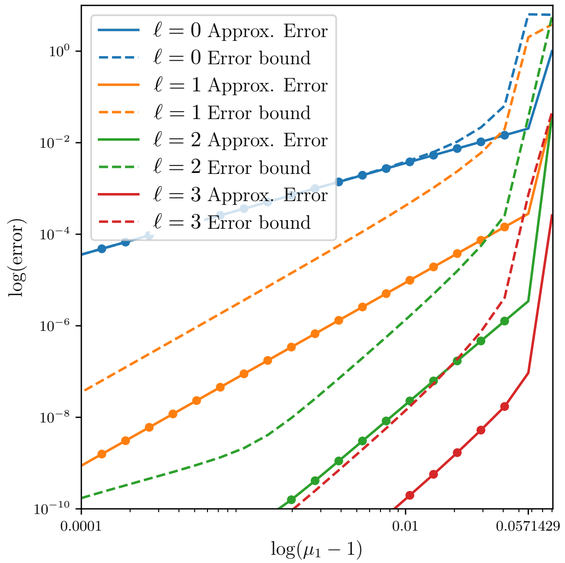

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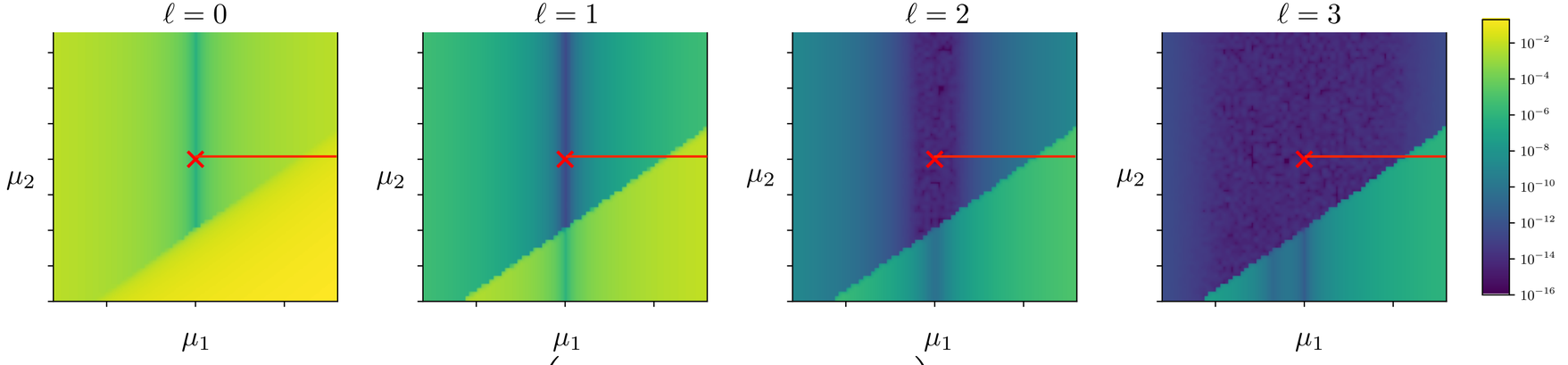

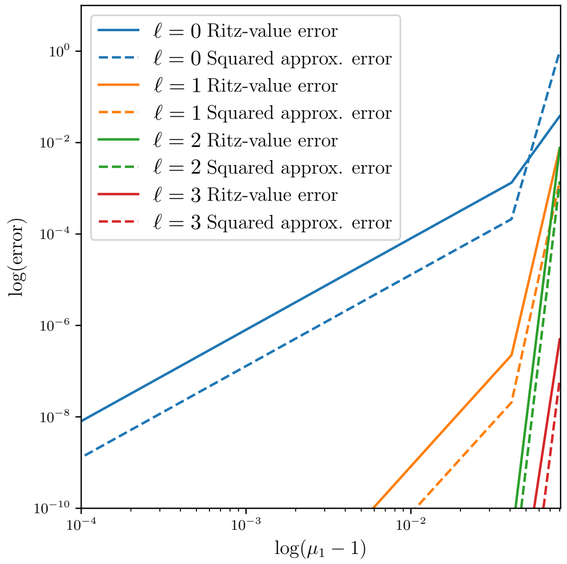

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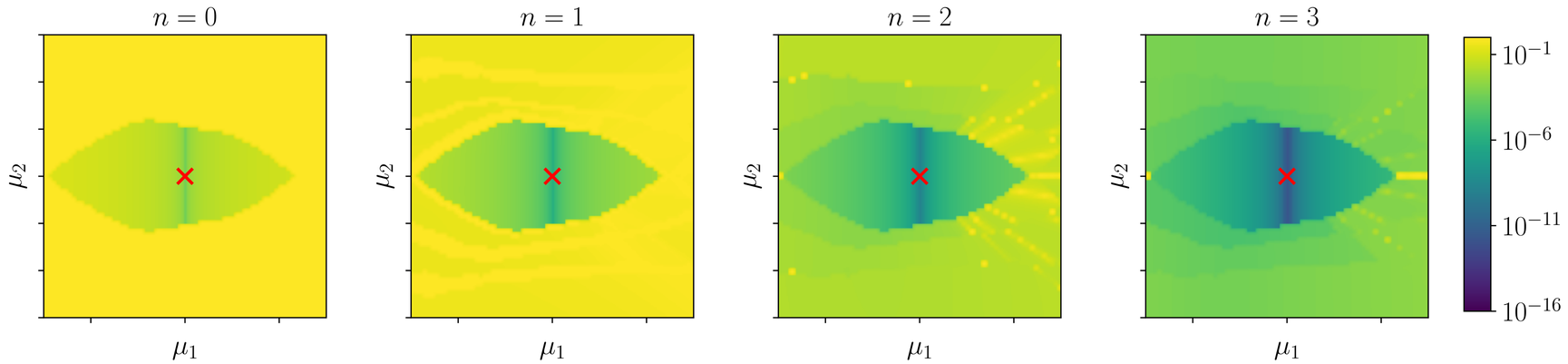
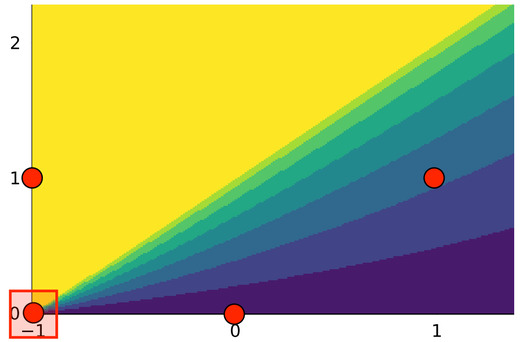
Taylor-RBM versus Perturbation Theory at $\mu_0 = (-1,0)$





RBM-Eigenprojector error $\|\mathbf{P}^{\text{rb}}(\boldsymbol{\mu}) - \mathbf{P}(\boldsymbol{\mu})\|$ for $(\boldsymbol{\mu} - \boldsymbol{\mu}_0) \in [-0.03, 0.03]^2$

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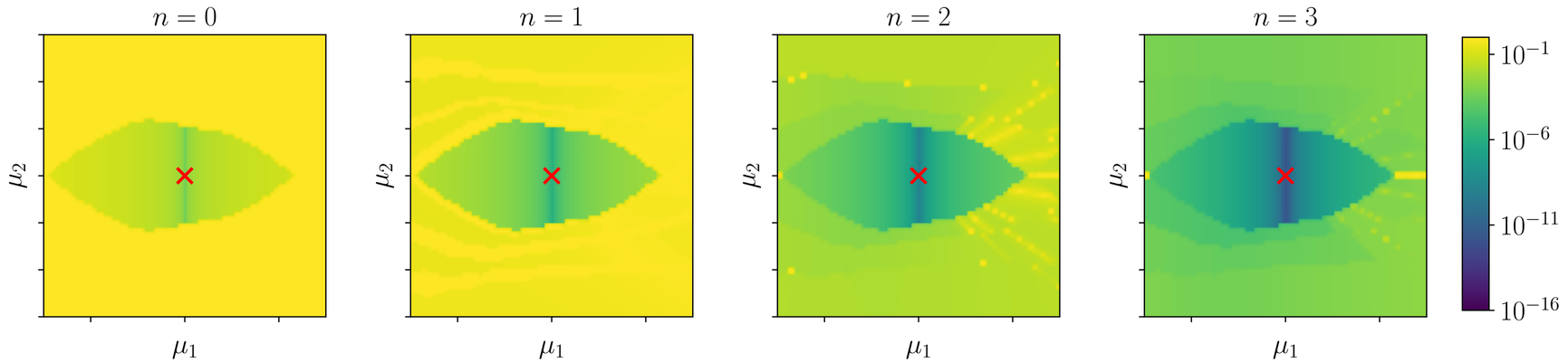

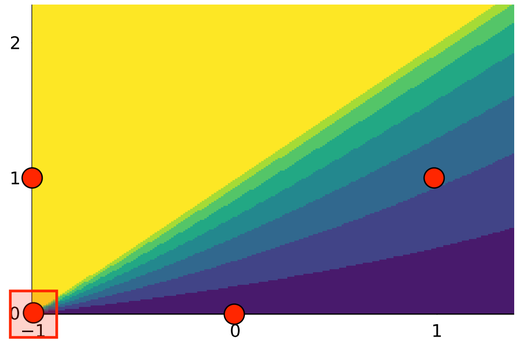

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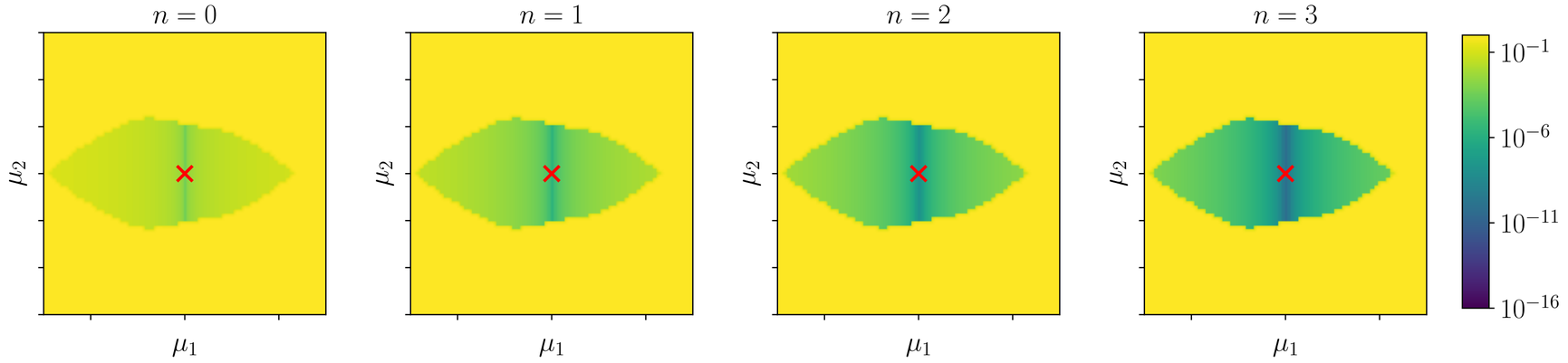

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Conclusions

- Eigenspaces resp. the projector onto them are the correct notion for eigenvalue problems
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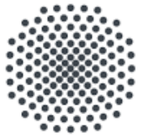

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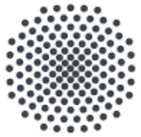

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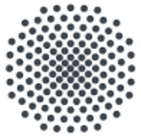

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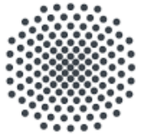

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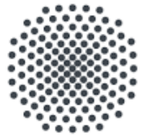

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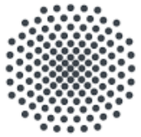

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