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Abstract

In the present paper, we propose and analyse a class of tensor methods for the efficient numerical computation of dynamics and spectrum of high-dimensional Hamiltonians. The main focus is on the complex-time evolution problems. We apply the recent quantized-TT (QTT) matrix product states tensor approximation that allows to represent N-d tensors generated by 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 spatial parts of 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 a class of "analytic" and low QTT-rank input data, our method allows to compute the solution at a fix point in time $t = T > 0$ with the asymptotic complexity of order $\mathcal{O}(d \log N \ln^q \frac{1}{\varepsilon})$, where $\varepsilon > 0$ is the error bound and q a fixed small number. The time-and-space separation method via the QTT-Cayley-transform enables us to construct the global m-term separable (x,t)-representation of a solution on very fine time-space grid with complexity of order $O(dm^4 \log N_t \log N)$, where N_t is the number of sampling points in time. The latter allows the efficient energy spectrum calculations by FFT (or QTT-FFT) of autocorrelation function computed on sufficiently long time interval $[0, T]$. Moreover, we show that the spectrum of 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 dynamics and 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. 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 represents a challenging problem due to the so-called "curse of dimensionality". Roughly speaking, the computational costs to find such a function grows exponentially as $d \to \infty$ even in the case if the function is analytical. If we restrict only to computation of high dimensional integrals then Quasi-Monte Carlo algorithms maight be efficient [39]. In some cases the curse of dimensionality can be circumvented by using the so-called sparse grid spaces, based on tensor product of d one-dimensional multiscale functions. In particular, in the case of high dimensional parabolic problems this approach has been successfully applied 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 course 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 the discrete problem should be represented as the tensor product of the solution operators of one-dimensional problems or a short sum of such tensor products. Some tensor-structured numerical methods based on this approach were proposed and analyzed in [8, 21, 20, 26]. In order to separate the time variable in nonstationary problems one may 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 [9, 10]. Various tensor-product techniques for separation of the spatial Hamiltonians were recently introduced [23, 27, 28, 19].

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

$$\dot{\psi}(t) = i\mathcal{H}\psi(t) + f(t), \quad \psi(0) = \psi_0 \in D(\mathcal{H}) \subset \mathbb{W}. \tag{1.1}$$

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, equation like (1.1) may represent the molecular or electronic Schrödinger equation in d dimensions that describes how the quantum state of a physical system evolves in time (see Example 2.2 below). In this case the many particle Hamiltonian $\mathcal{H}$ is given by a sum of $d-$dimensional Laplacian and certain interaction potential, say, potential energy surface [4, 31]. In general, in multidimensional setting, a separable approximation of the operator $S(t)$ in molecular dynamics is the 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 spatial Hamiltonian operator. This enables us to derive the low-parametric tensor structured representation to the solution $\psi(x,t)$ globally in t over fixed interval $0 \le t \le T$. Hence, at this stage a time discretization does not appear.

Specifically, we propose to approximate $S(t)$ by simplified operator family $S_m(t)$ obtained by the m-term truncated series expansion in the Laguerre t-polynomials. For a class of $\mathcal{H}$-analytic data ψ_0, we prove a super exponential convergence

$$\|S(t) - S_m(t)\| \le cm^{-1/12} e^{-c_1 m^{1/3}},$$

where $m \in \mathbb{N}$ is a truncation parameter. This ensures the rank-m time-space separability for a class of initial data. Even more important, this approach creates the robust adaptive basis for the so-called proper orthogonal decomposition (POD) being the building block in the model reduction techniques.

In order to compute $S_m(t)$ one should solve $\mathcal{O}(m)$ linear problems with the d-dimensional spatial Hamiltonian $\mathcal{H}+iI$ discretized over d-fold $N \times N \times ... \times N$ 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,

$$\mathcal{O}(dmW(N)|\ln \varepsilon|^q),$$

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 very fine time-space grid of size $N \times ... \times N \times N_t$ by simultaneous time-space low-parametric tensor representation, where N_t is the number of sampling points in time. Under certain regularity assumptions on ψ_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 $e^{-c_1 m^{1/3}}$, where the constant C scales at most quadratically in the tensor rank of $(\mathcal{H}+iI)^{-m}\psi_0$ (cf. Lemma 3.4). The latter allows the efficient energy spectrum calculations by FFT transform of autocorrelation function computed on sufficiently long time interval $[0,T]$. Moreover, we show that the spectrum of Hamiltonian can be also represented by the poles of Laplace transform of autocorrelation function. In particular, our approach can be an option to compute dynamics and spectrum of time-dependent molecular Schrödinger equations describing the molecular vibration [32].

The rest of the paper is organised as follows. In Section 2 we discuss the separation of the time and space variables via Cayley transform. The error analysis of m-term truncated series representation for certain class of initial data is presented. Section 3 discuss spatial tensor approximation of the solution $\psi(x,t)$ via TT/QTT formats. In particular, we prove the $\log - \log$ complexity tensor representation in time and space for a class of so-called $\mathcal{H}$-analytic initial data ψ_0 with the controlled tensor rank of $(\mathcal{H}+iI)^{-m}\psi_0$. The computation of the spectrum of d-dimensional Hamiltonian is addressed in Section 4.

2 Separation of the time variable via Cayley transform

2.1 Infinite series representation

The idea on separation of 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 α,

$$(1-z)^{-\alpha-1}e^{\frac{tz}{z-1}} = \sum_{p=0}^{\infty} L_p^{(\alpha)}(t)z^p.$$

After the formal substitution $z \to \lambda(\lambda+i)^{-1} := T(\lambda)$, 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 $\psi_0 \in D(\mathcal{H})$, i.e.,

$$\psi_0 = \sum_{k=0}^{\infty} a_k\phi_k, \quad \text{such that} \quad \sum_{k=0}^{\infty} |a_k|^2\lambda_k^2 < \infty, \tag{2.2}$$

the solution operator can be represented by

$$e^{i\mathcal{H}t} = i(\mathcal{H}+iI)^{-1}\sum_{p=0}^{\infty} L_p^{(0)}(t)T^p(\mathcal{H}), \tag{2.3}$$

where

$$T = T(\mathcal{H}) = \mathcal{H}(\mathcal{H}+iI)^{-1}$$

is the (non-classical) Cayley transform of the operator $\mathcal{H}$. This representation can be used for separation of 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

$$\psi(t) = \sum_{p=0}^{\infty} L_p^{(0)}(t)u_p \equiv i(\mathcal{H}+iI)^{-1}\sum_{p=0}^{\infty} L_p^{(0)}(t)T^p(\mathcal{H})\psi_0, \tag{2.4}$$

where the elements u_p can be found from the recursion

$$\begin{aligned} u_0 &= i(\mathcal{H}+iI)^{-1}\psi_0, \\ u_{p+1} &= \mathcal{H}(\mathcal{H}+iI)^{-1}u_p, \quad p = 0, 1, ... \end{aligned}$$

or, equivalently, as the solutions of the operator equations

$$\begin{aligned} (\mathcal{H}+iI)u_0 &= i\psi_0, \\ (\mathcal{H}+iI)u_{p+1} &= \mathcal{H}u_p, \quad p = 0, 1, ... \end{aligned} \tag{2.5}$$

Notice that the recursion $u_p = T^p u_0$, $p = 0, 1, 2, ...$ indicates the opportunity for optimization of the set $\{u_p\}$ by analogy to the Krylov subspace method commonly used in the numerical linear algebra.

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

Proof. First, we use the estimates (2.12) which yield $\lim_{p\to\infty} L_p^{(0)}(t) = O(p^{-1/4})$ for each fixed t. Then the following bound $\|u_{p+1}\| \le cp^{-\sigma/2}\|\mathcal{H}^\sigma\psi_0\|$ (see (2.15) below) proves that (2.4) is well defined. Furthermore, from (2.5) it follows that

$$u_p = i\mathcal{H}(u_p - u_{p-1}), \quad p = 0, 1, 2, ...; \quad u_{-1} = i\mathcal{H}^{-1}\psi_0. \tag{2.6}$$

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

$$\begin{aligned}
\psi(t) &= u_0 + i\mathcal{H}\sum_{p=1}^{\infty} L_p^{(0)}(t)(u_p - u_{p-1}) \\
&= u_0 - i\mathcal{H}u_0 L_0^{(0)}(t) - i\mathcal{H}\sum_{p=0}^{\infty}(L_{p+1}^{(0)}(t) - L_p^{(0)}(t))u_p \\
&= \psi_0 - i\mathcal{H}\sum_{p=0}^{\infty}(L_{p+1}^{(0)}(t) - L_p^{(0)}(t))u_p.
\end{aligned} \tag{2.7}$$

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) yields

$$\dot{\psi}(t) = i\mathcal{H}\sum_{p=0}^{\infty} L_p^{(0)}(t)u_p = i\mathcal{H}\psi(t), \tag{2.8}$$

which completes the proof. ∎

Example 2.2 *(Harmonic oscillator). In quantum mechanics the operator $\mathcal{H}$ in (1.1) might be the 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 ω is the angular frequency of the oscillator. The operator $\mathcal{H}$ in $\mathbb{W} = L_2(-\infty, \infty)$ is defined by*

$$\begin{aligned}
D(\mathcal{H}) &= \{u \in H^2(-\infty, \infty) : \psi(-\infty) = \psi(\infty) = 0\}, \\
\mathcal{H}\psi &= -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{m\omega^2}{2}x^2\psi \quad \forall \quad \psi \in D(\mathcal{H}).
\end{aligned} \tag{2.9}$$

It is known that the normalized eigenfunctions (subject to $\int_{-\infty}^{\infty}\phi^2(x)dx = 1$) are given by

$$\phi_n(x) = C_n e^{-\xi^2/2}H_n(\xi), \quad n = 0, 1, 2, ... \tag{2.10}$$

where $x = \alpha\xi, \alpha = \sqrt{\frac{\hbar}{m\omega}}, C_n = \frac{1}{\sqrt{\alpha}} \cdot \frac{1}{\sqrt{2^n n! \sqrt{\pi}}}$ *and* $H_n(\xi)$ *are the Hermite polynomials [41, 40]. These eigenfunctions correspond to the eigenvalues* $E_n = (n+1/2)\hbar\omega$. *In 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 1D Harmonic oscillator the operator $S(t)$ is easily diagonalisable, while for $d \geq 2$ it is a rank-1 separable, and thus the computational complexity of its tensor representation scales linearly in d. Hence, it provides the base for efficient preconditioner (see Section 3.5).

Remark 2.3 *In the case of 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

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

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

$$\begin{aligned}
&L_n^{(\alpha)}(t) = \pi^{-1/2} e^{t/2} t^{-\alpha/2-1/4} n^{\alpha/2-1/4} [\cos(2\sqrt{nt} - \beta\pi) + \mathcal{O}(n^{-1/2})], \\
&\text{for } t \in [a,b],\ 0 < a < b < \infty,\ \beta = (2\alpha+1)/4, \alpha > -1; \\
&|L_n^{(\alpha)}(t)| \leq c n^{\frac{\alpha}{2}-\frac{1}{4}} t^{-\frac{\alpha}{2}-\frac{1}{4}} e^{\frac{t}{2}} (1 + n^{-\frac{1}{4}} t^{\frac{5}{4}}), \alpha + \frac{1}{2} \geq 0, t \geq 0; \\
&|L_n^{(0)}| \leq e^{t/2}, t \geq 0,
\end{aligned} \tag{2.12}$$

where c is a constant independent of n and $0 < a < b$, are arbitrary fixed numbers. Moreover, it holds

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

uniformly in $t \in [0,T]$ (it follows from the representations $nL_n^\alpha(t) - (n+\alpha)L_{n-1}^\alpha(t) = t\frac{d}{dt}L_n^\alpha(t)$ and $\frac{d}{dt}L_n^\alpha(t) = -L_{n-1}^{\alpha+1}(t)$, 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 next theorem characterizes the convergence rate of the truncated series representation.

Theorem 2.4 *Let $\psi_0 \in D(\mathcal{H}^\sigma)$, with some $\sigma > 3/2$, then for fixed $T > 0$, the following estimate holds true,*

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

with some constant $c > 0$ independent of m.

Proof. First, we observe that for $\psi_0 = \sum\limits_{k=0}^{\infty} a_k\phi_k$ there holds

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

implying

$$\|u_{p+1}\| \le \max_{\lambda\in[\lambda_0,\infty)}\left|\lambda^{-\sigma}\left(\frac{\lambda}{\lambda+i}\right)^p\right|\|\mathcal{H}^\sigma\psi_0\| \le cp^{-\sigma/2}\|\mathcal{H}^\sigma\psi_0\|. \tag{2.15}$$

Now taking into account (2.13) we obtain the estimates

$$\begin{aligned} \|\psi(t) - \psi_m(t)\| &\le \sum_{p=m+1}^{\infty} |L_{p+1}^{(0)}(t) - L_p^{(0)}(t)|\|u_p\| \\ &\le c\|\mathcal{H}^\sigma\psi_0\|t^{\frac{1}{4}}e^{\frac{t}{2}}\sum_{p=m+1}^{\infty} p^{-\sigma/2-3/4} \\ &\le c\|\mathcal{H}^\sigma\psi_0\|t^{\frac{1}{4}}e^{\frac{t}{2}}m^{-\sigma/2+1/4}, \end{aligned}$$

which completes our proof. ∎

Theorem 2.4 shows that increase of σ in the $\mathcal{H}$-regularity condition $\psi_0 \in D(\mathcal{H}^\sigma)$ 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 $\mathcal{H}$-analytical input data to be introduced below.

Definition 2.5 *A vector $f = \sum\limits_{k=0}^{\infty} a_k\phi_k \in D(\mathcal{H})$ is called analytical for $\mathcal{H}$ ($\mathcal{H}$-analytic) if there is a constant $C = C(f) > 0$, such that*

$$\|\mathcal{H}^n f\| = \sqrt{\sum_{k=0}^{\infty} |a_k|^2\lambda_k^{2n}} \le C^n n! \quad \textit{for all} \quad n = 1,2,3,...$$

Remark 2.6 *For $\mathcal{H}$-analytic vector f the power series $\sum\limits_{n=0}^{\infty}\frac{s^n}{n!}\|\mathcal{H}^n f\| =: \|f\|_{s,\mathcal{H}}$ possesses a positive convergence radius $r > 0$, i.e., $\|f\|_{s,\mathcal{H}} < \infty$ if $0 \le s < r$.*

Proposition 2.7 *The finite sum* $u_0(x) = \sum_{k=0}^{m} \gamma_k \phi_k(x)$ *gives rise to the* $\mathcal{H}$*-analytic vector with* $C \approx \lambda_m$*. In particular, in Example 2.2, we have* $C \approx \hbar\omega(m + 1/2)$*.*

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

$$\begin{aligned} \|\mathcal{H}^n u_0\| &= \Big(\int_{-\infty}^{\infty} \Big| \sum_{k=0}^{m} \gamma_k \lambda_k^n \phi_k(x) \Big|^2 dx \Big)^{1/2} \\ &= \Big(\sum_{k=0}^{m} |\gamma_k|^2 \lambda_k^{2n} \Big)^{1/2} \le \lambda_m^n \Big(\sum_{k=0}^{m} |\gamma_k|^2 \Big)^{1/2} \le \lambda_m^n \|u_0\|, \end{aligned} \tag{2.16}$$

that ensures the required bound. ∎

The next theorem shows an exponential convergence of approximation (2.11) provided that the initial vector is $\mathcal{H}$-analytic.

Theorem 2.8 *Let* ψ_0 *be* $\mathcal{H}$*-analytic and let* $r > 0$ *be the convergence radius of the series* $\sum_{k=0}^{\infty} \frac{s^k}{k!} \|\mathcal{H}^k \psi_0\|$*. Then for every fixed* $s < r$*, and fixed* $T > 0$*, the approximation (2.11) converges exponentially in* m *implying the error estimate*

$$\|\psi(t) - \psi_m(t)\| \le c m^{-1/12} e^{-c_1 \sqrt[3]{m}} \|\psi_0\|_{s,\mathcal{H}}, \quad t \in [0, T], \tag{2.17}$$

where c, c_1 *are positive constants independent of* m*.*

Proof. First, we note that the estimates (2.12) yield for $t \in [\varepsilon, T]$

$$\|\psi(t) - \psi_m(t)\| \le c t^{-\frac{1}{4}} e^{\frac{t}{2}} \sum_{p=m+1}^{\infty} p^{-3/4} \|u_p\|, \tag{2.18}$$

where the iterand u_p allows the representation

$$\begin{aligned} u_{p+1} &= \sum_{k=0}^{\infty} a_k \Big(\frac{\lambda_k}{\lambda_k + i} \Big)^p \phi_k \\ &= \sum_{k=0}^{\infty} a_k e^{-\lambda_k s} \Big(\frac{\lambda_k}{\lambda_k + i} \Big)^p \Big(\sum_{n=0}^{\infty} \frac{\lambda_k^n s^n}{n!} \Big) \phi_k, \\ &= \sum_{k=0}^{\infty} a_k e^{-\lambda_k s} \Big(\frac{\lambda_k}{\lambda_k + i} \Big)^p \sum_{n=0}^{\infty} \frac{s^n}{n!} \mathcal{H}^n \phi_k, \\ &= \sum_{n=0}^{\infty} \frac{s^n}{n!} \mathcal{H}^n \Big(\sum_{k=0}^{\infty} a_k \Phi_s(\lambda_k) \phi_k \Big), \end{aligned} \tag{2.19}$$

with

$$\Phi_s(\lambda) := e^{-\lambda s} \Big(\frac{\lambda}{\lambda + i} \Big)^p.$$

Let us notice that

$$\|\mathcal{H}^n\Big(\sum_{k=0}^{\infty} a_k \Phi_s(\lambda_k)\phi_k\Big)\| \le \max_{\lambda\in[\lambda_0,\infty)} \Big|\Phi_s(\lambda)\Big| \|\mathcal{H}^n\psi_0\|.$$

Simple variational analysis indicates that the function $\Phi_s(\lambda)$ takes its maximum at a point λ_* that solves the equation $s = \frac{p}{\lambda(1+\lambda^2)}$ implying that $\lambda_* \asymp \sqrt[3]{p/s}$. 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

$$\max_{\lambda\in[\lambda_0,\infty)} \Big|\Phi_s(\lambda)\Big| = \max_{\lambda\in[\lambda_0,\infty)} e^{-\lambda s}\Big(\frac{\lambda^2}{1+\lambda^2}\Big)^{p/2} \le c e^{-c_1\sqrt[3]{p}},$$

thus implying

$$\|u_{p+1}\| \le c e^{-c_1\sqrt[3]{p}} \|\psi_0\|_{s,\mathcal{H}}. \tag{2.20}$$

Furthermore, we have

$$\begin{aligned} \|\psi(t) - \psi_m(t)\| &\le c t^{\frac{1}{4}} e^{\frac{t}{2}} \|\psi_0\|_{s,\mathcal{H}} \sum_{p=m+1}^{\infty} p^{-1/12} p^{-2/3} e^{-c_1\sqrt[3]{p}} \\ &\le c t^{\frac{1}{4}} e^{\frac{t}{2}} m^{-1/12} e^{-c_1\sqrt[3]{m}} \|\psi_0\|_{s,\mathcal{H}}, \end{aligned} \tag{2.21}$$

which completes our proof. ∎

Theorem 2.8 shows that for $\mathcal{H}$-analytic initial data the truncated Cayley transform ensures the time-space separation with ε-rank of order $m = O(\log^3 1/\varepsilon)$.

Remark 2.9 *We also observe that the set of vectors, $U := [u_0, u_1, ..., u_N]$, creates the robust adaptive basis for the so-called proper orthogonal decomposition (POD) being the 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 slightly/smoothly modified operator or initial value (parameter dependent problems).*

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

Remark 2.10 *The Cayley transform $T(\mathcal{H}) = \mathcal{H}(\mathcal{H}+I)^{-1}$ can be adapted to the real-time evolution equation*

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

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

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

with

$$\Phi_{1,s}(\lambda) := e^{-\lambda s}\Big(\frac{\lambda}{\lambda+1}\Big)^p.$$

Contrary to the case of function $\Phi_s(\lambda)$ *in (2.19) now* $\Phi_{1,s}(\lambda)$ *takes its maximum at a point* $\lambda_* \asymp \sqrt{p}$*, and we arrive at the estimate* $\|u_{p+1}\| \le ce^{-c_1\sqrt{p}}\|\psi_0\|_{s,\mathcal{H}}$*, implying (cf. (2.17))*

$$\begin{aligned}\|\psi(t)-\psi_m(t)\| &\le ct^{\frac{1}{4}}e^{\frac{t}{2}}\|\psi_0\|_{s,\mathcal{H}}\sum_{p=m+1}^{\infty} p^{-1/4}p^{-1/2}e^{-c_1\sqrt{p}} \\ &\le ct^{\frac{1}{4}}e^{\frac{t}{2}}m^{-1/4}e^{-c_1\sqrt{m}}\|\psi_0\|_{s,\mathcal{H}}.\end{aligned} \tag{2.24}$$

3 Spatial tensor approximation in 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 the 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 the multivariate spacial functions $u_p(x)$ and a vector obtained by sampling of the Laguerre polynomials $L_p(t)$ on uniform grid over $[0,T]$.

3.1 Tensor-product Hilbert spaces

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

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

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

$$\langle \mathbf{A}, \mathbf{B}\rangle := \sum_{\mathbf{i}\in\mathcal{I}} A(\mathbf{i})B(\mathbf{i}), \quad \mathbf{A},\mathbf{B} \in \mathbb{W}_{\mathbf{n}}.$$

The storage demand for N-d tensors scales exponentially in d, $\dim \mathbb{W}_{\mathbf{n},d} = N^d$ ("curse of dimensionality").

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

3.2 Matrix product states tensor model by 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 traditional Tucker model, but with essentially 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 chain corresponding to the case of periodic boundary condition in MPS, can be described by the following definition (cf. [24]).

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

$$\mathsf{V} = \{\times_\ell\}_{\ell=1}^{d} \mathsf{G}^{(\ell)} \quad \textit{with 3-tensors} \quad \mathsf{G}^{(\ell)} \in \mathbb{R}^{J_{\ell-1} \times I_\ell \times J_\ell}. \tag{3.1}$$

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

The beneficial properties of the TC/TT formats are due to 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 ℓ-mode TT-unfolding matrices (known in 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 $L = 1, 2, ...$ Next definition introduces the folding of N-d tensors into the 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* $2 \le p \le L$*,*

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

with $m_{\ell,1} = q^{L-p+1}$*, and* $m_{\ell,\nu} = q$ *for* $\nu = 2, ..., p$*, (*$\ell = 1, ..., d$*), that reshapes the initial* $\mathbf{n}$*-d tensor in* $\mathbb{W}_{\mathbf{n},d}$ *to the element in quantics space* $\mathbb{W}_{\mathbf{m},dp}$ *as follows:*
(A) For $d = 1$ *a vector* $\mathsf{X}_{(N,1)} = [X(i)]_{i \in I} \in \mathbb{W}_{N,1}$*, is reshaped to the element of* $\mathbb{W}_{q^{L-p+1},p}$ *by*

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

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* $j - 1$ *is the q-adic representation of* $i - 1$ *for* $i \in I$*, in radix-q system, such that* j_ν *takes values in* $\{1, ..., q\}$*.*
(B) For $d > 1$ *the construction is similar.*

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

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 Chebyshev grid can be represented by rank-2 quantics tensor, while the general polynomial vector sampled over 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 the high compressibility features of the QTT representation applied to 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 may reduce the storage complexity of spatial vectors u_p to log-volume size $O(d \log N) \ll N^d$, 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 complexity of order $O(dm \log N_t \log N)$, where N_t is the number of sampling points in time. The latter allows the efficient energy spectrum calculations by FFT transform (or QTT-FFT) of autocorrelation function (see Section 4.1) computed by our method on 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

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 the implementation of 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 scalar product) increase the separation rank of the resultant tensor. Hence, the complexity control requires further "projection" of such intermediate results to the set of tensors with smaller rank parameter (rank truncation).

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

$$\mathbf{A}_0 \in \mathbb{W}_{\mathbf{n},d} : \quad T_{\mathcal{S}}\mathbf{A}_0 = \mathrm{argmin}_{\mathbf{T}\in\mathcal{S}} \|\mathbf{A}_0 - \mathbf{T}\|_{\mathcal{S}}, \tag{3.2}$$

that is a challenging nonlinear approximation problem. In practice, the computation of the minimizer $T_{\mathcal{S}}\mathbf{A}_0$ can be performed only approximately. The replacement of $\mathbf{A}_0$ by its approximation in $\mathcal{S}$ is called the *tensor truncation* to $\mathcal{S}$ and denoted by $T_{\mathcal{S}}\mathbf{A}_0$. As it was already mentioned, in the case of TT/QTT formats it can be computed by 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 complex-time evolution equation arising in quantum molecular dynamics.

Example 3.3 *(Quantum molecular dynamics). 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),*

$$i\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\psi, \quad \mathcal{H} = T + V, \quad \psi(0) = \psi_0, \tag{3.3}$$

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

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

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

providing mean for application of the tensor-structured (say in 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 rather large step-size $\Delta T = O(1)$, hence 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 QTT-matrix exponential with uniform bound on the TT-ranks. However, for some classes of PES (for example the Henon-Heiles potential) the multivariate function $E(x_1, ..., x_d)$ can be represented with low QTT-rank [28], which makes it possible to apply our QTT-Cayley transform solver to the energy spectrum computations. Taking into account the exponentially convergent in m time-space separation scheme, the QTT approximability of a function $(\mathcal{H} + iI)^{-m}\psi_0$ then ensures the low complexity tensor representation of a 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 $\mathbb{W}_{\mathbf{n}} = \mathbb{R}^{\mathcal{I}}$ of dimension N^d, specified by the univariate "grid-size" N. Correspondingly, all multivariate functions $\psi_p(t) : \mathbb{R}^d \to \mathbb{R}$, $t \in [0, T]$, and u_p, will be substituted by N-d tensors, $\psi_p(t) \in \mathbb{W}_{\mathbf{n}}$, and $\mathbf{U}_p$, respectively.

Hence, the application of the operator $T = \mathcal{H}(\mathcal{H} + iI)^{-1}$, is reduced to the solution of huge linear system of equations

$$(\mathcal{H} + iI)\mathbf{U} = \mathbf{F}, \quad \mathbf{U}, \mathbf{F} \in \mathbb{W}_{\mathbf{n}}, \tag{3.4}$$

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

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

$$\Delta_d = A \otimes I_N \otimes ... \otimes I_N + I_N \otimes A \otimes I_N ... \otimes I_N + ... + I_N \otimes I_N ... \otimes A \in \mathbb{R}^{I^{\otimes d}\times I^{\otimes d}}, \quad (3.5)$$

with $A = \Delta_1 = \mathrm{tridiag}\{-1, 2, -1\} \in \mathbb{R}^{N\times N}$, and I_N being the $N \times N$ identity. The QTT (resp. TT) rank of the operator Δ_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 $\mathcal{S}$. As the main prerequisite, matrices $\mathcal{D}$ and $\mathcal{V}$, as well as the solution $\mathbf{U}$ and loading vector $\mathbf{F}$, are supposed to have a low $\mathcal{S}$-tensor rank representation uniformly in the main discretization/model parameters.

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

$$\mathbf{U}^{(0)} \in \mathcal{S}: \quad \widetilde{\mathbf{U}}^{(k+1)} = \mathbf{U}^{(k)} - \mathcal{B}((\mathcal{H}+iI)\mathbf{U}^{(k)} - \mathbf{F}), \quad \mathbf{U}^{(k+1)} := T_{\mathcal{S}}(\widetilde{\mathbf{U}}^{(k+1)}), \quad k = 0, 1, ... \quad (3.6)$$

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

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

uniformly in N, and it has the low $\mathcal{S}$-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 $\mathcal{B} = \mathcal{B}_M$ 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

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

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

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

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

Numerical examples on $O(d \log n)$ complexity scaling for QTT representation of the high-dimensional Laplacian can be found [25]. Here we do not count the (problem independent) preprocessing cost required to compute the QTT representation of a family of $1D$ matrix exponentials, $\{\exp(-t_k\Delta_1)\}$, $t_k > 0$, $k = -M, ..., M$, 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 on QTT-rank analysis of the d-dimensional harmonic oscillator as well as the more general multivariate polynomial potentials (see [28] for more detail). In particular, in Example 2.2 the operator $(\mathcal{H} + iI)^{-1}$ allows a 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 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 $\mathbf{U}_p$, $p = 0, 1, ..., m$. The QTT rank of a tensor will be called by $rank_{QTT}$.

Lemma 3.4 *The QTT-rank of a tensor* $\mathbf{P}_m = [\psi_m(t_0), ..., \psi_m(t_{N_t})]_{k=0}^{N_t} \in \mathbb{W}_{\mathbf{n}} \times \mathbb{R}^{N_t+1}$, $t_k = k\tau$, *is bounded by*

$$rank_{QTT}(\mathbf{P}_m) \le \sum_{p=0}^{m} (p+1) rank_{QTT}(T^p \psi_0).$$

For the harmonic oscillator we have for the QTT ε*-rank,*

$$rank_{QTT}(\mathbf{P}_m) \le Cm^2 |\log \varepsilon|^2 rank_{QTT}(\psi_0).$$

Proof. We notice that QTT-rank of the discretized Laguerre polynomial $L_p^{(0)}(t)$ sampled over 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 $[(L_{p+1}(t_k) - L_p(t_k))\mathbf{U}_p]_{k=0}^{N_t}$, $t_k = k\tau$, $(k = 0, 1, ..., N_t)$ in the discretized truncated series representation (2.11) has the QTT-rank bounded by $(p+1)rank_{QTT}\mathbf{U}_p$ 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. ∎

Lemma 3.4 combined with Theorem 2.8 ensures that for given $\varepsilon > 0$ there exists the m-term QTT ε-approximation $\mathbf{P}_m \in \mathbb{W}_{\mathbf{n}} \times \mathbb{R}^{N_t+1}$ 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

$$rank_{QTT}(\mathbf{P}_m) \le Cm^2 rank_{QTT}(T^m \psi_0), \quad \text{with } m = O(\log^3 \frac{1}{\varepsilon}),$$

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,

$$\psi_0 = \psi(0), \quad (I - \tau i\mathcal{H})\psi_{k+1} - \psi_k = 0, \quad k = 0, 1, ..., N_t - 1, \tag{3.8}$$

where $\psi_k \in \mathbb{W}_{\mathbf{n}}$ will approximate the value $\psi(t_k)$, 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)

$$\mathbf{P} = [\psi_0, \psi_1, ..., \psi_{N_t}] \in \mathbb{W}_{\mathbf{n}} \times \mathbb{R}^{N_t+1} \approx \mathbf{P}_m.$$

Similar approach can be applied to the Crank-Nicolson scheme.

The solution of 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 spectrum of Hamiltonian

4.1 Computing QTT-FFT of autocorrelation function

Autocorrelation function is given by

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

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

$$\Lambda(E) = \int_0^\infty a(t) e^{iEt} dt. \tag{4.2}$$

Assuming that each vector u_p, $(p = 0, ..., m)$ and ψ_0 allow the low-rank QTT representation (implicitly we assume the $\mathcal{H}$-analyticity of ψ_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

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

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

$$\begin{aligned} \Sigma(s) &= \sum_{p=0}^{\infty} \frac{(s-1)^p}{s^{p+1}} [\mathcal{H}(\mathcal{H} + iI)^{-1}]^{p-1} u_0 \\ &= \frac{s-1}{s^2} \left[I - \frac{s-1}{s} \left(\mathcal{H}(\mathcal{H} + iI)^{-1} \right) \right]^{-1} u_0, \end{aligned}$$

with $u_0 = i(\mathcal{H} + iI)^{-1}\psi_0$. Note that here the following 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 to evaluate 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 s variable.

Calculation by truncated representation leads to the m-term summation using a 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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