Intermediate report

Diagonalizing Spin Hamiltonians with the Lanczos Algorithm

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This report demonstrates the application of the *Lanczos algorithm* for approximating a hermitian matrix by a lower-dimensional tri-diagonal one. Given a tri-diagonal approximation on a low-dimensional subspace, standard methods for fully diagonalizing or computing matrix functions such as the exponential become feasible and usually give approximations for the corresponding objects of the original matrix. This method is especially efficient when applied to sparse matrices as typically arise in spin Hamiltonians. Here, we consider a system of many non-interacting two-level systems that couple equally to a harmonic oscillator—the Dicke model. The Dicke model features a so-called *super-radiant phase*, where there are states that spontaneously emit more photons than expected. This phenomenon is typically described by a transition amplitude of spontaneous emission scaling up to quadratically with the number of two-level systems. Here, we apply Lanczos algorithm in order to simulate dynamical properties of the Dicke model. In particular, the expectation value for the number of photons depending on time is compared for different initial states and different coupling strengths. Prior to its application to this problem, the algorithm itself is being discussed in detail and is implemented in the programming language `python`.

1. The Lanczos algorithm

The Lanczos method is a numerical method to approximate spectral properties of hermitian matrices. Given such a matrix $H \in \mathbb{C}^{N\times N}$, the method provides iteratively a d-dimensional approximation of H that is tri-diagonal after $d-1$ iterations and which can easily be diagonalized in $\mathcal{O}(N)$ time. The only necessary information specific to H is an oracle for the matrix-vector product $H \cdot v$. If the matrix is sparse, i.e. if the ratio of the number of non-zero and zero entries is constant in N and small, the matrix-vector product can be evaluated in $\mathcal{O}(N)$ time and storing such matrices takes $\mathcal{O}(N)$ memory [1]. Due to fast convergence of the method with respect to a growing number of iterations, approximating the lowest eigenvalue takes $\mathcal{O}(1)$ iterations and therefore $\mathcal{O}(N)$ memory and time [1]. In addition, eigenvectors and the matrix-exponential may also be approximated using this method.

The idea of the Lanczos algorithm is to find an orthonormal basis $\{v_i\}_{0\leq i\leq K}$ for the *Krylov space*

$$\mathcal{K}_H^{(K)}(v) = \operatorname{span}\big(\{v, Hv, H^2v, H^3v, \dots, H^Kv\}\big) \tag{1}$$

of order $K \leq N-1$ such that $(\langle v_i,\ Hv_j\rangle)_{0\leq i,j\leq K}$ is a tri-diagonal matrix. Then when extending this basis to a basis $(\tilde{v}_i)_{0\leq i\leq N}$ of C^N, the non-trivial part of the projection

$$P_{K+1}HP_{K+1} = H_{\mathcal{K}_H^{(K)}(v)} \oplus 0_{(\mathcal{K}_H^{(K)}(v))^\perp}, \quad P_n v \coloneqq \sum_{i=1}^{n} \langle v_i,\ v\rangle v_i \tag{2}$$

onto the first $K+1$ basis elements of $(\tilde{v}_i)_{0\leq i\leq N}$ is tri-diagonal. This projection is known as the *Galerkin approximation* of H and converges to H when $K \to N-1$.

The algorithm computes this orthonormal basis for $\mathcal{K}_H^{(K)}(v)$ is computed very similar to *Gram-Schmidt orthogonalization* but of an iteratively defined set of vectors. Set $v_0 = v/\|v\|$, for some arbitrary vector $v \in \mathbb{C}^N$. The next vector v_1 is the normalized Gram-Schmidt orthogonalization of Hv_0 with respect to v_0:

$$b_1 v_1 = \tilde{v}_1 = Hv_0 - \langle v_0,\ Hv_0\rangle v_0, \tag{3}$$

where we introduced the notation $b_n = \|\tilde{v}_n\|$. In general, v_{n+1} is defined as

$$b_{n+1}v_{n+1} = \tilde{v}_{n+1} = Hv_n - \sum_{i=0}^{n} \langle v_i,\ Hv_i\rangle v_i. \tag{4}$$

With this definition the desired property of $(\langle v_i,\ Hv_j\rangle)_{0\leq i,j\leq K}$ follows due to H being hermitian.

Lemma 1. *Let $H \in \mathbb{C}^{N\times N}$ for $N \in \mathbb{N}$ be a hermitian matrix, $v_0 = v/\|v\|$, and $K \leq N-1$. Define v_n recursively for $1 \leq n \leq K$ by*

$$b_{n+1}v_{n+1} = \tilde{v}_{n+1} = Hv_n - \sum_{i=0}^{n} \langle v_i,\ Hv_n\rangle v_i, \tag{5}$$

with $b_n = \|\tilde{v}_n\|$. Then

$$b_{n+1}v_{n+1} = Hv_n - a_n v_n - b_n v_{n-1} \tag{6}$$

for $n \leq K$ with $a_n = \langle v_n,\ Hv_n\rangle$, the set $(v_n)_{0\leq n\leq K}$ is a orthonormal basis for $\mathcal{K}_H^{(K)}(v)$, and its matrix representation

$$(\langle v_i,\ Hv_j\rangle)_{0\leq i,j\leq K} = \begin{pmatrix} a_0 & b_1 & & & & \\ b_1 & a_1 & b_2 & & 0 & \\ & b_2 & a_3 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & a_{K-1} & b_K \\ & & & & b_K & a_K \end{pmatrix} \tag{7}$$

is tri-diagonal.

The Lanczos algorithm consists of computing the basis $\{v_n\}$ according to eq. (6) iteratively. Per iteration one matrix-vector product needs to be computed, which is the computationally most expensive operation.

2. The Dicke Model

In this report we consider the application of Lanczos algorithm to the *Dicke model*. It models the collective interaction of a collection of $N \in \mathbb{N}$ identical two-level systems (e.g. spins) with a harmonic oscillator (e.g. a single mode of some bosonic field). It can be seen as a multi-particle generalization of the celebrated quantum Rabi-model [2] and was introduced by Dicke [3] in order to describe the spontaneous emission by a collection of molecules modelled as two-level systems. In his work, Dicke found that for certain states his model predicts unusual high emission rates—an effect known as *super-radiance*. This result was confirmed later by Hepp and Lieb [4], who proved the existence of a phase transition to a region where super-radiant states exist in the thermodynamic limit of $N \to \infty$.

The goal for this project is to investigate the super-radiance phenomenon numerically for large N. The full Dicke Hamiltonian on $(\mathbb{C}^2)^{\otimes N} \otimes L^2(\mathbb{R})$ is given by

$$H_{\mathrm{D}} = \frac{\Omega}{2} S_z \otimes \mathbb{1} + \omega\, \mathbb{1} \otimes \hat{n} + \lambda S_x \otimes \left(a + a^\dagger\right), \tag{8}$$

where Ω is the energy gap of the two-level systems, ω is the frequency of the bosonic mode. In the following we will only consider the fully resonant case $\Omega = \omega$. The creation and annihilation operators, $a^\dagger$ and a are defined as usual by acting on an orthonormal basis ϕ_n of $L^2(\mathbb{R})$ via $a^\dagger \phi_n = \sqrt{n+1}\phi_{n+1}$ and $a\phi_n = \sqrt{n}\phi_{n-1}$. The number operator with $\hat{n}\phi_n = n\phi_n$ is defined accordingly. The collective spin operators

$$S_a = \sum_{i=1}^{n} \sigma_a^{(i)}, \quad \sigma_a^{(i)} = \mathbb{1}^{\otimes i-1} \otimes \sigma_a \otimes \mathbb{1}^{\otimes N-i}, \tag{9}$$

with $a \in \{x, y, z\}$ act collectively with the corresponding single spin Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ and satisfy the commutation relations of the angular-momentum-algebra:

$$[S_k, S_l] = i2\epsilon_{k,l}{}^m S_m. \tag{10}$$

Thus they give a representation of $\mathfrak{so}(3)$ and there is a basis $|j, m\rangle$ of $(\mathbb{C}^2)^{\otimes N}$ with eigenvalues

$$(S_x^2 + S_y^2 + S_z^2)|j, m\rangle = j(j+1)|j, m\rangle \tag{11}$$

$$S_z|j, m\rangle = m|j, m\rangle \tag{12}$$

$$\langle j, m \mid j', m'\rangle = \delta_{j,j'}\delta_{m,m'} \tag{13}$$

with $j = 0, 1, \ldots, N/2$ and $m = -j, -j+1, \ldots, j-1, j$. In this context, these states are commonly known as *Dicke states*. The Hamiltonian H_D commutes with the total collective spin operator $S_x^2 + S_y^2 + S_z^2$ and thus its matrix elements offer a block diagonal structure with blocks for each value of j.

3. Description of the project

4. Roadmap

A. Proofs skipped in the main text

Proof of lemma 1. We proof eq. (6), orthogonality $\langle v_i,\ v_j\rangle = \delta_{i,j}, \forall i, j \leq n$, and $\langle v_i,\ Hv_j\rangle = \delta_{j,i-1}b_i + \delta_{i,j}a_i, \forall i, j \leq n$ by induction in n. Consider the case $n = 1$. Then

$$\langle v_0,\ v_1\rangle = \frac{1}{b_1}(\langle v_0,\ Hv_0\rangle - \langle v_0,\ Hv_0\rangle\langle v_0,\ v_0\rangle) = 0 \tag{14}$$

$$\langle v_i,\ v_i\rangle = \|v_i\| = \|\frac{\tilde{v}_i}{b_i}\| = \frac{1}{\|\tilde{v}_i\|}\|\tilde{v}_i\| = 1, \quad i = 1, 0 \tag{15}$$

$$\langle v_0,\ Hv_1\rangle = \langle H_v 0,\ v_1\rangle = \tag{16}$$

□

References

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[2] I. I. Rabi, 'Space Quantization in a Gyrating Magnetic Field', Physical Review **51**, 652–654 (1937).

[3] R. H. Dicke, 'Coherence in Spontaneous Radiation Processes', Physical Review **93**, 99–110 (1954).

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