Quantized-TT-Cayley Transform for Computing the Dynamics and the Spectrum of High-Dimensional Hamiltonians

Ivan Gavrilyuk · Boris Khoromskij

Abstract — In the present paper, we propose and analyse a class of tensor methods for the efficient numerical computation of the dynamics and spectrum of high-dimensional Hamiltonians. We focus on the complex-time evolution problems. We apply the quantized-TT (QTT) matrix product states type tensor approximation that allows to represent $N$-dimensional tensors generated by the grid representation of $d$-dimensional functions and operators with log-volume complexity, $O(d \log N)$, where $N$ is the univariate discretization parameter in space. Making use of the truncated Cayley transform method allows us to recursively separate the time and space variables and then introduce the efficient QTT representation of both the temporal and the spatial parts of the solution to the high-dimensional evolution equation. We prove the exponential convergence of the $m$-term time-space separation scheme and describe the efficient tensor-structured preconditioners for the arising system with multidimensional Hamiltonians. For the class of “analytic” and low QTT-rank input data, our method allows to compute the solution at a fixed point in time $t = T > 0$ with an asymptotic complexity of order $O(d \log N \ln^q \frac{1}{\varepsilon})$, where $\varepsilon > 0$ is the error bound and $q$ is a fixed small number. The time-and-space separation method via the QTT-Cayley-transform enables us to construct a global $m$-term separable $(x, t)$-representation of the solution on a very fine time-space grid with complexity of order $O(dm^4 \log N \log N)$, where $N$ is the number of sampling points in time. The latter allows efficient energy spectrum calculations by FFT (or QTT-FFT) of the autocorrelation function computed on a sufficiently long time interval $[0, T]$. Moreover, we show that the spectrum of the Hamiltonian can also be represented by the poles of the $t$-Laplace transform of a solution. In particular, the approach can be an option to compute the dynamics and the spectrum in the time-dependent molecular Schrödinger equation.

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1. Introduction

High dimensional problems whose solutions are functions of $d$ variables with large $d$ arise in many important applications, e.g., in electronic and molecular modeling, stochastic PDEs,
quantum computations, finance mathematics, etc. [4, 43, 38, 30, 13, 26, 18, 32]. Even with modern computers their solution presents a challenging problem due to the so-called “curse of dimensionality”. Roughly speaking, computational costs to find such a function grows exponentially as \( d \to \infty \) even in the case where the input data is analytical. If we restrict ourselves to the computation of high dimensional integrals, then Quasi-Monte Carlo algorithms can be efficient [39]. In some cases, the curse of dimensionality can be circumvented by using the so-called sparse grid spaces based on the tensor product of \( d \) one-dimensional multiscale functions. In particular, in the case of high dimensional parabolic problems, this approach was successfully used in [36, 14, 15]. In this way the additional complexity due to the in-stationarity can be avoided.

One of the new ideas to overcome the curse of dimensionality is to (approximately) separate the variables and reduce the solution process to \( d \) one-dimensional problems. One can say in the language of operator/matrix calculus: the solution operator of a discrete problem should be represented as a tensor product of the solution operators of one-dimensional problems or as a short sum of such tensor products. Some tensor-structured numerical methods based on this approach were proposed and analyzed in [8, 21, 17, 20, 26]. In order to separate the time variable in nonstationary problems, one can use the techniques based on the Cayley transform which were proposed for the first order (parabolic) differential equations with an operator coefficient in [2] and then developed for various other problems in [6, 9, 10]. Various tensor-product techniques for the separation of spatial Hamiltonians have been introduced recently [23, 27, 28, 19].

Let \( \mathbb{W} \) be a complex Hilbert space and \( \mathcal{H} \) be a self-adjoint positive definite operator with a domain \( D(\mathcal{H}) \) and a spectrum \( \Sigma(\mathcal{H}) \in [\lambda_0, \infty), \lambda_0 > 0 \). For ease of presentation, we further assume that the Hamiltonian operator \( \mathcal{H} \) has the complete eigenbasis, \( \mathbb{W} = \text{span}\{\phi_n\}_{n=0}^{\infty} \), with the real eigenvalues \( 0 < \lambda_0 \leq \lambda_1 \leq \ldots \). Let us consider the following initial value problem for the Schrödinger-type equation:

\[
\dot{\psi}(t) = i\mathcal{H}\psi(t) + f(t), \quad \psi(0) = \psi_0 \in D(\mathcal{H}) \subset \mathbb{W}.
\]

The solution operator of this problem is the operator exponential family \( S(t) = e^{i\mathcal{H}t} \), and the solution of the initial value problem is given by

\[
\psi(t) = e^{i\mathcal{H}t}\psi_0 + \int_0^t e^{i\mathcal{H}(t-\tau)}f(\tau)d\tau.
\]

In the following, we focus on the special case \( f = 0 \). The general case \( f = f(x, t) \) can be included in our scheme.

In quantum mechanics, an equation like (1.1) can represent a molecular or electronic Schrödinger equation in \( d \) dimensions that describes how the quantum state of a physical system evolves in time (see Example 2.1 below). In this case, the many particle Hamiltonian \( \mathcal{H} \) is given by the sum of a \( d \)-dimensional Laplacian and a certain interaction potential, say, potential energy surface [4, 31]. In general, in the multidimensional setting, the separable approximation of the operator \( S(t) \) in molecular dynamics is a challenging problem.

In the present paper, we apply the truncated Cayley transform combined with the quantics-TT (QTT) separable approximation of the evolving functions and the resolvent of the spatial Hamiltonian operator. This enables us to derive a low-parametric tensor structured representation of the solution \( \psi(x, t) \) globally in \( t \) over fixed interval \( 0 \leq t \leq T \). Hence, at this stage a time discretization does not appear.
Specifically, we propose to approximate \( S(t) \) by the simplified operator family \( S_m(t) \) obtained by the \( m \)-term truncated series expansion in the Laguerre \( t \)-polynomials. For the class of \( \mathcal{H} \)-analytic data \( \psi_0 \), we prove the super exponential convergence
\[
\|S(t) - S_m(t)\| \leq cm^{-1/12}e^{-c_1m^{1/3}},
\]
where \( m \in \mathbb{N} \) is a truncation parameter. This ensures the rank-\( m \) time-space separability for the class of initial data. What is more important, this approach creates a robust adaptive basis for the so-called proper orthogonal decomposition (POD) as a building block in the model reduction techniques.

In order to compute \( S_m(t) \), one should solve \( O(m) \) linear problems with the \( d \)-dimensional spatial Hamiltonian \( \mathcal{H} + iI \) discretized over the \( d \)-fold \( N \times N \times \ldots \times N \) tensor grid. Under certain separability assumptions on \( \mathcal{H} \), this will be reduced to the preconditioned iteration requiring the treatment of \( O(d) \) one-dimensional problems of size \( N \times N \). Thus, in order to achieve a prescribed accuracy \( \varepsilon > 0 \), an amount of computational work,
\[
O(dmW(N)\ln|\varepsilon|),
\]
is required, where \( W(N) \) is the computational cost to treat a single one-dimensional problem in the QTT format, and we arrive at a linear complexity scaling in \( d \).

The time-space separation method via QTT-Cayley-transform enables us to construct the global \((x, t)\)-representation of a solution on a very fine time-space grid of size \( N \times \ldots \times N \times N_t \) by simultaneous time-space low-parametric tensor representation, where \( N_t \) is the number of sampling points in time. Under certain regularity assumptions on \( \psi_0 \) we are able to prove the asymptotic complexity bound for the \((x, t)\) tensor representation, \( Cdm^4 \log N_t \log N \), ensuring the approximation error \( e^{-c_1m^{1/3}} \), where the constant \( C \) scales at most quadratically in the tensor rank of \( (\mathcal{H} + iI)^{-m} \psi_0 \) (cf. Lemma 3.1). The latter allows efficient energy spectrum calculations by the FFT transform of the autocorrelation function computed on a sufficiently long time interval \([0, T]\). Moreover, we show that the spectrum of the Hamiltonian can also be represented by the poles of the Laplace transform of the autocorrelation function. In particular, our approach can be an option to compute the dynamics and the spectrum of time-dependent molecular Schrödinger equations describing the molecular vibration [32].

The rest of the paper is organized as follows. In Section 2, we discuss the separation of time and space variables via the Cayley transform. An error analysis of the \( m \)-term truncated series representation for a certain class of initial data is presented. Section 3 discusses the spatial tensor approximation of the solution \( \psi(x, t) \) via the TT/QTT formats. In particular, we prove the \( \log - \log \) complexity tensor representation in time and space for the class of so-called \( \mathcal{H} \)-analytic initial data \( \psi_0 \) with a controlled tensor rank of \( (\mathcal{H} + iI)^{-m} \psi_0 \). The computation of the spectrum of the \( d \)-dimensional Hamiltonian is addressed in Section 4.

2. Separation of the time variable via the Cayley transform

2.1. Infinite series representation

The idea of separating the time and space variables is based on the well-known expansion [3, 40] for the generating (reproducing) function of the Laguerre polynomial of degree \( p \) with a parameter \( \alpha \),
\[
(1 - z)^{-\alpha - 1}e^{\frac{zt}{1 - t}} = \sum_{p=0}^{\infty} L_p^{(\alpha)}(t)z^p.
\]
After the formal substitution $z \rightarrow \lambda(\lambda + i)^{-1} := T(\lambda)$, and setting $\alpha = 0$, we obtain
\[ e^{i\lambda t} = i(\lambda + i)^{-1}\sum_{p=0}^{\infty} L_p^{(0)}(t)T^p(\lambda), \tag{2.1} \]
where $L_p^{(0)}(t) = L_p(t)$ is the Laguerre polynomial of degree $p$. Hence, on every initial vector $\psi_0 \in D(H)$, i.e.,
\[ \psi_0 = \sum_{k=0}^{\infty} a_k \phi_k, \text{ such that } \sum_{k=0}^{\infty} |a_k|^2 \lambda_k^2 < \infty, \tag{2.2} \]
the solution operator for the homogeneous equation (1.1) can be represented by
\[ e^{iHt} = i(H + iI)^{-1}\sum_{p=0}^{\infty} L_p^{(0)}(t)T^p(H), \tag{2.3} \]
where $T = T(H) = H(H + iI)^{-1}$ is the (non-classical) Cayley transform of the operator $H$. This representation can be used to separate the time variable $t$ from the spatial part of the solution. In fact, it can be seen that the solution of our initial value problem subject (2.2) can be represented as
\[ \psi(t) = \sum_{p=0}^{\infty} L_p^{(0)}(t)u_p \equiv i(H + iI)^{-1}\sum_{p=0}^{\infty} L_p^{(0)}(t)T^p(H)\psi_0, \tag{2.4} \]
where the elements $u_p$ can be found from the recursion
\[ u_0 = i(H + iI)^{-1}\psi_0, \]
\[ u_{p+1} = H(H + iI)^{-1}u_p, \quad p = 0, 1, \ldots \]
or, equivalently, as the solutions of the operator equations
\[ (H + iI)u_0 = i\psi_0, \]
\[ (H + iI)u_{p+1} = Hu_p, \quad p = 0, 1, \ldots . \tag{2.5} \]
Notice that the recursion $u_p = T^p u_0$, $p = 0, 1, 2, \ldots$ points to the opportunity of optimizing the set $\{u_p\}$ by analogy to the Krylov subspace method commonly used in numerical linear algebra.

**Lemma 2.1.** Let $\psi_0 \in D(H^\sigma)$ with some $\sigma > 3/2$, then representation (2.4) is well defined, and $\psi(t)$ solves equation (1.1).

**Proof.** First, we use estimates (2.12) that yield $\lim_{p \to \infty} L_p^{(0)}(t) = O(p^{-1/4})$ for each fixed $t$. Then the following bound $\|u_{p+1}\| \leq cp^{-\sigma/2}\|H^\sigma \psi_0\|$ (see (2.15) below) proves that (2.4) is well defined. Furthermore, from (2.5) it follows that
\[ u_p = iH(u_p - u_{p-1}), \quad p = 0, 1, 2, \ldots; \quad u_{-1} = iH^{-1}\psi_0. \tag{2.6} \]
Substituting this representation into (2.4) and using the summation by parts
\[ \sum_{n=1}^{N} u_n v_n = u_N v_N - u_0 v_0 + \sum_{n=0}^{N-1} u_n v_n, \]
we obtain
\[
\psi(t) = u_0 + i \mathcal{H} \sum_{p=1}^{\infty} L_p^{(0)}(t)(u_p - u_{p-1})
\]
\[
= u_0 - i \mathcal{H} u_0 L_0^{(0)}(t) - i \mathcal{H} \sum_{p=0}^{\infty} (L_{p+1}^{(0)}(t) - L_p^{(0)}(t)) u_p
\]
\[
= \psi_0 - i \mathcal{H} \sum_{p=0}^{\infty} (L_{p+1}^{(0)}(t) - L_p^{(0)}(t)) u_p.
\]
(2.7)

Now using the well-known relation [40, 3]
\[
\frac{d}{dt} \left[ L_{p+1}^{(0)}(t) - L_p^{(0)}(t) \right] = -L_p^{(0)}(t),
\]
combined with (2.7), we get
\[
\dot{\psi}(t) = i \mathcal{H} \sum_{p=0}^{\infty} L_p^{(0)}(t) u_p = i \mathcal{H} \psi(t),
\]
(2.8)
which completes the proof.

**Example 2.1.** (Harmonic oscillator). In quantum mechanics the operator \( \mathcal{H} \) in (1.1) can be a Hamiltonian of an oscillated particle of mass \( m \) subject to a potential \( V(x) \) given by
\[
V(x) = \frac{1}{2} m \omega^2 x^2,
\]
where \( \omega \) is the angular frequency of the oscillator. The operator \( \mathcal{H} \) in \( \mathbb{W} = L_2(-\infty, \infty) \) is defined by
\[
D(\mathcal{H}) = \{ u \in H^2(-\infty, \infty) : \psi(-\infty) = \psi(\infty) = 0 \},
\]
\[
\mathcal{H} \psi = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{m \omega^2}{2} x^2 \psi \quad \forall \ \psi \in D(\mathcal{H}).
\]
(2.9)
It is known that the normalized eigenfunctions (subject to \( \int_{-\infty}^{\infty} \phi^2(x) dx = 1 \)) are given by
\[
\phi_n(x) = C_n e^{-\xi^2/2} H_n(\xi), \quad n = 0, 1, 2, \ldots,
\]
(2.10)
where \( x = \alpha \xi, \alpha = \sqrt{\frac{\hbar}{m \omega}}, C_n = \frac{1}{\sqrt{n!}} \frac{1}{\sqrt{2^{n+1} \pi}} \) and \( H_n(\xi) \) are Hermite polynomials [41, 40].

These eigenfunctions correspond to the eigenvalues \( E_n = (n + 1/2) \hbar \omega \). In the \( d \)-dimensional setting, we have \( \mathbb{W} = L_2^d(-\infty, \infty) \) and the separable Hamiltonian \( \mathcal{H} = \sum_{k=1}^{d} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx_k^2} + \frac{m \omega^2}{2} x_k^2 \right) \).

The Harmonic oscillator plays the same role in quantum mechanics as Newton’s law in classical mechanics. For the 1D Harmonic oscillator, the operator \( S(t) \) is easily diagonalisable, while for \( d \geq 2 \) it is rank-1 separable, and thus the computational complexity of its tensor representation scales linearly in \( d \). Hence, it provides the basis for an efficient preconditioner (see Section 3.5).

**Remark 2.1.** In the case of a non-homogeneous right hand side, \( f = f(x, t) \), the Cayley transform representation (2.4) can be adapted if we are given the converging decomposition
\[
f(x, t) = \sum_{p=0}^{\infty} L_p^{(0)}(t) f_p(x), \quad f_p \in D(\mathcal{H}).
\]
2.2. Truncated series representation and error bounds

As a computable approximation to the exact solution, we consider the m-term truncated series representation

$$\psi_m(t) = \psi_0 - i\mathcal{H}\sum_{p=0}^{m}(L_{p+1}^{(0)}(t) - L_p^{(0)}(t))u_p.$$  \hspace{1cm} (2.11)

We start the error analysis by collecting some standard properties of the Laguerre polynomials (see, e.g., [40, p. 243, 248] and [3, vol. 2, Ch. 10.18]):

$$L_n^{(0)}(t) = \pi^{-1/2}e^{t/2}t^{-n/4}n^{n/2-1/4}\cos(2\sqrt{n}t - \beta\pi) + O(n^{-1/2}),$$

for \(t \in [a, b] \), \(0 < a < b < \infty \), \(\beta = (2\alpha + 1)/4, \alpha > -1; \)

$$|L_n^{(0)}(t)| \leq c_n a^{-n/2}t^{1/2}e^{t}(1 + n^{-1/2}t^{2}), \alpha + \frac{1}{2} \geq 0, t \geq 0;$$

$$|L_n^{(0)}| \leq c t^{1/2}, t \geq 0,$$

where \(c\) is a constant independent of \(n\) and \(0 < a < b\) are arbitrary fixed numbers. Moreover,

$$|L_n^{(0)}(t) - L_{n-1}^{(0)}(t)| = \frac{t}{n}|L_{n-1}^{(1)}(1)\leq ct^{1/4}e^{t/2}n^{-3/4}(1 + n^{-1/4}t^{5/4}),$$  \hspace{1cm} (2.13)

uniformly in \(t \in [0, T]\) holds (it follows from the representations \(nL_n^{(0)}(t) - (n + \alpha)L_{n-1}^{(0)}(t) = t\frac{d}{dt}L_n^{(0)}(t)\) and \(\frac{d}{dt}L_n^{(0)}(t) = -L_{n-1}^{(0)}(t)\)) (see [40], p.226).

We say that \(u = \sum_{k=0}^{\infty} a_k \phi_k \in D(\mathcal{H}^{\sigma})\) with \(\sigma > 0\), if \(\sum_{k=0}^{\infty} a_k^2 \lambda_k^{2\sigma} < \infty\). The following theorem characterizes the convergence rate of the truncated series representation.

**Theorem 2.1.** Let \(\psi_0 \in D(\mathcal{H}^{\sigma})\), with some \(\sigma > 3/2\), then for fixed \(T > 0\), the following estimate holds true:

$$\| \psi(t) - \psi_m(t) \| \leq cm^{-\sigma/2+1/4}\|\mathcal{H}^\sigma \psi_0\|, \hspace{1cm} t \in [0, T],$$  \hspace{1cm} (2.14)

with some constant \(c > 0\) independent of \(m\).

**Proof.** First, we observe that for \(\psi_0 = \sum_{k=0}^{\infty} a_k \phi_k\) there holds

$$u_{p+1} = i(\mathcal{H} + iI)^{-1}[\mathcal{H}(\mathcal{H} + iI)^{-1}]^{p}\psi_0 = \sum_{k=0}^{\infty} a_k \frac{i}{\lambda_k + i} \left(\frac{\lambda_k}{\lambda_k + i}\right)^p \phi_k$$

$$= \sum_{k=0}^{\infty} a_k \lambda_k^{-\sigma} \frac{i}{\lambda_k + i} \left(\frac{\lambda_k}{\lambda_k + i}\right)^p \lambda_k^\sigma \phi_k,$$

implying

$$\|u_{p+1}\| \leq \max_{\lambda \in [\lambda_0, \infty)} \left|\lambda^{-\sigma} \left(\frac{\lambda}{\lambda + i}\right)^p \right|\|\mathcal{H}^\sigma \psi_0\| \leq cp^{-\sigma/2}\|\mathcal{H}^\sigma \psi_0\|. \hspace{1cm} (2.15)$$
Now, taking into account (2.13), we obtain the estimates

\[ \|\psi(t) - \psi_m(t)\| \leq \sum_{p=m+1}^{\infty} |L_p^{(0)}(t) - L_p^{(0)}(t)|\|u_p\|, \]

\[ \leq c\|H^\sigma \psi_0\| t^{1/4}e^{t^{1/2}} \sum_{p=m+1}^{\infty} p^{-\sigma/2-3/4}, \]

which completes our proof. \( \square \)

Theorem 2.1 shows that an increase in \( \sigma \) in the \( H \)-regularity condition \( \psi_0 \in D(H^\sigma) \) will provide an arbitrary high polynomial rate of convergence in the truncated series representation.

In the following, we show that approximation (2.11) leads to an exponential convergence rate for the \( H \)-analytical input data to be introduced below.

**Definition 2.1.** A vector \( f = \sum_{k=0}^{\infty} a_k \phi_k \in D(H) \) is called analytical for \( H \) (\( H \)-analytic) if there is a constant \( C = C(f) > 0 \), such that

\[ \|H^n f\| = \sqrt{\sum_{k=0}^{\infty} |a_k|^2 \lambda_k^{2n}} \leq C^n n! \quad \text{for all} \quad n = 1, 2, 3, ... \]

**Remark 2.2.** For the \( H \)-analytic vector \( f \) the power series \( \sum_{n=0}^{\infty} s^n \|H^n f\| =: \|f\|_{s,H} \) possesses a positive convergence radius \( r > 0 \), i.e., \( \|f\|_{s,H} < \infty \) if \( 0 \leq s < r \).

**Proposition 2.2.** The finite sum \( u_0(x) = \sum_{k=0}^{m} \gamma_k \phi_k(x) \) gives rise to an \( H \)-analytic vector with \( C \approx \lambda_m \). In particular, in Example 2.1, we have \( C \approx \hbar \omega (m + 1/2) \).

**Proof.** The representation \( H^n u_0 = \sum_{k=0}^{m} \gamma_k \lambda_k^n \phi_k(x) \) leads to the following estimate:

\[ \|H^n u_0\| = \left( \int_{-\infty}^{\infty} \left| \sum_{k=0}^{m} \gamma_k \lambda_k^n \phi_k(x) \right|^2 dx \right)^{1/2} \]

\[ = \left( \sum_{k=0}^{m} |\gamma_k|^{2} \lambda_k^{2n} \right)^{1/2} \leq \lambda_m \left( \sum_{k=0}^{m} |\gamma_k|^2 \right)^{1/2} \leq \lambda_m \|u_0\|, \] (2.16)

that ensures the required bound. \( \square \)

The following theorem shows an exponential convergence of approximation (2.11) provided that the initial vector is \( H \)-analytic.

**Theorem 2.3.** Let \( \psi_0 \) be \( H \)-analytic and let \( r > 0 \) be the convergence radius of the series \( \sum_{k=0}^{\infty} s^n \|H^k \psi_0\| \). Then for every fixed \( s < r \) and fixed \( T > 0 \), approximation (2.11) converges exponentially in \( m \) implying the error estimate

\[ \|\psi(t) - \psi_m(t)\| \leq cm^{-1/12} e^{-c_1 \sqrt{m}} \|\psi_0\|_{s,H}, \quad t \in [0,T], \] (2.17)

where \( c, c_1 \) are positive constants independent of \( m \).
Proof. First, we note that estimates (2.12) yield for \( t \in [\varepsilon, T] \)
\[
\|\psi(t) - \psi_m(t)\| \leq ct^{-\frac{1}{4}} e^{\frac{t}{2}} \sum_{p=m+1}^{\infty} p^{-3/4} \|u_p\|,
\] (2.18)
where the iterand \( u_p \) allows the representation
\[
u_{p+1} = \sum_{k=0}^{\infty} a_k \left( \frac{\lambda_k}{\lambda_k + i} \right)^p \phi_k
\]
\[
= \sum_{k=0}^{\infty} a_k e^{-\lambda_k s} \left( \frac{\lambda_k}{\lambda_k + i} \right)^p \left( \sum_{n=0}^{\infty} \frac{\lambda_k^n}{n!} \right) \phi_k,
\]
\[
= \sum_{k=0}^{\infty} a_k e^{-\lambda_k s} \left( \frac{\lambda_k}{\lambda_k + i} \right)^p \sum_{n=0}^{\infty} \frac{s^n}{n!} H^n \phi_k,
\]
\[
= \sum_{n=0}^{\infty} \frac{s^n}{n!} H^n \left( \sum_{k=0}^{\infty} a_k \Phi_s(\lambda_k) \phi_k \right),
\] (2.19)
with
\[
\Phi_s(\lambda) := e^{-\lambda s} \left( \frac{\lambda}{\lambda + i} \right)^p.
\]
Let us notice that
\[
\|H^n \left( \sum_{k=0}^{\infty} a_k \Phi_s(\lambda_k) \phi_k \right)\| \leq \max_{\lambda \in [\lambda_0, \infty)} \left| \Phi_s(\lambda) \right| \|H^n \psi_0\|.
\]
Simple variational analysis indicates that the function \( \Phi_s(\lambda) \) takes its maximum at point \( \lambda_\ast \) that solves the equation \( s = \frac{p}{\lambda(1+\lambda^2)} \) implying that \( \lambda_\ast \approx \sqrt{p/s} \). The latter ensures the existence of positive constants \( c, c_1 \) independent of \( p \) (but \( c_1 \approx s^{2/3} \) depends on \( s \)) such that
\[
\max_{\lambda \in [\lambda_0, \infty)} \left| \Phi_s(\lambda) \right| = \max_{\lambda \in [\lambda_0, \infty)} e^{-\lambda s} \left( \frac{\lambda^2}{1 + \lambda^2} \right)^{p/2} \leq ce^{-c_1 \sqrt[3]{p}},
\]
thus implying
\[
\|u_{p+1}\| \leq ce^{-c_1 \sqrt[3]{p}} \|\psi_0\|_{s,H}.
\] (2.20)
Furthermore, we have
\[
\|\psi(t) - \psi_m(t)\| \leq ct^{\frac{1}{4}} e^{\frac{t}{2}} \|\psi_0\|_{s,H} \sum_{p=m+1}^{\infty} p^{-1/12} p^{-2/3} e^{-c_1 \sqrt[3]{p}}
\]
\[
\leq ct^{\frac{1}{4}} m^{-1/12} e^{-c_1 \sqrt[3]{p}} \|\psi_0\|_{s,H},
\] (2.21)
which completes our proof. \( \square \)

Theorem 2.3 shows that for \( H \)-analytic initial data the truncated Cayley transform ensures the time-space separation with \( \varepsilon \)-rank of order \( m = O(\log^3 1/\varepsilon) \).
Remark 2.3. We also observe that the set of vectors, \( U := [u_0, u_1, ..., u_N] \), creates a robust adaptive basis for the so-called proper orthogonal decomposition (POD) as a building block in the model reduction techniques for parabolic problems. In fact, the set \( U \) can be orthonormalised and further used for solving a problem with a slightly/smoothly modified operator or initial value (parameter dependent problems).

The Cayley transform method is also applicable to the real-time evolution problems.

Remark 2.4. The Cayley transform \( T(H) = H(H + I)^{-1} \) can be adapted to the real-time evolution equation

\[
\dot{\psi}(t) = -H\psi(t), \quad \psi(0) = \psi_0 \in D(H) \subset W, \tag{2.22}
\]

where \( H \) is a self-adjoint positive definite operator. The infinite series representation is then a simple modification of (2.4) but providing better approximation properties (cf. (2.19))

\[
u_{p+1} = \sum_{n=0}^{\infty} \frac{s^n}{n!} \mathcal{H}^n \left( \sum_{k=0}^{\infty} a_k \Phi_{1,s}(\lambda_k) \phi_k \right), \tag{2.23}
\]

with

\[
\Phi_{1,s}(\lambda) := e^{-\lambda s} \left( \frac{\lambda}{\lambda + 1} \right)^p.
\]

Contrary to the case of the function \( \Phi_s(\lambda) \) in (2.19) now \( \Phi_{1,s}(\lambda) \) takes its maximum at point \( \lambda_s \approx \sqrt{p} \), and we arrive at the estimate \( \|u_{p+1}\| \leq c e^{-c_1 \sqrt{p}} \|\psi_0\|_{s,H} \), implying (cf. (2.17))

\[
\|\psi(t) - \psi_m(t)\| \leq c t^\frac{1}{4} e^\frac{t}{4} m^{-1/4} e^{-c_1 \sqrt{m}} \|\psi_0\|_{s,H}. \tag{2.24}
\]

3. Spatial tensor approximation in the TT/QTT format

Theorems 2.4 and 2.8 prove the separability of time-space variables. In the following, based on these results, we propose a low-parametric tensor representation of the solution \( \psi(x,t) \) in time and space. In this way, we analyse the so-called TT/QTT tensor decomposition of multivariate spatial functions \( u_p(x) \) and the vector obtained by sampling the Laguerre polynomials \( L_p(t) \) on a uniform grid over \([0,T]\).

3.1. Tensor-product Hilbert spaces

Tensors of order \( d \) are defined as elements of the finite dimensional tensor-product Hilbert space (TPHS) \( \mathbb{W}_n \equiv \mathbb{W}_{n,d} \) of the \( d \)-fold, \( N_1 \times ... \times N_d \) real-valued arrays that can be represented componentwise:

\[
A = [A(i_1, ..., i_d)] \quad \text{with} \quad i_\ell \in I_\ell := \{1, ..., N_\ell\}, \quad \text{and} \quad n = (N_1, ..., N_d).
\]

For ease of presentation, we consider mainly equal-size tensors, i.e., \( I_\ell = \{1, ..., N\} \) (\( \ell = 1, ..., d \)). We call the elements of \( \mathbb{W}_n = \mathbb{R}^\mathcal{I} \) with \( \mathcal{I} = I_1 \times ... \times I_d \), \( N \times N \) tensors. The Euclidean scalar product, \( \langle \cdot, \cdot \rangle : \mathbb{W}_n \times \mathbb{W}_n \to \mathbb{R} \), is defined by

\[
\langle A, B \rangle := \sum_{i \in \mathcal{I}} A(i)B(i), \quad A, B \in \mathbb{W}_n.
\]
The storage demand for \(N\)-\(d\) tensors scales exponentially in \(d\), \(\dim \mathbb{W}_{n,d} = N^d\) ("curse of dimensionality").

In the case of complex-valued TPHS, \(\mathbb{W}_{n,d} = \mathbb{C}^n\), the description is similar.

### 3.2. Matrix product states tensor model by the QTT format

To get rid of the "curse of dimensionality", we apply modern tensor formats based on the dimension splitting via factorized representation, matrix product states (MPS) (see [44, 42, 37]). In the recent mathematical literature, such a construction appeared as the tensor train (TT) format [33, 35] corresponding to the case of so-called "open" boundary conditions in the matrix product state.

The rank-\(r\) TT format is defined in the spirit of the traditional Tucker model, but with considerably reduced "connectivity" constraints (see [35]). Its storage size scales linearly in both \(d\) and \(N\). The generalisation of the TT-format to the case of connected index chains corresponding to the case of periodic boundary conditions in MPS, can be described by the following definition (cf. [24]).

**Definition 3.1.** (Tensor chain/train formats). Given the rank parameter \(r = (r_0, ..., r_d)\) and the respective index sets \(J_\ell = \{1, ..., r_\ell\} (\ell = 0, 1, ..., d)\), with the periodicity constraints \(J_0 = J_d\). The rank-\(r\) tensor chain (TC) format contains all elements \(\mathbf{V} \in \mathbb{W}_n = \mathbb{R}^2\) which can be represented as a chain of contracted products of 3-tensors over the \(d\)-fold product index set \(\mathcal{J} := \times_{\ell=1}^d J_\ell:\)

\[
\mathbf{V} = \{\times_{\ell=1}^d \mathbf{G}(\ell)\} \quad \text{with 3-tensors} \quad \mathbf{G}(\ell) \in \mathbb{R}^{d_{\ell-1} \times d_{\ell} \times d_{\ell+1}}.
\]

Denote this set of tensors by \(\mathbf{TC}[r,d] \subset \mathbb{W}_n\). In the case \(J_0 = J_d = \{1\}\) (disconnected chain), the TC-format coincides with the corresponding definition of the TT format, implying \(\mathbf{TT}[r,d] \subset \mathbf{TC}[r,d]\).

The beneficial properties of the TC/TT formats are due to the linear storage complexity in \(d\), \(dr^2N\), with \(r = \max_{\ell} r_\ell\). Moreover, the approximation of the canonical or TT-tensor by using the low TT-rank elements (rank truncation) can be fulfilled by the SVD/QR decompositions [33] applied to \(\ell\)-mode TT-unfolding matrices (known in the MPS literature as the Schmidt decomposition (cf. [42])).

In the rest of this subsection, we describe the quantics transform (linear isometry) of \(N\)-\(d\) tensors to higher dimensional tensor space with \(D = d \log N\). Given \(q = 2, 3, ...,\) we suppose that \(N = q^L\) with some \(L = 1, 2, ...\). The following definition introduces the folding of \(N\)-\(d\) tensors into elements of auxiliary higher-dimensional tensor space with dimension \(D = d \log_q N > d\).

**Definition 3.2.** ([24]) Introduce the \(q\)-adic folding transform of degree \(2 \leq p \leq L\),

\[
\mathcal{F}_{q,d,p} : \mathbb{W}_{n,d} \to \mathbb{W}_{m_{dp}}, \quad \mathbf{m} = (\mathbf{m}_1, ..., \mathbf{m}_d), \quad \mathbf{m}_\ell = (m_{\ell,1}, ..., m_{\ell,p}),
\]

with \(m_{\ell,1} = q^{L-p+1}\), and \(m_{\ell,\nu} = q\) for \(\nu = 2, ..., p\), \((\ell = 1, ..., d)\), that reshapes the initial \(n\)-tensor in \(\mathbb{W}_{n,d}\) to the element in quantics space \(\mathbb{W}_{m_{dp}}\) as follows:

(A) For \(d = 1\) a vector \(\mathbf{X}_{(N,1)} = [X(i)]_{i \in I} \in \mathbb{W}_{N,1}\), is reshaped to the element of \(\mathbb{W}_{q^{L-p+1},p}\) by

\[
\mathcal{F}_{q,1,p} : \mathbf{X}_{(N,1)} \to \mathbf{Y}(\mathbf{m},p) = [Y(j)] := [X(i)], \quad j = \{j_1, ..., j_p\},
\]

with \(j_1 \in \{1, ..., q^{L-p+1}\}\), and \(j_\nu \in \{1, ..., q\}\) for \(\nu = 2, ..., p\). For fixed \(i\), \(j_\nu = j_\nu(i)\) is defined by \(j_\nu = 1 + C\) \(L-p-1+\nu\), \((\nu = 1, ..., p)\), where the \(C\) \(L-p-1+\nu\) are found from the partial radix-\(q\)
representation of \( i - 1 \),
\[
i - 1 = C_{L-p} + C_{L-p+1} q^{L-p+1} + \cdots + C_{L-1} q^{L-1}.
\]

For the maximal degree folding corresponding to \( p = L \), the multi-index \( i - 1 \) is a \( q \)-adic representation of \( i - 1 \) for \( i \in I \), in the radix-\( q \) system, such that \( j_{\nu} \) takes values in \( \{1, \ldots, q\} \).

(B) For \( d > 1 \), the construction is similar.

For the sake of higher compressibility, the maximal degree folding, \( F_{q,d,L} \), can be applied. The high-dimensional image \( F_{q,d,L} A \in \mathbb{W}_{q,dL} \) is called the quantics transform of \( A \in \mathbb{W}_{N,d} \). An element in \( \mathbb{W}_{q,dL} \) can be represented/approximated in the TT format called the quantics-TT or quantized-TT (QTT) representation of the tensor \( A \in \mathbb{W}_{N,d} \).

The computational efficiency of the QTT format is substantiated by the basic approximation properties (see [24]): the class of discrete exponential (resp. trigonometric) \( N \)-vectors allows the rank-1 (resp. rank-2) \( q \)-folding representation, reducing the storage complexity \( O(N) \) to the logarithmic scale \( O(q \log_q N) \). Moreover, it can be shown [24] that Chebyshev polynomials sampled over the Chebyshev grid can be represented by rank-2 quantics tensor, while the general polynomial vector sampled over a uniform grid has the rank-(\( m + 1 \)) QTT representation for any polynomial of degree \( m \) (see also [12] for related results). Combined with the well-known sinc-approximation results, this ensures high compressibility features of the QTT representation applied to a large class of function related tensors. Moreover, we are able to compute the fast QTT-FFT and QTT-convolution transforms of large \( N \)-vectors, as well as to represent the classes of multidimensional operators (Hamiltonians) effectively (see [25] for more detailed discussion).

We summarize that, on the one hand, the QTT representation can reduce the storage complexity of spatial vectors \( u_p \) to the log-volume size \( O(d \log N) \ll N^d \), and, on the other hand, this enables us to construct the global \((x,t)\)-representation of \( \psi(x,t) \) on very fine time/space grids with a complexity of order \( O(dm \log N_t \log N) \), where \( N_t \) is the number of sampling points in time. The latter allows efficient energy spectrum calculations by the FFT (or QTT-FFT) transform of the autocorrelation function (see Section 4.1) computed by our method on a sufficiently long time interval \([0, T]\). In the case of long-time integration, the restarted version of the Cayley-QTT representation can be applied on smaller subintervals of the initial time interval \([0, T]\).

3.3. Tensor Truncation

The representation of tensors in low separation rank formats is the key point in the design of fast tensor-structured numerical methods in higher dimension. In fact, it allows implementing the basic linear and bilinear algebraic operations on tensors such as addition, scalar, Hadamard and convolution products with linear complexity in the univariate tensor size (see [22, 25, 19, 20, 5]).

These tensor operations (excepting the scalar product) increase the separation rank of the resultant tensor. Hence, the complexity control requires further “projection” of such intermediate results onto the set of tensors with a smaller rank parameter (rank truncation).

To perform computation over a nonlinear set of rank-structured tensors \( S \) (say, in the truncated iteration), we need to perform a “projection” of the current iterand onto that set \( S \). The latter may represent the Tucker, canonical, TT or QTT formats. This action is fulfilled by implementing the tensor truncation operator \( T_S : \mathbb{W}_{n,d} \to S \) defined by

\[
A_0 \in \mathbb{W}_{n,d} : \quad T_S A_0 = \text{argmin}_{T \in S} \| A_0 - T \|_S.
\]
that is a challenging nonlinear approximation problem. In practice, the computation of the minimizer $T_S A_0$ can be performed only approximately. The replacement of $A_0$ by its approximation in $S$ is called the tensor truncation to $S$ and denoted by $T_S A_0$. As it was already mentioned, in the case of the TT/QTT formats, it can be computed by the conventional QR/SVD algorithm.

### 3.4. QTT-Cayley approach for complex-time evolution equations

Below, we discuss the more general (than the harmonic oscillator) example of the complex-time evolution equation arising in quantum molecular dynamics.

**Example 3.1. (Quantum molecular dynamics).** An important example in molecular dynamics is given by the Schrödinger equation for the motion of $d$ nuclei obtained from the Born-Oppenheimer approximation (see [4, 31, 32] for more detail),

$$i\hbar \frac{\partial \psi}{\partial t} = \mathcal{H} \psi, \quad \mathcal{H} = T + V, \quad \psi(0) = \psi_0,$$

with kinetic energy $T = -\sum_{\ell=1}^d \frac{\hbar^2}{2M} \Delta x_\ell$ and a potential $V = V(x_1, \ldots, x_d), x_\ell \in \mathbb{R}^3 (\ell = 1, \ldots, d)$ being an approximation to the electronic potential energy surface $E(x_1, \ldots, x_d)$.

In some cases, the possible tensor approximation of the solution $\psi(x, T)$ can be computed without time stepping by the direct approximation of the solution operator via the tensor representation of the matrix exponential family

$$\psi(t) = e^{-\mathcal{H} t} \psi_0 \approx T_S (e^{-\mathcal{H} t}) \psi_0, \quad t \geq 0,$$

providing a means for the application of the tensor-structured (say, in the QTT format) matrix exponential to each fixed $t > 0$ [27].

This approach allows a considerable coarsening in the time stepping by restarting the algorithm with a rather large step-size $\Delta T = O(1)$, thus reducing the number of grid points in the time domain to $O(\log T)$, in order to compute the solution at $t = T$. In the case of moderate $T$, the time stepping can be avoided completely.

In general, the solution operator $e^{-i\mathcal{H} t}$ could not be approximated by a QTT-matrix exponential with a uniform bound on the TT-ranks. However, for some classes of PES (for example, the Henon-Heiles potential) the multivariate function $E(x_1, \ldots, x_d)$ can be represented with a low QTT-rank [28], which makes it possible to apply our QTT-Cayley transform solver to energy spectrum computations. Taking into account the time-space separation scheme exponentially convergent in $m$, the QTT approximability of the function $(\mathcal{H} + iI)^{-1} \psi_0$ ensures a low complexity tensor representation of the solution $\psi(x, t)$.

### 3.5. On QTT approximation of $(\mathcal{H} + iI)^{-1}$

To perform the algorithm (2.4), (2.5) efficiently in multidimensional setting, we switch to semi-discrete formulation and assume that $\mathcal{H}$ is a matrix acting in the real-valued TPHS $\mathbb{W}_n = \mathbb{R}^d$ of dimension $N^d$, specified by the univariate “grid-size” $N$. Accordingly, all multivariate functions $\psi_p(t) : \mathbb{R}^d \rightarrow \mathbb{R}, t \in [0, T]$, and $u_p$, will be substituted by $N\cdot d$ tensors, $\psi_p(t) \in \mathbb{W}_n$, and $U_p$, respectively.
Hence, the application of the operator $T = \mathcal{H}(\mathcal{H} + iI)^{-1}$ is reduced to the solution of a huge linear system of equations

$$(\mathcal{H} + iI)\mathbf{U} = \mathbf{F}, \quad \mathbf{U}, \mathbf{F} \in \mathbb{W}_n,$$  \hspace{1cm} (3.4)

projected onto the low-parametric tensor manifold $S \in \{TT, QTT\}$.

Along the line of [23], we consider the model discrete elliptic problem of stationary type with $\mathcal{H} = \mathcal{D} + \mathcal{V}$, where $\mathcal{D} \in \mathbb{R}^{I \times I}$ represents the elliptic diffusion operator, $-\nabla^T a(x) \nabla$, $0 < a_0 \leq a(x) \leq a_1 \in \mathbb{R}^{d \times d}$, defined on the tensor-product domain in $\mathbb{R}^d$, and the matrix $\mathcal{V} \in \mathbb{R}^{I^2 \times I^2}$, represents some physically relevant potential. In particular, the scaled finite difference negative $d$-Laplacian over a uniform tensor grid is known to have the Kronecker rank-$d$ representation

$$\Delta_d = A \otimes I_N \otimes \ldots \otimes I_N + I_N \otimes A \otimes I_N \ldots \otimes I_N + \ldots + I_N \otimes I_N \ldots \otimes A \in \mathbb{R}^{I^d \times I^d},$$  \hspace{1cm} (3.5)

with $A = \Delta_1 = \text{tridiag}\{-1, 2, -1\} \in \mathbb{R}^{N \times N}$ and $I_N$ being the $N \times N$ identity. The QTT (resp. TT) rank of the operator $\Delta_d$ is equal to 4 (resp. 2) for any $d$ (see [19]).

Our goal is to solve equation (3.4) in the tensor-structured format $S$. As the main prerequisite, the matrices $\mathcal{D}$ and $\mathcal{V}$, as well as the solution $\mathbf{U}$ and the loading vector $\mathbf{F}$, are supposed to have a low $S$-tensor rank representation uniformly in the main discretization/model parameters.

For the linear system (3.4) the simple truncated preconditioned iteration takes the form

$$\mathbf{U}^{(0)} \in S: \quad \mathbf{U}^{(k+1)} = \mathbf{U}^{(k)} - \mathbf{B}((\mathcal{H} + iI)\mathbf{U}^{(k)} - \mathbf{F}), \quad \mathbf{U}^{(k+1)} := \mathcal{T}_S(\mathbf{U}^{(k+1)}), \quad k = 0, 1, \ldots \hspace{1cm} (3.6)$$

Now we assume that the preconditioner $\mathbf{B}$ is constructed in such a way that

$$\rho(I - \mathbf{B}(\mathcal{H} + iI)) < 1,$$

uniformly in $N$, and it has a low $S$-tensor rank. Then with the adaptive choice of the tensor rank (controlled by the chosen approximation error of the discrete scheme), the truncated iteration (3.6) can be proved to converge geometrically [17]. The preconditioner $\mathbf{B} = \mathbf{B}_M$ can be chosen as:

(a) the shifted anisotropic $d$-Laplacian inverse, or
(b) the shifted $d$-dimensional harmonic oscillator inverse.

In case (a), the rank-$(2M + 1)$, canonical tensor approximation is given by

$$\Delta_d^{-1} \simeq \mathcal{B}_M := \sum_{k=-M}^{M} c_k \bigotimes_{\ell=1}^{d} \exp(-t_k \Delta_1 + iI_1),$$  \hspace{1cm} (3.7)

$$t_k = e^{kh}, \quad c_k = \hbar t_k, \quad \hbar = \pi/\sqrt{M}, \quad \Delta_1 \in \mathbb{R}^{N \times N},$$

providing the exponential convergence rate in the canonical rank (cf. sinc-method in [8]),

$$\|\Delta_d^{-1} - \mathcal{B}_M\| \leq Ce^{-\pi\sqrt{M}}\|\Delta_d^{-1}\|.$$

Numerical examples on $O(d \log n)$ complexity scaling for the QTT representation of the high-dimensional Laplacian can be found in [25]. Here we do not count the (problem-independent) preprocessing cost required to compute the QTT representation of a family of 1D matrix...
exponentials, \{\exp(-t_k \Delta_t)\}, \, t_k > 0, \, k = -M, ..., M, of size \(N \times N\) (the latter can be precomputed once and stored). The total numerical cost is estimated by \(O(d \log \varepsilon^{-1} \log N)\).

In case (b) one can apply the results of the QTT-rank analysis of the \(d\)-dimensional harmonic oscillator as well as of the more general multivariate polynomial potentials (see [28] for more detail). In particular, in Example 2.2 the operator \((\mathcal{H} + iI)^{-1}\) allows the rank-(\(2M + 1\)) canonical approximation obtained along the line of (3.7).

### 3.6. Simultaneous QTT representation in time and space

Now we are in a position to prove the principal result on the low-rank simultaneous time-and-space QTT decomposition as maintained in the following lemma. In the following discussion, we assume that \(\psi_m(t)\) represents a \(d\)-dimensional tensor obtained by the truncated series representation (2.11) in terms of discretized solutions \(u_p(x)\), further denoted by \(U, p = 0, 1, ..., m\). The QTT rank of the tensor will be called \(\text{rank}_{\text{QTT}}\).

**Lemma 3.1.** The QTT-rank of the tensor \(P_m = [\psi_m(t_0), ..., \psi_m(t_{N_t})]_{k=0}^{N_t} \in \mathbb{W}_n \times \mathbb{R}^{N_t+1}, t_k = k\tau, \) is bounded by

\[
\text{rank}_{\text{QTT}}(P_m) \leq \sum_{p=0}^{m} (p+1)\text{rank}_{\text{QTT}}(T^p\psi_0).
\]

For the harmonic oscillator, we have for the QTT \(\varepsilon\)-rank:

\[
\text{rank}_{\text{QTT}}(P_m) \leq C m^2 |\log \varepsilon|^2 \text{rank}_{\text{QTT}}(\psi_0).
\]

**Proof.** We notice that the QTT-rank of the discretized Laguerre polynomial \(L_p^{(0)}(t)\) sampled over a uniform grid is bounded by \(p + 1\) independently of the number of sampling points \(N_t\) in the time variable (see §3.2). This means that each tensor term \([(L_{p+1}(t_k) - L_p(t_k))U_p]_{k=0}^{N_t}, t_k = k\tau, (k = 0, 1, ..., N_t)\) in the discretized truncated series representation (2.11) has the QTT-rank bounded by \((p+1)\text{rank}_{\text{QTT}}U_p\) ensuring the low-rank simultaneous time-and-space QTT decomposition as stated by lemma. The second assertion follows from the observation that in the case of harmonic oscillator the rank-(\(2M + 1\)) representation like (3.7) can be adapted. \(\square\)

Lemma 3.1 combined with Theorem 2.3 ensures that for given \(\varepsilon > 0\) there exists the \(m\)-term QTT \(\varepsilon\)-approximation \(P_m \in \mathbb{W}_n \times \mathbb{R}^{N_t+1}\) to the exact solution \(\psi(x, t)\) defined on the time-grid \(t_k = k\tau, (k = 0, 1, ..., N_t)\) whose QTT-rank can be controlled by

\[
\text{rank}_{\text{QTT}}(P_m) \leq C m^2 \text{rank}_{\text{QTT}}(T^m\psi_0), \quad \text{with} \quad m = O(\log^3 \frac{1}{\varepsilon}),
\]

independently of \(d\) and the spatial and time grid parameters \(N\) and \(N_t\).

Hence, we conclude that the block two-diagonal system of equations defined, say, by the implicit Euler scheme

\[
\psi_0 = \psi(0), \quad (I - \tau i \mathcal{H})\psi_{k+1} = \psi_k, \quad k = 0, 1, ..., N_t - 1,
\]

(3.8)

where \(\psi_k \in \mathbb{W}_n\) will approximate the value of \(\psi(t_k)\), has a low QTT rank solution with \(O(d \log N \log N_t)\) complexity scaling. Consequently, (3.8) can be solved in the QTT format as the global system of equations with respect to the unknown space-time vector (tensor)

\[
P = [\psi_0, \psi_1, ..., \psi_{N_t}] \in \mathbb{W}_n \times \mathbb{R}^{N_t+1} \approx P_m.
\]
A similar approach can be applied to the Crank-Nicolson scheme.

The solution of the global system (3.8) can be approached by either tensor-truncated preconditioned iteration (say, GMRES) or by DMRG iteration, both in the $D$-dimensional space with the virtual dimension $D = d \log N \log N_t$ (work in progress).

4. Computation of the Hamiltonian spectrum

4.1. Computing QTT-FFT of the autocorrelation function

The autocorrelation function is given by

$$a(t) = \langle \psi(t), \psi(0) \rangle = \sum_{p=0}^{m} (L_{p+1}^{(0)}(t) - L_p^{(0)}(t)) \langle u_p, \psi_0 \rangle, \quad 0 \leq t \leq T. \quad (4.1)$$

Given vectors $u_p$, $p = 0, 1, ..., m$, the function $a(t)$ can be sampled on a very fine time-grid $t_0, t_1, ..., t_N_t$ and with a low cost. The energy spectrum can be then recovered by means of the Fourier transform (in practice by the FFT):

$$\Lambda(E) = \int_{0}^{\infty} a(t) e^{iEt} dt. \quad (4.2)$$

Assuming that each vector $u_p$, $(p = 0, ..., m)$ and $\psi_0$ allow the low-rank QTT representation (implicitly we assume the $\mathcal{H}$-analyticity of $\psi_0$), and making use of FFT for the truncated sum in (4.1), the total asymptotical cost of spectrum calculations can be estimated by $O(dm \log N_t \log N)$.

4.2. Spectrum recovering by the QTT-Cayley-Laplace transform

Using the well-known correspondence for the Laplace transform

$$\mathcal{L}\{ t^{\alpha-1} e^{at} \} = \frac{\Gamma(n)}{(s - a)^n},$$

as well as the relation

$$\mathcal{L}\{ t^\alpha L_n^{(\alpha)}(t) \} = \frac{\Gamma(\alpha + n + 1)(s - 1)^n}{n! s^{\alpha+n+1}}, \quad \Re \alpha > -1, \ Re s > 0,$$

which for $\alpha = 0$ reads as

$$\mathcal{L}\{ L_n^{(0)}(t) \} = \frac{(s - 1)^n}{s^{n+1}},$$

we obtain for the complete series representation (2.4)

$$\mathcal{L}\{ e^{i\mathcal{H}t} \psi_0 \} = \mathcal{L}\{ \sum_{p=0}^{\infty} L_p^{(0)}(t) u_p \} = \sum_{p=0}^{\infty} \mathcal{L} L_p^{(0)}(t) u_p =: \Sigma(s),$$

where

$$\Sigma(s) = \sum_{p=0}^{\infty} \frac{(s - 1)^p}{s^{p+1}} [\mathcal{H}(\mathcal{H} + iI)^{-1}]^{p-1} u_0$$

$$= \frac{s - 1}{s^2} \left[ I - \frac{s - 1}{s} \left( \mathcal{H}(\mathcal{H} + iI)^{-1} \right) \right]^{-1} u_0,$$
with \( u_0 = i(\mathcal{H} + iI)^{-1} \psi_0 \). Note that here the conditions \( \| \mathcal{H}(\mathcal{H} + iI)^{-1} \| \leq 1 \) and \( \left| \frac{s-1}{s} \right| < 1 \) for \( \Re s > 1/2 \) have to be satisfied as soon as the formula for the sum of the infinite geometrical series has been used.

Thus, the discrete spectrum of the Schrödinger operator coincides with the poles of the function \( \| \Sigma(s) \| \) multiplied by \( -i \). The total cost now is determined by the complexity of evaluating the elements \( \left[ I - \frac{s-1}{s} \left( \mathcal{H}(\mathcal{H} + iI)^{-1} \right) \right]^{-1} u_0 \) at all sampling points in the \( s \) variable.

The calculation by the truncated representation leads to the \( m \)-term summation using the function \( \Sigma_m(s) = \sum_{p=0}^{m} \frac{(s-1)^p}{s^{p+1}} u_p \approx \Sigma(s) \).

Finally, we notice that numerical illustrations on the proposed approach will be presented in the forthcoming papers.

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References


Quantized-TT-Cayley transform for high-dimensional Hamiltonians


