Quantum many-body systems: Numerical aspects

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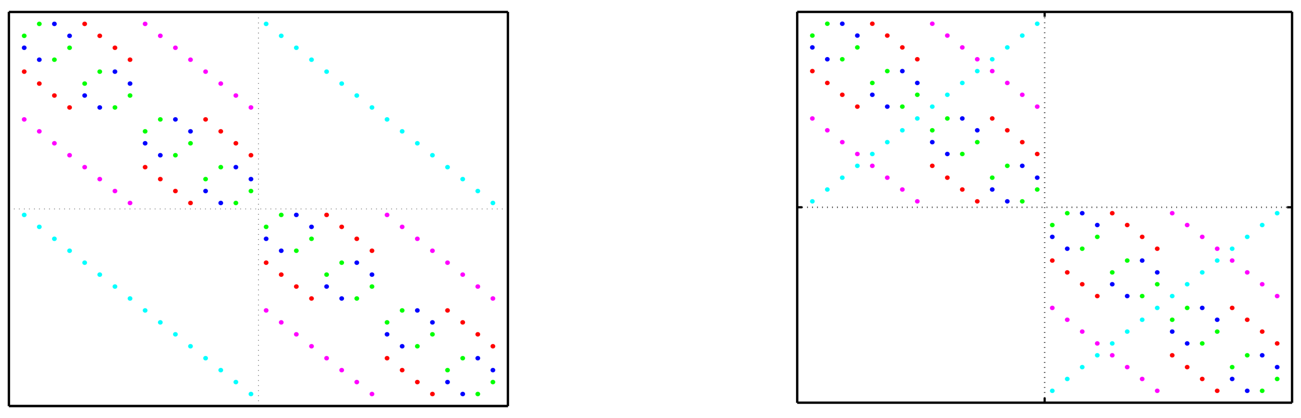
Computation of the matrix exponential

Motivation

The matrix exponential is the most-studied matrix function and plays a key role in quantum applications as it describes the physical time evolution. The matrix exponential is known as an intrinsically hard problem; methods for the computation, such as Padé approximation are often known to be "dubious". A polynomial ansatz based on Chebyshev polynomials leads to an efficient method which outruns the standard methods by a factor of 30% and only requires elementary matrix operations.

Description of the problem

- Compute $U = e^{-i\Delta t \mathbf{H}} = \sum_{k=0}^{\infty} (-i\Delta t)^k \frac{\mathbf{H}^k}{k!}$
- Make use of the structure of the matrix:



Numerical methods for the matrix exponential

- **Eigen decomposition:** For $\mathbf{H} = \mathbf{V}\mathrm{diag}(d_1, \dots, d_n)\mathbf{V}^\dagger$

$$e^{-i\Delta t \mathbf{H}} = \mathbf{V} \begin{pmatrix} e^{-i\Delta t d_1} & & \\ & \ddots & \\ & & e^{-i\Delta t d_n} \end{pmatrix} \mathbf{V}^\dagger$$

- **Padé approximation:**

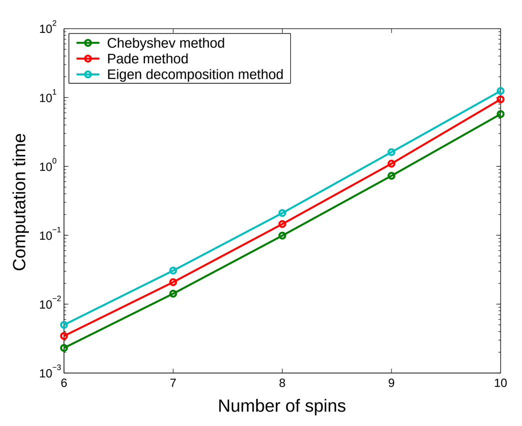
$$e^{-i\Delta t \mathbf{H}} = \lim_{m\to\infty} \left(\sum_{j=0}^{m} \frac{(2m-j)!}{(m-j)!} \frac{(i\Delta t \mathbf{H})^j}{j!} \right)^{-1} \left(\sum_{j=0}^{m} \frac{(2m-j)!}{(m-j)!} \frac{(-i\Delta t \mathbf{H})^j}{j!} \right)$$

- **New: Chebyshev series expansion:** For $\Delta t \|H\| < 2^p$

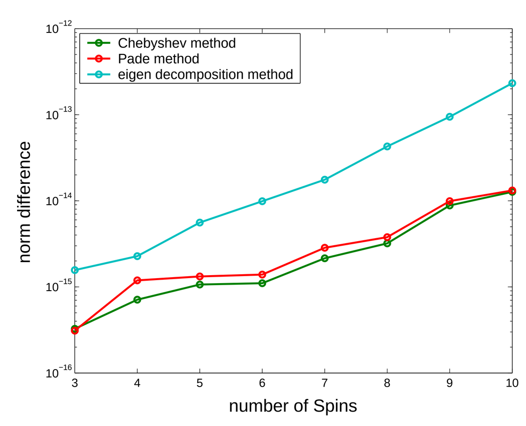
$$e^{-i\Delta t \mathbf{H}} = \left(J_0(i)\mathbf{I} + 2 \sum_{k=1}^{\infty} i^k J_k(-i) \cdot T_k \left(-i\Delta t \cdot \frac{\mathbf{H}}{2^p} \right) \right)^{2^p}$$

Comparison of the different methods

Computation time



Accuracy



Advantages of the Chebyshev series expansion

- Fast convergence of the expansion
- 30% faster than Padé or eigen decomposition methods
- Only elementary matrix operations required
- Efficient evaluation of matrix polynomials by reordering of the factors possible
- Only products of the form Dense * Sparse appear

References

[1] T. Gradl, A.K. Spörl, T. Huckle, S. J. Glaser, and T. Schulte-Herbrüggen: *Parallelising Matrix Operations on Clusters for an Optimal Control-Based Quantum Compiler*, Lecture Notes 4128 751 (2006)

[2] K. Waldherr: *Die Matrix-Exponentialabbildung: Eigenschaften und Algorithmen*, Diploma thesis (2007)

[3] T. Huckle, K. Waldherr: *Chebyshev methods for the matrix exponential* (in preparation)

[4] C. Moler, C. Van Loan: *Nineteen dubious ways to compute the exponential of a matrix*, SIAM Review, Vol. 20, No. 4. (1978)

[5] T. Huckle, T. Schulte-Herbrüggen, A. Spörl, K. Waldherr und S. Glaser: *Using the HLRB-II Cluster as a Quantum CISC-Compiler*, Springer, Berlin (2007)

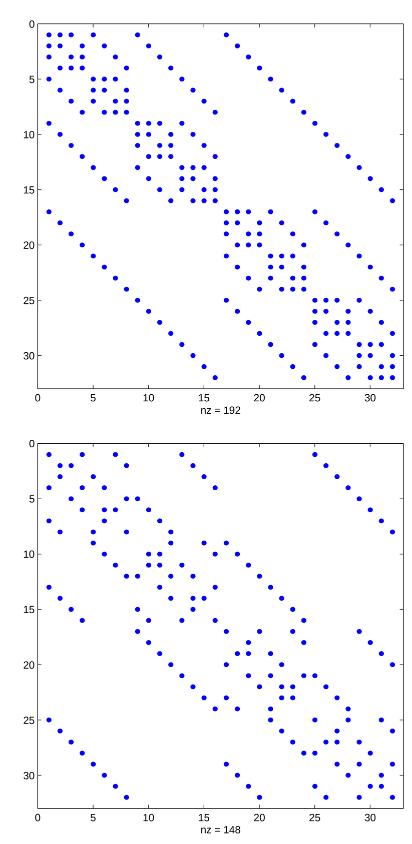
Current challenge: Computation of ground states

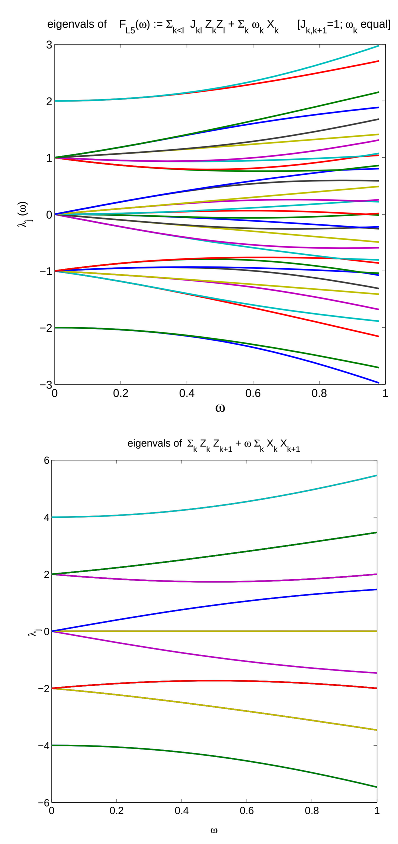
Description of the problem

- Find the smallest eigenvalue of Hamiltonian $\mathbf{H}$
- Principle of variations: $\min_{\|x\|=1} x^\dagger \mathbf{H} x$
- $\mathbf{H}$ is very large, sparse and hermitian
- Computation of the complete eigen decomposition too expensive
- Iterative methods required

Example of eigenvalue spreadings

Sparsity pattern — **Spreading of the eigenvalues**





Numerical methods (conventional)

- Rayleigh quotient iteration (Inverse vector iteration with shift)

$$(\mathbf{H} - \lambda_{k-1}\mathbf{I})x = q_{k-1} \to q_k := \frac{x}{\|x\|} \to \lambda_k := q_k^\dagger \mathbf{H} q_k$$

- Lanczos iteration

$$\mathbf{T}_m = \begin{pmatrix} \alpha_1 & \beta_2 & & \\ \beta_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_m \\ & & \beta_m & \alpha_m \end{pmatrix} = \mathbf{V}_m^\dagger \mathbf{H} \mathbf{V}_m$$

- Jacobi-Davidson (In combination with appropriate preconditioner)

$$\left(\mathbf{I} - u_j u_j^\dagger\right)(\mathbf{H} - \theta_j \mathbf{I})\left(\mathbf{I} - u_j u_j^\dagger\right) t_j = -(\mathbf{H} - \theta_j \mathbf{I})\, u_j$$

Physically motivated approaches

Make use of efficient representations based on

- Matrix product states (MPS)
- Density matrix renormalization group (DMRG)
- Protected entangled pair states (PEPS)
- Multi-Scale Entanglement Renormalisation Ansatz (MERA)

References

[1] I. Gohberg, P. Lancaster, L. Rodman: *Invariant Subspaces of Matrices with Applications*, SIAM Review, Vol. 30, No. 4 (1988)

[2] R. Horn, C. Johnson: *Matrix analysis*, Cambrigde University Press (1991)

Further collaborations

- Comparison of numerical and physical approaches for the eigenvalue problem in cooperation with Norbert Schuch and Uwe Sander
- Analysing variational techniques (e.g. Gradient flow algorithms) for the eigenvalue problem in cooperation with Thomas Schulte-Herbrüggen and Steffen Glaser
- Improving numerical algorithms in cooperation with Thomas Huckle