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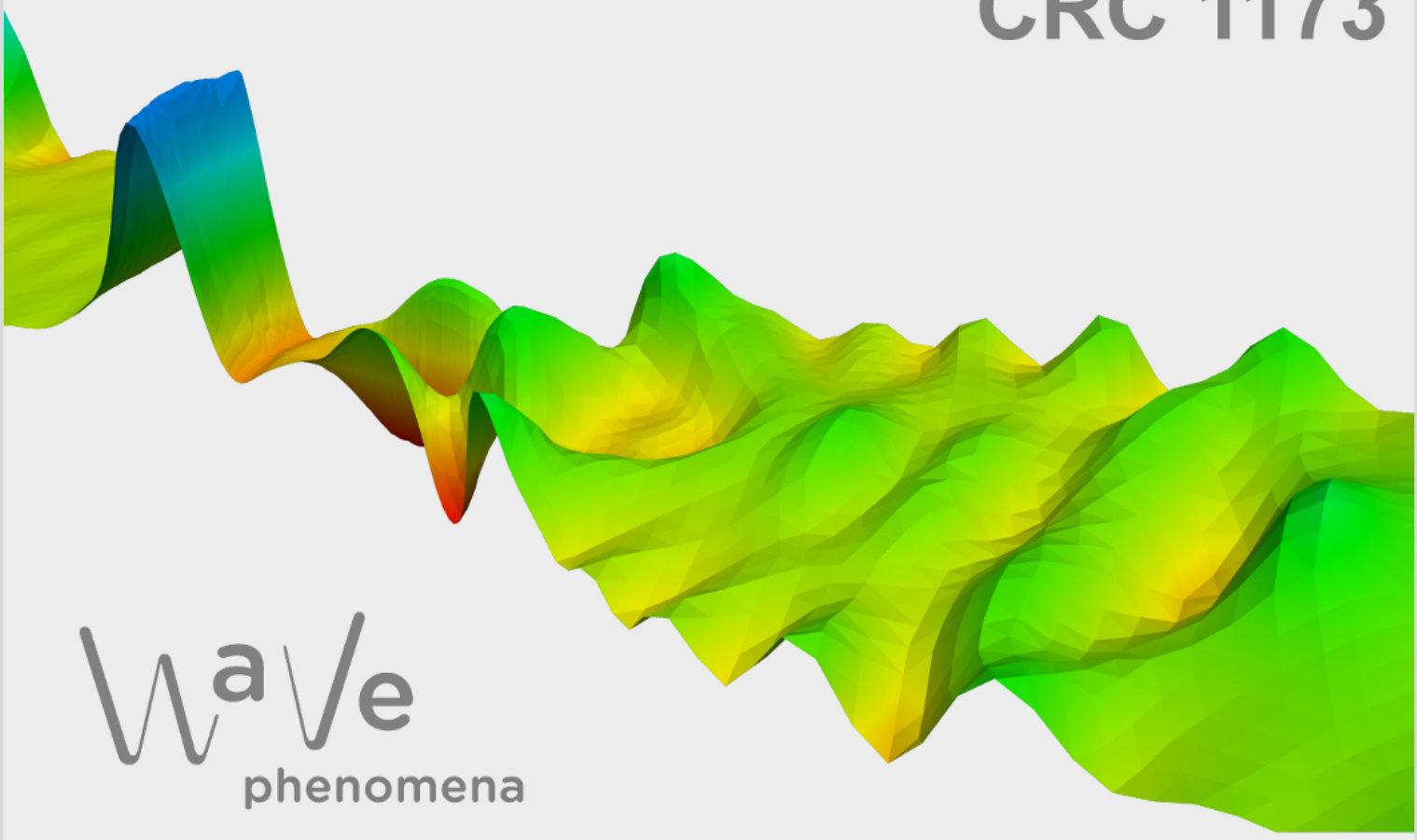

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A multi-level stochastic collocation method for Schrödinger equations with a random potential*

Tobias Jahnke† and Benny Stein†

Abstract. We propose and analyze a numerical method for time-dependent linear Schrödinger equations with uncertain parameters in both the potential and the initial data. The random parameters are discretized by stochastic collocation on a sparse grid, and the sample solutions in the nodes are approximated with the Strang splitting method. The computational work is reduced by a multi-level strategy, i.e. by combining information obtained from sample solutions computed on different refinement levels of the discretization. We prove new error bounds for the time discretization which take the finite regularity in the stochastic variable into account, and which are crucial to obtain convergence of the multi-level approach. The predicted cost savings of the multi-level stochastic collocation method are verified by numerical examples.

Key words. Uncertainty quantification, splitting methods, Strang splitting, Schrödinger equation, sparse grids, stochastic collocation method, multi-level method

AMS subject classifications. 65M12, 65M15, 65M70, 65D05, 65C20, 35Q41

1. Introduction.

In recent years the influence of uncertain parameters on the behaviour and the simulation of partial differential equations (PDEs) has received increasing attention. A central goal of *uncertainty quantification* is to understand these influences in any PDE occuring in real-life phenomena. An important example is the *time-dependent linear Schrödinger equation* which describes the evolution of the wave function of a quantum-mechanical system. The wave function is the key to compute observables such as, e.g., positions and momenta, or the probability to find the system in a given subset of the state space. Since solving the full molecular Schrödinger equation is typically impossible, the classical approach is to use the Born-Oppenheimer approximation to separate the slow motion of the heavy nuclei from the fast dynamics of the electrons. This leads to a lower-dimensional Schrödinger equation for the nuclei on an electronic energy surface; cf. [19, II.2.]. The potential of the reduced equation, however, is obtained by a number of approximations and simplifications, and is thus affected by a significant degree of uncertainty. Additional uncertainties arise from the fact that the initial state of the system can only be measured with limited accuracy. A reliable numerical treatment of these uncertainties in numerical simulations is desirable and necessary.

From all non-intrusive methods for uncertainty quantification, the arguably most studied classes are *stochastic collocation methods* and *Monte Carlo type methods* – at least from the numerical analyst's point of view. Both of these classes rely on sample solutions obtained from solving the same deterministic PDE with different values of the parameters. From these sample solutions one may derive, e.g., expectations, variances, higher-order moments

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or other statistical quantities of the solution. In the case of stochastic collocation methods, one may even obtain a surrogate for the unknown solution itself via a generalised polynomial chaos approximation or interpolation. Non-intrusive methods have the advantage that any suitable traditional numerical method can be used to solve the deterministic PDEs, and that parallelization is trivial because the sample solutions are uncoupled. Stochastic collocation schemes are discussed, e.g., in [2, 22, 20, 28]. One of the most important extensions of the standard Monte Carlo approach are Multi-Level Monte Carlo methods [7, 6, 8]. These methods use information obtained from sample solutions computed on different refinement levels of the discretization, which decreases the computational work significantly under certain conditions. For stochastic collocation methods such a multi-level procedure has been introduced and developed in [25, 26, 12]. In these references it was shown that multi-level stochastic collocation (MLSC) methods need much lower computational costs than standard collocation methods if a high accuracy is desired and the regularity of the solution with respect to the parameters is rather low. The method we propose in this work is closely related to [25].

The multi-index stochastic collocation approach from [10, 9] is perhaps the most important extension of MLSC. This approach computes an estimator based on mixed difference operators in all individual spatiotemporal and stochastic dimensions. This is more general than in the MLSC method described here, where the refinement in the stochastic dimensions is determined by a single parameter (and the temporal discretisation, too). By solving a simplified knapsack problem, a quasi optimal multi-index set for the difference operators is selected based on profits computed from a priori work and error bounds. Another extension of MLSC is presented in [17], where the approach from [25] was extended in such a way that the adaptive (spatial) mesh refinement is allowed to vary with the samples. This allows an optimization of the computational work in each stochastic collocation point which was shown to be superior to strategies which are only adaptive in the spatial or stochastic discretisation, but ignore properties of individual samples.

Many stochastic and deterministic PDEs or ODEs can be decomposed into two or more parts which can be solved numerically with significantly lower computational costs than the entire problem. Splitting methods exploit this property and provide a family of time-integrators which are both efficient and easy to implement. The accuracy, stability, and the geometric properties of splitting methods have been thoroughly analyzed in a large number of papers; examples in the context of the linear Schrödinger equation are, e.g., [1, 5, 11, 14, 18, 19, 21] and references therein. Applying splitting methods to PDEs with uncertain parameters is straightforward if a non-intrusive method is chosen to deal with the randomness. Moreover, error bounds for the full discretization are readily obtained by combining the available error bounds for splitting methods and for the space discretization with the known convergence results for non-intrusive methods. This is *not* true for multi-level stochastic collocation methods, because here convergence of the method used for computing the sample solutions does *not* imply convergence of the multi-level approximation. To obtain convergence of the multi-level method, certain conditions must be fulfilled, which are required to combine the information computed on different levels. These conditions involve a stronger norm with respect to the random parameters, and for splitting methods and other time-integrators, these conditions cannot be verified with standard results from the literature.

Goals and results. We propose and analyze a multi-level stochastic collocation method on sparse grids for time-dependent linear Schrödinger equations with an uncertain potential and uncertain initial data. We assume that the dimension of the state space is moderate, but that the parameter set which models the uncertainty can be high-dimensional. The sample solutions at the nodes of the sparse grid are computed with time discretization by the Strang splitting method. This yields a method which is efficient and easy to implement. The focus of our work, however, is on the convergence analysis. We prove new error bounds for the time discretization, which are the cornerstone to verify conditions for convergence of the multi-level stochastic collocation method. The main challenge is the fact that the linear Schrödinger equation is neither elliptic nor parabolic, such that typical solutions *have only finite regularity.* Our work is the first convergence analysis for a multi-level stochastic collocation method with time discretization by a splitting method. Splitting methods within the framework of stochastic *Galerkin* methods – which are not the subject of our paper – have been analyzed, e.g., in [16, 27, 4].

Structure of this paper. In Section 2 the problem setting is introduced. The Strang splitting method and stochastic collocation methods on sparse grids are reviewed in Subsections 3.1 and 3.2, respectively. In Subsection 3.3 we explain how the techniques can be combined to obtain a single-level method. This approach is then extended to a multi-level version in Subsection 4.1. In particular, conditions for convergence of the multi-level stochastic collocation method are formulated; cf. Assumptions 2 and 3. In Subsection 4.2 we present our main result (Theorem 3) and show that the conditions for convergence can be verified with this theorem. Since the proof is rather long and technical, it is postponed to Section 7. The efficiency of the method is discussed in Section 5 and the computational savings are confirmed by numerical examples in Section 6.

2. Linear Schrödinger equations with random data.

We consider the parametric linear Schrödinger equation

$$\partial_t u(t,x,y) = \mathrm{i}\Delta u(t,x,y) + \mathrm{i}V(x,y)u(t,x,y), \qquad t\in[0,T],\ x\in\mathbb{T}^D,\ y\in\Gamma, \tag{2.1a}$$

$$u(0,x,y) = u_0(x,y), \qquad x\in\mathbb{T}^D,\ y\in\Gamma, \tag{2.1b}$$

with solution $u\colon [0,T]\times\mathbb{T}^D\times\Gamma\to\mathbb{C}$, where T is the length of the time interval, $\mathbb{T}^D=(\mathbb{R}/\mathbb{Z})^D$ denotes the D-dimensional torus, Γ is some compact parameter set and $V(\cdot,y)\in L^\infty(\mathbb{T}^D)$ is a bounded real-valued potential. With no loss of generality we assume that $\Gamma=[-1,1]^d$. The solution $u=u(t,x,y)$ depends on the temporal variable t, the spatial variable x, and on a parameter vector y which accounts for uncertainty in the potential V and the initial data u_0. These uncertainties are caused, e.g., by modelling or measurement errors.

The focus of this paper is on the t- and y-discretizations, whereas no discretization in x is made. The space discretization of (2.1) can be carried out with standard methods, which is briefly addressed in the context of the numerical experiments in Section 6. Most of the time, the spatial variable x will be hidden in our notation: instead of denoting the solution by $u=u(t,x,y)$, we consider $u(t,y):x\mapsto u(t,x,y)$ as an element in the Hilbert space $X=L^2(\mathbb{T}^D)$. With this convention, (2.1) can be formulated as a parameter-dependent

abstract Cauchy problem

$$\partial_t u(t,y) = \mathrm{i}\Delta u(t,y) + \mathrm{i}V(y)u(t,y), \qquad t \in [0,T],\ y \in \Gamma, \tag{2.2a}$$

$$u(0,y) = u_0(y), \qquad y \in \Gamma, \tag{2.2b}$$

with solution $u\colon [0,T] \times \Gamma \to X$. The operator

$$H(y_\star) = \Delta + V(y_\star)\colon H^2(\mathbb{T}^D) \to X$$

is self-adjoint for every $y_\star \in \Gamma$ by the Kato-Rellich theorem [15, Chapter V.4.1, Theorem 4.3]. Hence, $\mathrm{i}H(y_\star)$ generates a strongly continuous unitary group $(\mathrm{e}^{\mathrm{i}tH(y_\star)})_{t\in\mathbb{R}}$ by Stone's theorem [24, Chapter 1.10, Theorem 10.8], which means that for every $y_\star$, (2.2) has a unique solution $u(t,y_\star) = \mathrm{e}^{\mathrm{i}tH(y_\star)}u_0(y_\star)$ with constant norm. Throughout we assume that $\|u_0(y)\|_X = 1$ for all y, such that $\|u(t,y)\|_X = 1$ for all t and all y.

The following assumption on the parameter space is made henceforth.

Assumption 1. *The variable $y \in \Gamma$ corresponds to a realization of a random variable $Y \sim \mathcal{U}(-1,1)^d$ with uniform probability density $\varrho(y) = \frac{1}{2^d}$.*

This assumption is made in order to use a particular error estimate for the sparse grid interpolation which is given in Subsection 3.2. Our results could also be adapted to other choices of Γ and ϱ. In particular, every bounded probability density $\hat\varrho$ on $\Gamma = [-1,1]^d$ can be handled, since it defines a weaker norm. If $\hat\varrho$ is also bounded from below, then the induced norms are even equivalent. Problems with, e.g., different probability measures and different abscissas in each direction could also be treated. The requirement that Γ is compact, however, is essential.

3. Discretization of time and of the parameter set.

3.1. Time discretization with the Strang splitting method. In this subsection we consider (2.2) without uncertainty or, equivalently, for a *fixed* vector $y = y_\star \in \Gamma$. In this case, a very popular and widely used method to approximate the solution is the Strang splitting method

$$\widetilde{u}_n(y_\star) = \Phi_\tau(y_\star)\widetilde{u}_{n-1}(y_\star) := \mathrm{e}^{\mathrm{i}\tau V(y_\star)/2}\mathrm{e}^{\mathrm{i}\tau\Delta}\mathrm{e}^{\mathrm{i}\tau V(y_\star)/2}\widetilde{u}_{n-1}(y_\star), \qquad n = 1,2,\dots, \tag{3.1}$$

which successively computes approximations $\widetilde{u}_n(y_\star) \approx u(t_n,y_\star)$ at times $t_n = n\tau$ with a given step-size $\tau > 0$; see, e.g., [1, 5, 11, 14, 18, 19, 21] and references therein. Note that $\widetilde{u}_n(y_\star) = \Phi_\tau^n(y_\star)u_0(y_\star)$ for $n \in \mathbb{N}_0$ with the notation $\Phi_\tau^0(y_\star) = \mathrm{Id}$ and $\Phi_\tau^n(y_\star) = \Phi_\tau(y_\star)(\Phi_\tau(y_\star))^{n-1}$. The Strang splitting is a time-reversible second-order method with a unitary numerical flow. This method is particularly efficient when combined with a pseudo-spectral method for space discretization, because then $\mathrm{e}^{\mathrm{i}\tau\Delta}$ can be computed by means of the Fast Fourier transform; see, e.g., Section II.1.3 in [19].

The accuracy of the Strang splitting was analyzed, e.g., in [19, III.3.2] and in a more general setting in [14, Section 2-3]. In these references, the following error bounds are shown. Here and below, the commutator of two operators A and B is denoted by $[A,B] = AB - BA$, and $\|\cdot\|_X$ is the usual norm of $X = L^2(\mathbb{T}^D)$.

Theorem 1. *Let $y = y_\star \in \Gamma$ be fixed and let $u(t,y_\star) = \mathrm{e}^{\mathrm{i}tH(y_\star)}u_0(y_\star)$ be the exact solution of (2.2).*

(i) If $V(y_\star) \in L^\infty(\mathbb{T}^D)$ and if the commutator bound

$$\|[V(y_\star), \Delta]w\|_X \leq C\|w\|_{H^1(\mathbb{T}^D)}, \tag{3.2}$$

holds for all $w \in H^1(\mathbb{T}^D)$, then there is a constant C_1 such that

$$\|\mathrm{e}^{\mathrm{i}\tau H(y_\star)}w - \Phi_\tau w\|_X \leq C_1\tau^2\|w\|_{H^1(\mathbb{T}^D)} \tag{3.3}$$

for every $w \in H^1(\mathbb{T}^D)$. If in addition $u_0(y_\star) \in H^1(\mathbb{T}^D)$, then there is a constant C_2 such that

$$\|u(t_n, y_\star) - \Phi_\tau^n u_0(y_\star)\|_X \leq C_2 t_n \tau \max_{s\in[0,T]} \|u(s, y_\star)\|_{H^1(\mathbb{T}^D)}. \tag{3.4}$$

for all $n \in \mathbb{N}_0$ with $t_n = n\tau \in [0, T]$. The constants C_1 and C_2 depend on $\|V(y_\star)\|_{L^\infty(\mathbb{T}^D)}$ and on C from (3.2), but not on τ.

(ii) Suppose that the assumptions from part (i) hold. If the commutator bound

$$\|[[V(y_\star), \Delta], \Delta]w\|_X \leq C\|w\|_{H^2(\mathbb{T}^D)}, \tag{3.5}$$

holds for all $w \in H^2(\mathbb{T}^D)$, then there is a constant C_1 such that

$$\|\mathrm{e}^{\mathrm{i}\tau H(y_\star)}w - \Phi_\tau w\|_X \leq C_1\tau^3\|w\|_{H^2(\mathbb{T}^D)}, \tag{3.6}$$

for every $w \in H^2(\mathbb{T}^D)$. If in addition $u_0(y_\star) \in H^2(\mathbb{T}^D)$, then there is a constant C_2 such that

$$\|u(t_n, y_\star) - \Phi_\tau^n u_0(y_\star)\|_X \leq C_2 t_n \tau^2 \max_{s\in[0,T]} \|u(s, y_\star)\|_{H^2(\mathbb{T}^D)}. \tag{3.7}$$

for all $n \in \mathbb{N}_0$ with $t_n = n\tau \in [0, T]$. The constants C_1 and C_2 depend on $\|V(y_\star)\|_{L^\infty(\mathbb{T}^D)}$ and on the constants in the commutator bounds (3.2) and (3.5), but not on τ.

The inequalities (3.3) and (3.6) are bounds for the *local* error, i.e. for the error after only one time-step. The *global* error after many time-steps is estimated in (3.4) and (3.7). The convergence rate in part (ii) is higher: (3.7) yields second order convergence with respect to τ, whereas (3.4) yields only convergence with order one. On the other hand, the assumptions in part (ii) are stronger.

Remark 1. *The commutator bounds are related to the spatial regularity of the potential $V(y_\star)$. If $V(y_\star) \in W^{2,\infty}(\mathbb{T}^D)$, then the commutator*

$$\begin{aligned}[\Delta, V(y_\star)]w &= (\Delta V(y_\star))w + 2\nabla V(y_\star)\cdot\nabla w + V(y_\star)\Delta w - V(y_\star)\Delta w \\ &= (\Delta V(y_\star))w + 2\nabla V(y_\star)\cdot\nabla w\end{aligned}$$

is only a first-order differential operator – it involves second-order derivatives of $V(y_\star)$, but only first-order derivatives of the function w to which the commutator is applied. Hence, the commutator bound (3.2) holds with a constant which depends on $\|V(y_\star)\|_{W^{2,\infty}(\mathbb{T}^D)}$. In a similar way, it can be checked by a tedious but straightforward calculation that the double commutator $[[\Delta, V(y_\star)], \Delta]$ is only a second-order differential operator if $V(y_\star) \in W^{4,\infty}(\mathbb{T}^D)$, because the fourth-order derivatives cancel; cf. [19, page 99]. As a consequence, the commutator bound (3.5) holds with a constant which depends on $\|V(y_\star)\|_{W^{4,\infty}(\mathbb{T}^D)}$.

3.2. Sparse grid discretization of the parameter set. The Strang splitting allows us to compute accurate approximations $\Phi_\tau^n u_0(y_\star) \approx \mathrm{e}^{\mathrm{i}t_n H(y_\star)} u_0(y_\star)$ to the solution of (2.2) for every *single* $y_\star \in \Gamma$. However, this is not enough, since our goal is to approximate $y \mapsto u(t_n, y)$ for all values of y *simultaneously*. The principle of stochastic collocation is to compute $\Phi_\tau^n u_0(y_i) \approx u(t_n, y_i)$ for finitely many vectors $y_1, \dots, y_\eta \in \Gamma$, and then to use these values to construct an interpolant. But since the dimension d of the parameter space $\Gamma = [-1,1]^d$ is typically not small, one has to choose the collocation points $y_1, \dots, y_\eta$ carefully to avoid the *curse of dimension*, i.e. the effect that for a fixed accuracy the number of nodes η has to grow exponentially in d. We use sparse grids to choose $y_1, \dots, y_\eta$ in order to alleviate the curse of dimension to a certain extent.

The following description of the interpolation process follows the presentation in [23, Sec. 2.1]. Let $\mathbb{P}_{m_i}(X) = \mathbb{P}_{m_i} \otimes X$, where $\mathbb{P}_{m_i}$ is the space of univariate polynomials on $[-1,1]$ with complex coefficients and degree not larger than m_i. For any index $i \in \mathbb{N}$, let $y_1^i, \dots, y_{m_i}^i \in [-1,1]$ be a set of abscissas and let

$$Q_i \colon C([-1,1], X) \to \mathbb{P}_{m_i}(X), \qquad Q_i w(y) = \sum_{j=1}^{m_i} w(y_j^i) \ell_j^i(y), \tag{3.8}$$

be the corresponding interpolation operator. Here, ℓ_j^i, $j = 1, \dots, m_i$, are the Lagrange polynomials corresponding to the abscissas $y_1^i, \dots, y_{m_i}^i$. The index i determines the accuracy of the interpolation, while m_i is the corresponding number of nodes actually used by Q_i. The mapping $i \mapsto m_i$ is called growth rule.

In the multivariate setting the full tensor product interpolation formula corresponding to a multi-index $\mathbf{i} = (i_1, \dots, i_d) \in \mathbb{N}^d$ is given by

$$Q_{\mathbf{i}} w = (Q_{i_1} \otimes \cdots \otimes Q_{i_d}) w = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} w(y_{j_1}^{i_1}, \dots, y_{j_d}^{i_d}) (\ell_{j_1}^{i_1} \otimes \cdots \otimes \ell_{j_d}^{i_d})$$

for $w \in C([-1,1]^d, X)$. Clearly, $m_{i_1} m_{i_2} \cdots m_{i_d}$ function evaluations of w are necessary to compute $Q_{\mathbf{i}} w$. The sparse grid interpolation with level parameter ℓ is now defined via Smolyak's formula

$$\mathcal{A}(\ell, d) w = \sum_{\mathbf{i} \in \mathcal{I}_\ell} (-1)^{\ell + d - |\mathbf{i}|} \binom{d-1}{\ell + d - |\mathbf{i}|} Q_{\mathbf{i}} w, \qquad w \in C([-1,1]^d, X), \tag{3.9}$$

where $\mathcal{I}_\ell = \{\mathbf{i} \in \mathbb{N}^d \mid \ell + 1 \le |\mathbf{i}| \le \ell + d\}$. The nodes of the sparse grid are all points where w is evaluated, i.e.

$$\Big\{ (y_{j_1}^{i_1}, \dots, y_{j_d}^{i_d}) \colon \mathbf{i} \in \mathcal{I}_\ell,\ j_k \in \{1, \dots, m_{i_k}\},\ k \in \{1, \dots, d\}. \Big\}$$

More points and hence more accurate approximations are obtained with a larger value of ℓ. The notation $\mathcal{A}(\ell, d)$ is often used in the literature, but in the following sections, $\mathcal{A}(\ell, d)$ will be denoted by $\mathcal{Q}_\ell$ (without indicating the dimension) in order to express its relation to the

one-dimensional constituents Q_{j_i}. The number of points needed to evaluate $\mathcal{Q}_\ell w = \mathcal{A}(\ell, d)w$ is denoted by η_ℓ.

Now the collocation points $y_1, \dots, y_\eta$ of the stochastic collocation method are simply chosen to be the nodes (3.2) of a sparse grid with a suitable enumeration. These nodes, however, depend on the abscissas y_j^i, which can be chosen in several ways. We decide for the Clenshaw-Curtis abscissas

$$y_j^i = -\cos\left(\frac{\pi(j-1)}{m_i - 1}\right), \qquad j = 1, \dots, m_i, \tag{3.10}$$

for $i > 1$ and $y_j^1 = 0$ with the usual weights, and with growth rule

$$m_1 = 1, \qquad m_i = 2^{i-1} + 1, \qquad i > 1. \tag{3.11}$$

This choice implies that the abscissas for Q_i are a subset of the abscissas for Q_{i+1} and hence the corresponding grids are *nested*. In [3, Prop. 6], it was shown that the corresponding sparse grid interpolation operator $\mathcal{Q}_\ell = \mathcal{A}(\ell, d)$ is actually interpolatory whenever the one-dimensional interpolation grids are nested, which is not clear from the definition (3.9) itself.

For $k \in \mathbb{N}_0$ we consider spaces of continuously differentiable functions given by

$$C^k_{\mathrm{mix}}(\Gamma, X) = \left\{ w \colon \Gamma \to X \;\middle|\; \partial_y^{\mathbf{j}} w \in C(\Gamma, X),\ \mathbf{j} = (j_1, \dots, j_d) \in \mathbb{N}_0^d,\ |\mathbf{j}|_\infty \le k \right\}$$

with norm

$$\|w\|_{C^k_{\mathrm{mix}}(\Gamma,X)} = \max_{|\mathbf{j}|_\infty \le k} \left\|\partial_y^{\mathbf{j}} w\right\|_{C(\Gamma,X)}, \qquad \|w\|_{C(\Gamma,X)} = \sup_{y\in\Gamma} \|w(y)\|_X.$$

These spaces are typically used to establish error bounds for interpolation on sparse grids, see e.g. [3] and [23]. Note that $C^k_{\mathrm{mix}}(\Gamma, X)$ is larger than the classical function space $C^k(\Gamma, X)$, which is defined with $|\mathbf{j}|_1 \le k$ instead of $|\mathbf{j}|_\infty \le k$. Let I denote the identity operator. For $w \in C^k_{\mathrm{mix}}(\Gamma, X)$ with $k \in \mathbb{N}$, Eq. (3.28) in [23] yields the bound

$$\begin{aligned} \|(I - \mathcal{Q}_\ell)w\|_{C(\Gamma,X)} &\le \frac{C}{|C(1+2^k) - 1|}(C(1+2^k))^d(\ell+1)^{2d}2^{-k\ell}\|w\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \\ &\le C(k,d)(\ell+1)^{2d}2^{-k\ell}\|w\|_{C^k_{\mathrm{mix}}(\Gamma,X)}. \end{aligned} \tag{3.12}$$

One may also obtain a version of (3.12) where accuracy is expressed in terms of the number of nodes $\eta = \eta_\ell$ in the sparse grid. In [3], the estimate

$$\|(I - \mathcal{Q}_\ell)w\|_{C(\Gamma,X)} \le C(k,d)\eta^{-k}(\log(\eta))^{(k+2)(d-1)+1}\|w\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \tag{3.13}$$

was given. Slightly better (but more complicated) estimates were stated in [23, Sec. 3.1.1].

3.3. Single-level stochastic collocation method. The sparse grid discretization of Γ can now be combined with the time discretization from 3.1. This yields the following stochastic collocation method.

1. Choose a level parameter $\ell \in \mathbb{N}$, $\eta = \eta_\ell$ and compute the nodes $y_1, \dots, y_\eta \in \Gamma$ of the associated sparse grid. Choose $N \in \mathbb{N}$ and set the step-size to $\tau = T/N$.

2. For every $j = 1, \dots, \eta$ and every $n = 1, \dots, N$ compute approximations

$$\widetilde{u}_n(y_j) = \Phi_\tau^n(y_j) u_0(y_j) \approx u(t_n, y_j)$$

with the Strang splitting.

3. For every $n = 1, \dots, N$ compute the interpolation polynomial $\mathcal{Q}_\ell \Phi_\tau^n u_0$ of the data $(y_j, \widetilde{u}_n(y_j))$, $j = 1, \dots, \eta$. This yields an approximation to $y \mapsto u(t_n, y)$.

The step-size $\tau = T/N$ determines the accuracy of the temporal approximations, whereas the accuracy of the y-approximations depends on the level parameter ℓ from the previous subsection.

4. Multi-level stochastic collocation with Strang splitting. The single-level stochastic collocation method can be used to approximate $y \mapsto u(t_n, y)$ at every time point t_n. In situations where a very accurate approximation is sought-after or where the regularity in y is low such that a very fine sparse grid is required, the efficiency can be improved considerably by multi-level stochastic collocation methods – at least if certain conditions are met. Such methods have been proposed and analyzed in [25, 26, 12]. For more recent works containing remarkable extensions of the approach consider [10, 9, 17].

In the next subsection, we briefly outline how to construct such a multi-level method for (2.2). We closely follow the presentation in [25], where an elliptic problem was considered.

4.1. The multi-level method and conditions for convergence. In the previous section, the sparse grid interpolation operator on level ℓ was denoted by $\mathcal{Q}_\ell$, and the number of nodes by η_ℓ. Because of (3.13), however, we will henceforth index the interpolation operator by the number of points of the sparse grid, i.e. we use the notation $\mathcal{Q}_{\eta_\ell}$ instead of $\mathcal{Q}_\ell$. Moreover, we pretend that $\mathcal{Q}_\eta$ could be defined for *arbitrary* $\eta \in \mathbb{N}$, although this is actually only true if η is the number of nodes of a sparse grid.

Assume for simplicity that only an approximation at the final time T is supposed to be computed; approximations at several times are discussed in Remark 2 below. Given a set of collocation points $y_1, \dots, y_\eta \in \Gamma$ and a number $N \in \mathbb{N}$, the numerical solution at $T = t_N = N\tau$ computed with step-size $\tau = T/N$ is denoted by

$$u_{\eta,\tau}^{(\mathrm{SL})} = \mathcal{Q}_\eta \Phi_\tau^N u_0.$$

The upper index "(SL)" stands for single-level, referring to the fact that only a single point set $\{y_q \colon q = 1, \dots, \eta\}$ and a single step-size τ are used to compute $u_{\eta,\tau}^{(\mathrm{SL})}$. In contrast, multi-level collocation is based on computations with several different step-sizes and point sets.

Choose $N_0 \in \mathbb{N}$, set $\tau_0 = T/N_0$, and $\tau_j = 2^{-j}\tau_0$ for $j \in \mathbb{N}_0$, such that $(\tau_j)_{j \in \mathbb{N}_0}$ is a decreasing sequence of step-sizes. Each of these step-sizes induces a numerical flow Φ_{τ_j} and a number of time-steps $N_j = 2^j N_0$ to reach the final time $T = \tau_j N_j$. For simplicity, the notation

$$u_{\tau_j} = \Phi_{\tau_j}^{N_j} u_0 \approx u(T, \cdot)$$

is used henceforth. As $u_0 = u_0(y)$, $u(T, y)$ and $\Phi_\tau = \Phi_\tau(y)$ depend on y, the approximations $u_{\eta,\tau}^{(\mathrm{SL})} = u_{\eta,\tau}^{(\mathrm{SL})}(y)$ and $u_{\tau_j} = u_{\tau_j}(y)$ are functions in y as well, but the argument "(y)" will often be omitted to improve readability.

Assumption 2. *Suppose that there exists constants $\alpha, C_T > 0$ such that*

$$\|u(T,\cdot) - u_{\tau_j}\|_{C(\Gamma,X)} \leq C_T \tau_j^\alpha$$

for all $j \in \mathbb{N}_0$.

Let $(\eta_\ell)_{\ell\in\mathbb{N}_0}$ be an increasing (but not necessarily strictly increasing) sequence of integers, and let $\mathcal{Q}_{\eta_\ell}$ be an interpolation operator based on η_ℓ nodes. According to (3.13) we expect that $\mathcal{Q}_{\eta_{\ell+1}}$ is more accurate than $\mathcal{Q}_{\eta_\ell}$ if $\eta_{\ell+1} > \eta_\ell$. On the other hand, the cost of one evaluation of $\mathcal{Q}_{\eta_\ell}$ is proportional to η_ℓ. The following assumption is very similar to the assumptions made in [25].

Assumption 3. *There exist constants $C_I, C_\star, \beta, \mu > 0$ and an index $k \in \mathbb{N}$ such that the following holds:*

$$\|v - \mathcal{Q}_{\eta_\ell} v\|_{C(\Gamma,X)} \leq C_I \eta_\ell^{-\mu} \|v\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \qquad \text{for all } v \in C^k_{\mathrm{mix}}(\Gamma,X), \tag{4.1a}$$

$$u_{\tau_j} = \Phi_{\tau_j}^{N_j} u_0 \in C^k_{\mathrm{mix}}(\Gamma,X) \qquad \text{for all } j \in \mathbb{N}_0, \tag{4.1b}$$

$$\|u_{\tau_j}\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \leq C_\star \tau_0^\beta \qquad \text{for all } j \in \mathbb{N}_0, \tag{4.1c}$$

$$\|u_{\tau_{j+1}} - u_{\tau_j}\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \leq C_\star \tau_{j+1}^\beta \qquad \text{for all } j \in \mathbb{N}_0. \tag{4.1d}$$

After these preparations we are in a position to formulate the multi-level stocastic collocation (MLSC) method. We set $u_{\tau_{-1}} = 0$ and start with the telescoping sum

$$u_{\tau_J} = \sum_{j=0}^{J} (u_{\tau_j} - u_{\tau_{j-1}}), \qquad u_{\tau_j} = \Phi_{\tau_j}^{N_j} u_0. \tag{4.2}$$

In practice, only an interpolation of each u_{τ_j} can be computed, not u_{τ_j} itself. The most obvious approach would be to interpolate every difference under the sum with the same interpolation operator. In order to reach a given accuracy, however, it is much more efficient to balance the two errors caused by time-integration and interpolation in a near-optimal way. If j increases, then (4.1d) implies that the difference $u_{\tau_j} - u_{\tau_{j-1}}$ decreases and can thus be interpolated with a coarser (but cheaper) interpolation operator. Conversely, a more accurate interpolation has to be used for the summands with small j, but for those terms, the time-integration is less costly. This suggests to define the multi-level approximation $u_J^{(\mathrm{ML})}$ by

$$u_J^{(\mathrm{ML})} = \sum_{j=0}^{J} \mathcal{Q}_{\eta_{J-j}} [u_{\tau_j} - u_{\tau_{j-1}}] = \sum_{j=0}^{J} \left(u^{(\mathrm{SL})}_{\eta_{J-j},\tau_j} - u^{(\mathrm{SL})}_{\eta_{J-j},\tau_{j-1}} \right). \tag{4.3}$$

Next, the sequence $(\eta_j)_{j\in\mathbb{N}_0}$ has to be specified. Applying the triangle inequality to the global error yields

$$\|u(T,\cdot) - u_J^{(\mathrm{ML})}\|_{C(\Gamma,X)} \leq \|u(T,\cdot) - u_{\tau_J}\|_{C(\Gamma,X)} + \|u_{\tau_J} - u_J^{(\mathrm{ML})}\|_{C(\Gamma,X)} = (\mathtt{I}) + (\mathtt{II}).$$

We show that for a suitable choice of $(\eta_j)_{j\in\mathbb{N}_0}$, the error components (I) and (II) converge at the same rate, which implies convergence of the multi-level approximation.

The term $(\mathtt{I}) = \|u(T,\cdot) - u_{\tau_J}\|_{C(\Gamma,X)}$ is the error of the time discretization with the splitting method. By Assumption 2 there are parameters $\alpha, C_T > 0$ independent of τ_J such that $(\mathtt{I}) \le C_T \tau_J^\alpha$. From (4.2) and Assumption 3, we may estimate the stochastic collocation error as

$$(\mathtt{II}) \le \sum_{j=0}^{J} \big\| (u_{\tau_j} - u_{\tau_{j-1}}) - \mathcal{Q}_{\eta_{J-j}}(u_{\tau_j} - u_{\tau_{j-1}}) \big\|_{C(\Gamma,X)} \le \sum_{j=0}^{J} C_I C_\star \eta_{J-j}^{-\mu} \tau_j^\beta.$$

Choosing a sequence $(\eta_j)_{j\in\mathbb{N}_0}$ with

$$\eta_{J-j}^{-\mu} \le C_T \big((J+1) C_I C_\star\big)^{-1} \tau_J^\alpha \tau_j^{-\beta} \tag{4.4}$$

yields $(\mathtt{II}) \le C_T \tau_J^\alpha$, such that the error contribution from $(\mathtt{II})$ and $(\mathtt{I})$ is basically the same. It follows that

$$\|u(T,\cdot) - u_J^{(\mathrm{ML})}\|_{C(\Gamma,X)} \le 2 C_T \tau_J^\alpha, \tag{4.5}$$

which means that the multi-level approximation converges as $J \to \infty$. However, the convergence relies on the somewhat abstract Assumptions 2 and 3. The next step is to verify these assumptions for the Strang splitting applied to (2.2).

Remark 2. *In exactly the same way approximations at the times $\tau_0, 2\tau_0, 3\tau_0, \dots, N_0\tau_0 = T$ could be computed. However, the efficiency of the multi-level method comes from the fact that some approximations are made with a rather large step-size $\tau_j \le \tau_0$. If N_0 is rather large and thus even the maximal step-size $\tau_0 = T/N$ is rather small, then the efficiency is typically reduced.*

4.2. Verification of the conditions for convergence. Theorem 1 yields the pointwise error bound

$$\|u(T,y_\star) - u_{\tau_j}(y_\star)\|_X = \|u(T,y_\star) - \Phi_{\tau_j}^{N_j} u_0(y_\star)\|_X \le C \tau_j^\alpha \tag{4.6}$$

for every single $y_\star$ with $\alpha = 1$ or $\alpha = 2$, depending on the spatial regularity of the initial data and the potential. Extending this result to an error bound in $\|\cdot\|_{C(\Gamma,X)}$ is straightforward if the regularity assumptions in Theorem 1 hold uniformly in y, which will be shown below.

For functions $v\colon \Gamma \to X$ which admit a holomorphic extension to a complex polyellipse it can be shown that $\|v - \mathcal{Q}_{\eta_\ell} v\|_{C(\Gamma,X)} \le \mathcal{O}(\eta_\ell^{-\mu})$, but for functions of finite regularity, as in our case, the error estimate (3.13) contains a logarithmic factor $\log(\eta_\ell)^E$ with $E = (k+2)(d-1)+1$. To the best of our knowledge, it is not really possible to include this factor into the construction of the multi-level method and into the analysis in Section 5.1. To get around this problem one can simply use that $\log(\eta_\ell)^E \le C\eta_\ell$ for a constant C which depends on k and d, but not on η_ℓ. Hence, the estimate (4.1a) in Assumption 3 holds with $\mu = k - 1$. Of course, the loss of one order of convergence is often way too pessimistic.

The main challenge is to prove that the remaining parts of Assumption 3 are true. According to (4.1b) it has to be shown that the numerical solution has a certain degree of smoothness with respect to y. In order to confirm (4.1d) the difference between two appoximations with

different step-sizes has to be bounded in the stronger norm. Such a result cannot be deduced from the classical pointwise error bound (4.6). The larger k, the faster is the convergence of the sparse grid interpolation in (4.1a) (since we can choose $\mu = k - 1$), but the stronger are the conditions (4.1b), (4.1c), and (4.1d).

Our main result is Theorem 3 below. It implies in particular that Assumptions 2 and 3 hold if the initial data and the potential are sufficiently regular. The corresponding conditions are now formulated in detail.

Assumption 4. *Let $u_0 \in C^k_{\mathrm{mix}}(\Gamma, H^2(\mathbb{T}^D))$ for some $k \in \mathbb{N}_0$.*

Assumption 5. *Let $V \in C^k_{\mathrm{mix}}(\Gamma, W^{2,\infty}(\mathbb{T}^D))$ for some $k \in \mathbb{N}_0$.*

Assumption 5 means that

$$\|\partial_x^{\mathbf{r}} \partial_y^{\mathbf{m}} V\|_{C(\Gamma, L^\infty(\mathbb{T}^D))} \leq C, \qquad |\mathbf{r}|_1 \leq s, \quad |\mathbf{m}|_\infty \leq k. \tag{4.7}$$

holds for $s = 2$. Replacing $V(y_\star)$ in Remark 1 by $\partial_y^{\mathbf{m}} V(y)$ and using that partial derivatives with respect to x and y are independent shows that (4.7) implies the commutator bound

$$\|[\partial_y^{\mathbf{m}} V, \Delta] w\|_{C(\Gamma, X)} \leq C \|w\|_{C(\Gamma, H^1(\mathbb{T}^D))}, \qquad |\mathbf{m}|_\infty \leq k \tag{4.8}$$

for all $w \in C(\Gamma, H^1(\mathbb{T}^D))$. Assumption 4 and the commutator bound (4.8) are generalizations of the assumptions made in part (i) of Theorem 1. We will show that this is sufficient to verify (4.1c) and (4.1d) in Assumption 3 for $\beta = 1$. In order to obtain $\beta = 2$ in (4.1c) and (4.1d), more regularity is required, i.e. Assumption 5 has to be replaced by the following one.

Assumption 6. *Let $V \in C^k_{\mathrm{mix}}(\Gamma, W^{4,\infty}(\mathbb{T}^D))$ for some $k \in \mathbb{N}_0$.*

Assumption 6 implies Assumption 5 and, as in Remark 1, the commutator bound

$$\|[[\partial_y^{\mathbf{m}} V, \Delta], \Delta] w\|_{C(\Gamma, X)} \leq C \|w\|_{C(\Gamma, H^2(\mathbb{T}^D))}, \qquad |\mathbf{m}|_\infty \leq k \tag{4.9}$$

for all $w \in C(\Gamma, H^2(\mathbb{T}^D))$, which is a generalization of (3.5).

Assumption 4, 5, and 6 can be easily checked in practice, because these assumptions concern the *given* initial data and the *given* potential. In contrast, the abstract conditions (4.1b), (4.1c), and (4.1d) refer to the numerical solution, which is not known *a priori*.

Theorem 2. *Suppose that Assumption 4 and Assumption 5 hold for some $k \in \mathbb{N}_0$. Then, the classical solution of the initial value problem (2.2) has the regularity*

$$u \in C^1\big([0,T], C^k_{\mathrm{mix}}(\Gamma, X)\big) \cap C\big([0,T], C^k_{\mathrm{mix}}(\Gamma, H^2(\mathbb{T}^D))\big).$$

The proof of Theorem 2 is based on classical techniques from semigroup theory and can be found in the supplementary material, Section SM1. A consequence of Theorem 2 is that

$$M_k^{(s)} = \max_{t \in [0,T]} \|u(t,\cdot)\|_{C^k_{\mathrm{mix}}(\Gamma, H^s(\mathbb{T}^D))} \tag{4.10}$$

is well-defined for $s \in \{1, 2\}$.

We are now ready to state our main results. The proofs are quite long and therefore postponed to later sections.

Theorem 3. *Let $0 < \tau \le 1$ and set $t_n = n\tau$. Let $H(y) = \Delta + V(y)$ such that the exact solution of (2.2) is $u(t,y) = \mathrm{e}^{\mathrm{i}tH(y)}u_0(y)$.*

(i) If Assumption 4 and Assumption 5 are true with the same $k \in \mathbb{N}_0$, then $\Phi_\tau^n u_0 \in C^k_{\mathrm{mix}}(\Gamma, X)$ for all n. Moreover, there is a constant C such that

$$\|u(t_n,\cdot) - \Phi_\tau^n u_0\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \le C M_k^{(1)} \tau \qquad \text{for} \qquad t_n = n\tau \in [0,T]$$

with $M_k^{(1)}$ defined by (4.10). The constant C depends on T and on the constants in (4.8) and (4.7) with $s = 2$.

(ii) If, in addition, Assumption 6 is true with the same $k \in \mathbb{N}_0$, then there is a constant C such that

$$\|u(t_n,\cdot) - \Phi_\tau^n u_0\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \le C M_k^{(2)} \tau^2 \qquad \text{for} \qquad t_n = n\tau \in [0,T]$$

with $M_k^{(2)}$ defined by (4.10). The constant C depends on T and on the constants in (4.9) and (4.7) with $s = 4$.

The proof of Theorem 3 is given in Section 7. Choosing $k = 0$ shows that Assumption 2 holds with $\alpha = \beta = 1$ in case (i) and $\alpha = \beta = 2$ in case (ii).

Verification of (4.1b), (4.1c), and (4.1d). Applying Theorem 3 with $n = N_j$, $\tau = \tau_j = T/N_j$ and $t_n = T$ verifies (4.1b) and yields the bound

$$\|u(T,\cdot) - u_{\tau_j}\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \le C M_k^{(\beta)} \tau_j^\beta$$

with $\beta = 1$ in case (i) and $\beta = 2$ in case (ii). With $\tau_{j+1}^\beta + \tau_j^\beta = (1+2^\beta)\tau_{j+1}^\beta$ it follows that

$$\begin{aligned}\|u_{\tau_{j+1}} - u_{\tau_j}\|_{C^k_{\mathrm{mix}}(\Gamma,X)} &\le \|u_{\tau_{j+1}} - u(T,\cdot)\|_{C^k_{\mathrm{mix}}(\Gamma,X)} + \|u(T,\cdot) - u_{\tau_j}\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \\ &\le C M_k^{(\beta)} (1+2^\beta) \tau_{j+1}^\beta\end{aligned}$$

such that (4.1d) is true. Moreover, the estimate

$$\|u_{\tau_j}\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \le \|u_{\tau_j} - u(T,\cdot)\|_{C^k_{\mathrm{mix}}(\Gamma,X)} + \|u(T,\cdot)\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \le \left(C M_k^{(\beta)} + \frac{M_k^{(0)}}{\tau_0^\beta} \right) \tau_0^\beta$$

shows that (4.1c) holds for a sufficiently large $C_\star$.

5. Efficiency of the multi-level approximation.

5.1. Computational costs for a given accuracy.

Here we consider the computational cost required to achieve a desired accuracy ε with the MLSC method. This analysis relies on the convergence rates from Assumptions 2 and 3.

In the rest of this section we use the following notation: It holds $a \lesssim b$ if and only if $a \le Cb$ for some constant C which is independent of the step-size τ, the number of interpolation points η, the level j, and the accuracy ε. Similarly, we have $a \eqsim b$ if and only if $a = Cb$ for some constant C with the same properties.

Let C_j denote the cost of "evaluating" $u_{\tau_j} - u_{\tau_{j-1}}$ at a sample y. Since the number of time steps of the splitting method is $N_j = T/\tau_j$, it is natural to assume the following.

Assumption 7. $C_j \lesssim \tau_j^{-1}$.

The *total computational cost* of the MLSC approximation (4.3) is defined as

$$C^{(\mathrm{ML})} = \sum_{j=0}^{J} \eta_{J-j} C_j. \tag{5.1}$$

The following result quantifies the cost which is needed to achieve an accuracy of ε with the MLSC method.

Theorem 4. *Suppose that Assumption 4 – 7 hold and assume that $\alpha \geq \min\{\beta, \mu\}$. Then, for given $\varepsilon < \mathrm{e}^{-1}$, there exists $J \in \mathbb{N}_0$ and a sequence $(\eta_j)_{j=0}^J$ of real numbers such that*

$$\|u(T,\cdot) - u_J^{(ML)}\|_{C(\Gamma,X)} \leq \varepsilon \tag{5.2}$$

and simultaneously

$$C_\varepsilon^{(ML)} \lesssim \begin{cases} \varepsilon^{-\frac{1}{\mu}}, & \mu < \beta, \\ \varepsilon^{-\frac{1}{\mu}} |\log(\varepsilon)|^{1+\frac{1}{\mu}}, & \mu = \beta, \\ \varepsilon^{-\frac{1}{\mu} - \frac{\mu-\beta}{\alpha\mu}}, & \mu > \beta. \end{cases}$$

The sequence $(\eta_j)_{j=0}^J$ is explicitly given by

$$\eta_{J-j} = (2C_I C_\star \max\{\tau_0^\beta, 1\} \mathcal{S}(J))^{1/\mu} \varepsilon^{-1/\mu} 2^{-j(\beta+1)/(\mu+1)}, \qquad j = 0, \dots, J, \tag{5.3}$$

where

$$\mathcal{S}(J) = \sum_{j=0}^{J} 2^{-j(\beta-\mu)/(\mu+1)}.$$

Proof. The proof is the same as in [25, Thm. 4.2]. ∎

In Subsection 4.2 we have seen that Theorem 3 yields $\alpha = \beta = 1$ (under Assumption 4 and 5) or $\alpha = \beta = 2$ (under Assumption 4 and 6). In both cases the requirement $\alpha \geq \min\{\beta, \mu\}$ is satisfied. For $\alpha = \beta = 2$, Theorem 4 implies that $\|u(T,\cdot) - u_J^{(\mathrm{ML})}\|_{C(\Gamma,X)} \leq \varepsilon$ holds with

$$C_\varepsilon^{(\mathrm{ML})} \lesssim \begin{cases} \varepsilon^{-\frac{1}{\mu}}, & \mu < 2, \\ \varepsilon^{-\frac{1}{2}} |\log(\varepsilon)|^{\frac{3}{2}}, & \mu = 2, \\ \varepsilon^{-\frac{1}{2}}, & \mu > 2. \end{cases}$$

The optimal choice for η_{J-j} gives in general only a real number, not an integer. In practice, however, the interpolation operators $\mathcal{Q}_m$ are only available for certain integer levels ℓ corresponding to $m = m_\ell$, the number of interpolation points on that level. To determine a practicable family $(\widetilde{\eta}_j)_{j=0}^J$ as a replacement for $(\eta_j)_{j=0}^J$, one could simply choose the next integer $\widetilde{\eta}_j = m_{\ell(j)}$ for which an interpolation operator (and hence an associated sparse grid) is available, i.e.

$$\widetilde{\eta}_j = \min\{m_\ell \colon \ell \in \mathbb{N},\ \eta_j \leq m_\ell\}, \quad j = 0, \dots, J. \tag{5.4}$$

This choice may not lead precisely to the cost estimate from Theorem 4, but in practice one often observes that the cost behaves nearly as predicted. However, one should be aware of the fact that the sequence $(m_\ell)_{\ell\in\mathbb{N}}$ usually grows exponentially in case of nested point sequences, see e.g. (3.11) for the growth rule which is usually applied with Clenshaw-Curtis points. Hence, $\widetilde{\eta}_j$ might be up to twice as large as η_j in some cases, which could be crucial if the stochastic dimensions d is large, or if very accurate solutions (and hence large values of η_J) are required. In such cases, the simple choice (5.4) could severely influence the cost behaviour of the MLSC method. This is the main reason why other strategies to determine $(\widetilde{\eta}_j)_{j=0}^J$ are discussed in [25, Rem. 6.1, 6.3]. In our numerical experiments, we will also use the strategy described as "up/down" in their article.

In some applications the goal is not to approximate the wave function u itself, but rather a quantity of interest. Typical quantities of interest in case of a single particle are its *position*

$$P\colon X \to \mathbb{R}^D, \qquad u \mapsto \int_{\mathbb{T}^D} x|u(x)|^2 \mathrm{d}x, \tag{5.5}$$

or the probability that the particle is located in a set $S \subset \mathbb{T}^D$,

$$M_S\colon X \to \mathbb{R}, \qquad u \mapsto \int_S |u(x)|^2 \mathrm{d}x. \tag{5.6}$$

For continuously Fréchet differentiable observables $\chi(u)$ of the wave function u, the rate of convergence is at least as good as for the wave function itself, and Theorem 4 is true if $\|u(T,\cdot) - u_J^{(\mathrm{ML})}\|_{C(\Gamma,X)}$ is replaced by the corresponding expected error in the quantity of interest. We omit the details.

5.2. Comparison with single level collocation methods. Under the assumptions of Theorem 4, the error of the single-level collocation method can be bounded by

$$\|u(T,\cdot) - u_{\eta_*,\tau_*}^{(\mathrm{SL})}\| \le C_T \tau_*^\alpha + C_I \|u_{\tau_*}\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \eta_*^{-\mu}$$

for any admissible $\eta_* \in \mathbb{N}$ and $\tau_* > 0$. To make both contributions equal to $\varepsilon/2$ (or ε, since we ignore constants anyway), one can choose $\tau_* \eqsim \varepsilon^{\frac{1}{\alpha}}$ and $\eta_* \eqsim \varepsilon^{-\frac{1}{\mu}}$. The computational cost to achieve the total error ε is then bounded by

$$C_\varepsilon^{(\mathrm{SL})} \eqsim \frac{\eta_*}{\tau_*} \eqsim \varepsilon^{-\frac{1}{\mu}-\frac{1}{\alpha}}. \tag{5.7}$$

To compare this with Theorem 4, we consider the quotient $C_\varepsilon^{(\mathrm{ML})}/C_\varepsilon^{(\mathrm{SL})}$ which indicates the *cost reduction* of the multi-level approach compared to the single-level approach. By Theorem 4 and (5.7), we have

$$\frac{C_\varepsilon^{(\mathrm{ML})}}{C_\varepsilon^{(\mathrm{SL})}} \eqsim \begin{cases} \varepsilon^{\frac{1}{\alpha}}, & \mu < \beta, \\ \varepsilon^{\frac{1}{\alpha}} |\log(\varepsilon)|^{1+\frac{1}{\mu}}, & \mu = \beta, \\ \varepsilon^{\frac{\beta}{\alpha\mu}}, & \mu > \beta. \end{cases} \tag{5.8}$$

Note that only the decay rate in ε and μ is meaningful in the above discussion of the cost savings, because constants which appear in $C_\varepsilon^{(\mathrm{ML})}$ and $C_\varepsilon^{(\mathrm{SL})}$ have been ignored.

For $\alpha = \beta = 2$ we observe that the cost reductions are $\varepsilon^{\frac{1}{\alpha}} = \varepsilon^{\frac{1}{2}}$ for low regularity ($\mu < 2$), $\varepsilon^{\frac{1}{\alpha}} |\log(\varepsilon)|^{3/2}$ for $\mu = 2$ and $\varepsilon^{\frac{\beta}{\alpha\mu}} = \varepsilon^{\frac{1}{\mu}}$ for higher regularity ($\mu > 2$). Clearly, the savings are most noticeable if the regularity μ of the solution is rather low (and hence generally more levels are required) and the tolerance is small. Figure 1 below gives a picture of this situation (dark blue is best, yellow means "no savings"). Note that (5.8) considered as a function in μ and ε has a discontinuity at $\mu = \beta = 2$ due to the logarithmic term. Since this case corresponds to a null set, however, we have plotted (5.8) only for $\mu > 2$ and $\mu < 2$ for better visibility.

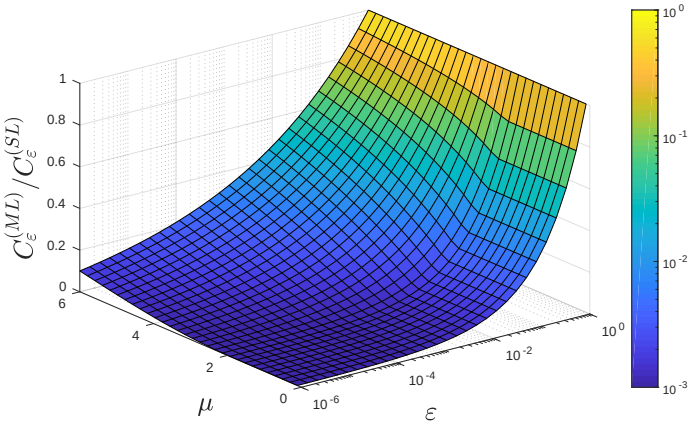


Figure 1. *Cost reduction* (5.8) *of the multi-level approach*

6. Numerical experiments.

For the following numerical tests we consider the equation

$$\partial_t u(t,x,y) = \frac{\mathrm{i}}{2}\partial_x^2 u(t,x,y) + \mathrm{i}V(x,y)u(t,x,y), \qquad t \in [0,T],\ x \in \mathbb{T},\ y \in \Gamma, \tag{6.1a}$$

$$u(0,x,y) = u_0(x,y), \qquad x \in \mathbb{T},\ y \in \Gamma. \tag{6.1b}$$

Recall that the random variables $Y_1, \dots, Y_d$ which correspond to the parameters $y_1, \dots, y_d$ are uniformly distributed on $[-1,1]$ by Assumption 1.

In order to study the convergence of the MLSC method we compare the final approximation at time T with a reference solution $u_{\mathrm{ref}}(T,\cdot,\cdot)$. Now we explain how such a reference solution may be obtained. In order to simplify the corresponding formulas, the factor $1/2$ in front of the second derivative was introduced in (6.1a). This factor was missing in (2.1) but does not affect the preceding analysis substantially.

Reference solution. If we replace the torus $\mathbb{T}$ by $\mathbb{R}$ and assume that the potential is a polynomial of degree 2 with representation

$$V(x,y) = -\nu(y)(x - \kappa(y))^2 - \gamma(y), \tag{6.2}$$

then a family of solutions to the linear Schrödinger equation is given by parametrized Gaussians

$$u(t,x,y) = \exp(w(t,x,y)) \tag{6.3a}$$

$$\text{with} \qquad w(t,x,y) = \frac{\mathrm{i}}{2}C(t,y)(x-q(t,y))^2 + \mathrm{i}p(t,y)(x-q(t,y)) + \mathrm{i}\xi(t,y), \tag{6.3b}$$

cf. [19, Sec. II.4.1]. The functions $p(t,y), q(t,y) \in \mathbb{R}$ and $C(t,y), \xi(t,y) \in \mathbb{C}$ are related via the four ODEs

$$\partial_t q(t,y) = p(t,y), \tag{6.4a}$$

$$\partial_t p(t,y) = -2\nu(y)(q(t,y) - \kappa(y)), \tag{6.4b}$$

$$\partial_t \xi(t,y) = \frac{\mathrm{i}C(t,y)}{2} + \frac{1}{2}p(t,y)^2 - \nu(y)(q(t,y)-\kappa(y))^2 - \gamma(y), \tag{6.4c}$$

$$\partial_t C(t,y) = -C(t,y)^2 - 2\nu(y), \tag{6.4d}$$

supplied with initial values. If the imaginary part of $C(t,y)$ is strictly positive for $t = 0$, then this is the case for all t, such that $|u(t,\cdot,y)|$ is a real Gaussian. However, neither the potential (6.2) nor the solution (6.3) are periodic in space, and thus this construction does not seem to be compatible with the PDE (6.1) on the torus. But the complex Gaussian (6.3) decays exponentially, and as long as it is almost zero outside the interval $[-L, L]$ for all t and y, the error caused by imposing periodic boundary conditions at $\pm L$ is negligible; cf. [19, p. 75]. Hence, (6.3) provides highly accurate solutions to the Schrödinger equation on the torus if the interval $[-L, L]$ is sufficiently large. For the same reason, one can expect that the error bounds from Theorem 3 remain true although the underlying assumptions are, strictly speaking, not met.

In order to obtain a reference solution to (6.1)–(6.2) with initial data $u_0(x,y) = \exp(w(0,x,y))$, $N_{\mathrm{ref}} = 10.000$ (pseudo-)random vectors $y^1, \dots, y^{N_{\mathrm{ref}}} \in \Gamma$ were drawn from the joint distribution of $Y \sim \mathcal{U}((-1,1)^d)$. For each y^j the ODE system (6.4) was solved with a Dormand-Prince method with relative error tolerance set to 10^{-10}. This approach was chosen in order to keep the reference solution independent of the concepts used for the MLSC method (splitting, sparse grids, collocation). Since we focus on the error induced by discretizing the parameter set Γ and time, however, we have used the same space discretization for the reference solution and for the MLSC method, namely Fourier collocation with $M = 2^{10}$ grid points. Computations were made on the time interval $[0,1]$ and the spatial domain $[-3\pi, 3\pi]$ with periodic boundary conditions. All errors were computed at the endpoint $t = T = 1$ of the time interval.

Two-dimensional example. As a first test, we chose the following parametrization in $d = 2$ dimensions. For $y = (y_1, y_2) \in \Gamma$ the potential (6.2) with

$$\nu(y) = 1 + \frac{\delta}{3}(y_1 + 2y_2), \qquad \kappa(y) = \frac{1}{2}\left(1 + \frac{\delta}{2}(y_1 + y_2)\right), \qquad \gamma(y) = 1 + \frac{\delta}{3}(y_1 + y_2^2)$$

and noise parameter $\delta = \frac{1}{20}$ was used. The initial values at time $t = 0$ were set to

$$\Big(C(0,y), q(0,y), p(0,y), \xi(0,y)\Big) = \left(1 + \frac{\delta}{4}y_2^2 + \mathrm{i}, -2 + \delta y_1^2 y_2^2, 2, 1\right),$$

which defines $u(0,x,y)$ via (6.3).

Since the potential and the initial data are smooth enough, Theorem 3 can be applied with $\alpha = \beta = 2$, which justifies Assumption 2 and 3. In order to illustrate Theorem 4, however, the values of μ and of the product $C_I C_\star$ had to be determined numerically, because the optimal choice of η_{J-j} in (5.3) relies on these values and on the maximal step-size $\tau_0 = 0.1$. Our numerical data confirmed Assumption 2 with $C_T = 1.23$ and $\alpha = 1.96$, and, after setting $\beta = \alpha$, Assumption 3 with $\mu = 1.80$ and $C = C_I C_\star = 8.78$. The values of μ and C were obtained by extrapolating from error diagrams of the quantities in Assumption 3. Only 3 or 4 levels are usually required to observe good values for the constants and rates. For details, we refer to [25, Sec. 6]. The value $\alpha = 1.96$ agrees very well with the order 2 expected according to Theorem 3(ii). In this example the "up/down" rounding strategy was used.

In (4.5) and in (5.2) the error is measured in the norm $\|\cdot\|_{C(\Gamma,X)}$ with $X = L^2(\mathbb{T}^D)$. In the numerical tests, this norm has to be replaced by its discrete counterpart

$$\max_{j=1}^{N_{\mathrm{ref}}} \Big(\frac{6\pi}{M} \sum_{k=1}^{M} |u_J^{(\mathrm{ML})}(T,x_k,y^j) - u_{\mathrm{ref}}(T,x_k,y^j)|^2 \Big)^{1/2} \approx \|u_J^{(\mathrm{ML})}(T,\cdot,\cdot) - u_{\mathrm{ref}}(T,\cdot,\cdot)\|_{C(\Gamma,X)}$$

where x_k, $k = 1,\dots,M$ are the Fourier collocation points in the spatial domain. The fact that Γ is bounded implies the bound $\|w\|_{L^2_\varrho(\Gamma,X)} \le \|w\|_{C(\Gamma,X)}$ for every $w \in C(\Gamma,X)$, with L^2_ϱ denoting the L^2 space with weight ϱ. For this reason, we have also computed the error in the discrete norm

$$\begin{aligned} &\Big(\frac{6\pi}{N_{\mathrm{ref}} M} \sum_{j=1}^{N_{\mathrm{ref}}} \sum_{k=1}^{M} |u_J^{(\mathrm{ML})}(T,x_k,y^j) - u_{\mathrm{ref}}(T,x_k,y^j)|^2 \Big)^{1/2} \\ &\approx \Big(\mathbb{E}\Big[\|u_J^{(\mathrm{ML})}(T,\cdot,\cdot) - u_{\mathrm{ref}}(T,\cdot,\cdot)\|_X^2 \Big] \Big)^{1/2} = \|u_J^{(\mathrm{ML})}(T,\cdot,\cdot) - u_{\mathrm{ref}}(T,\cdot,\cdot)\|_{L^2_\varrho(\Gamma,X)}. \end{aligned}$$

In Figure 2 these two alternatives are indicated by "error in $C(\Gamma,X)$" and "error in $L^2_\varrho(\Gamma,X)$". Moreover, we have investigated two other types of error, namely the error in the expected value

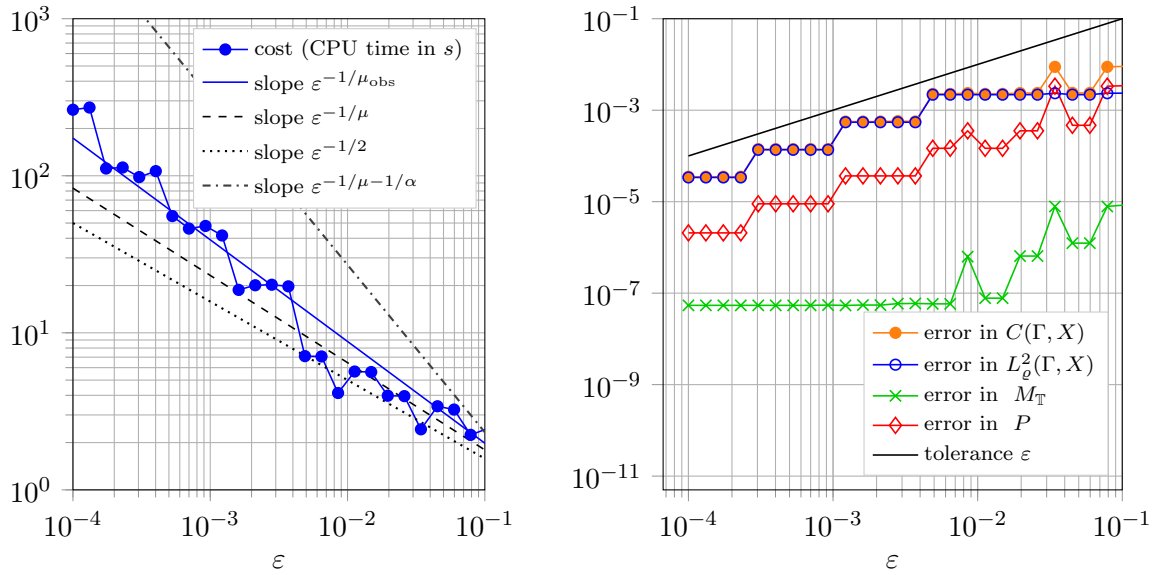
$$\Big| \mathbb{E}\Big[M_{\mathbb{T}}\Big(u_J^{(\mathrm{ML})}(T,\cdot) \Big) - M_{\mathbb{T}}(u_{\mathrm{ref}}(T,\cdot)) \Big] \Big| \tag{6.5}$$

in the quantity of interest $M_{\mathbb{T}}$ defined in (5.6) and the error

$$\Big| \mathbb{E}\Big[P\Big(u_J^{(\mathrm{ML})}(T,\cdot) \Big) - P(u_{\mathrm{ref}}(T,\cdot)) \Big] \Big| \tag{6.6}$$

in the quantity of interest P defined in (5.5). In Figure 2 these two errors are denoted by "error in $M_{\mathbb{T}}$" and "error in P", respectively. Of course, (6.5) and (6.6) must also be replaced by a suitable discretization in the numerical examples. It can be shown that (6.5) is not larger than $\|u_J^{(\mathrm{ML})}(T,\cdot) - u_{\mathrm{ref}}(T,\cdot)\|_{C(\Gamma,X)}$. For (6.6) the situation is more complicated because the functional P is nonlinear. In most situations, however, it is to be expected that (6.6) is much smaller than $\|u_J^{(\mathrm{ML})}(T,\cdot) - u_{\mathrm{ref}}(T,\cdot)\|_{C(\Gamma,X)}$, because applying P can be seen as an averaging which usually cancels a lot of contributions to the error.

Figure 2(b) confirms that the error in $\|\cdot\|_{C(\Gamma,X)}$ stays indeed below the tolerance ε, and that same is true for the other three types of error. Since $2 = \beta > \mu = 1.80$, we expect from Theorem 4 that the computational cost scales as $\varepsilon^{-1/\mu}$. Figure 2(a) shows, however, that the CPU time of the method (blue circles) scales rather as $\varepsilon^{-1/\mu_{\text{obs}}}$ (blue line) with the slightly smaller value $\mu_{\text{obs}} = 1.544$. For comparison, we included the theoretical slope $\varepsilon^{-1/\mu-1/\alpha}$ of the single-level stochastic collocation method from (5.7), too.



(a) Cost vs. error (b) Error vs. ε

Figure 2. *Validation of the MLSC method in the two-dimensional example ($\mu = 1.80$, $\mu_{obs} = 1.544$).*

In the iterative process of finding the correct value of J from Theorem 4 described in [25, Sec. 6.3], one has to compute the multi-level approximations $u_{\widetilde{J}}^{(\text{ML})}$ for all $\widetilde{J} = 0, \dots, J-1$, too. This is included in the CPU time depicted in Figure 2(a), but was not included in the cost from Theorem 4. This could explain why slightly more effort than expected is necessary for smaller tolerances ε. On the other hand, one can reuse most of the approximations computed for $\widetilde{J}$ between 0 and $J-1$ for the multi-level approximation $u_J^{(\text{ML})}$. Another effect which contributes to the slightly worse cost behaviour which we observe is the crude overestimation of the quantity η_{J-j} explained in the text below equation (5.4).

Ten-dimensional example. To check the performance of the method in $d = 10$ dimensions, we considered the quadratic potential (6.2) with

$$\nu(y) = 1 + \frac{\delta}{3}(y_1 + 2y_2), \qquad \kappa(y) = \frac{1}{2}\left(1 + \frac{\delta}{2}(y_3 + y_4)\right), \qquad \gamma(y) = 1 + \frac{\delta}{3}(y_5 + y_6^2)$$

for $y = (y_1, \dots, y_{10}) \in \Gamma$, and with noise parameter $\delta = \frac{1}{20}$. The initial values at time $t = 0$ were

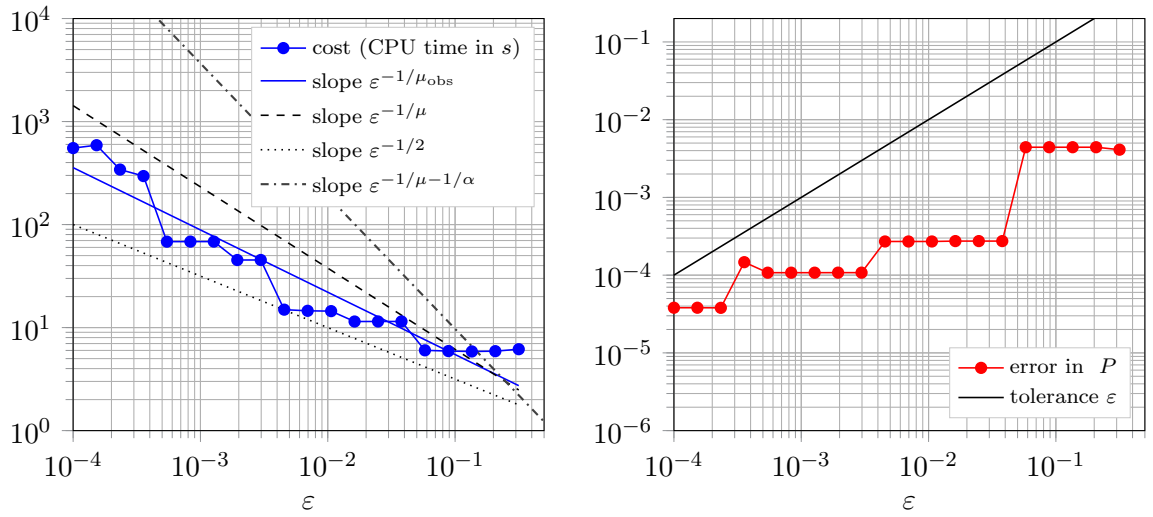
$$\Big(C(0,y), q(0,y), p(0,y), \xi(0,y)\Big) = \left(1 + \frac{\delta}{4}y_7^2 + \mathrm{i}, -2 + \delta y_8^2 y_9^2, 2 + \delta y_{10}, 1\right).$$

The remaining parameters were the same as in the two-dimensional example before.

This time, we apply the multi-level approach to approximate the functional P from (5.5) of the solution instead of the solution itself. Thus, our goal is now to achieve

$$|\mathbb{E}[P(u(T,\cdot)) - P(u_J^{(\mathrm{ML})})]| \leq \varepsilon \qquad \text{instead of} \qquad \|u(T,\cdot) - u_J^{(\mathrm{ML})}\|_{C(\Gamma,X)} \leq \varepsilon.$$

The procedure to achieve this is very similar, and we refer to [25, Sec. 4.3] for details. Approximating the functional P with a given accuracy is typically easier than approximating the solution itself, but the challenge here is the large dimension of the parameter set Γ. The



(a) Cost vs. error (b) Error vs. ε

Figure 3. *Validation of the MLSC method in the ten-dimensional example ($\mu = 1.268$, $\mu_{obs} = 1.654$).*

P-analogues of Assumptions 2 and 3 were confirmed numerically with constants and parameters $\mu = 1.268$, $C = C_I C_\star = 1.361$, $C_T = 0.0055$ and $\alpha = 2$. This time, we use the rounding strategy which always rounds down, because we expect that the overhead of rounding up in this dimension would be too large.

Figure 3(a) shows that the computational costs (blue circles) scale as $\varepsilon^{-1/\mu_{\mathrm{obs}}}$ with $\mu_{\mathrm{obs}} = 1.654$ (blue line). This is significantly better than expected, because Theorem 4 states that the computational costs grow proportional to $\varepsilon^{-1/\mu}$ (black dashed) when $\varepsilon \to 0$. Figure 3(b) shows that the error in the observable P stays below the tolerance for all ε. Thus the results agree with the theoretical statement from Theorem 4.

7. Proof of Theorem 3. In order to prove part (ii) of Theorem 3 a bound for the local error (Lemma 8) and a stability result (Lemma 9) are combined to show the global error bound. For part (i), Lemma 8 is replaced by Lemma 7. Since both lemmas can be shown with essentially the same procedure, we only prove Lemma 8. The proof of Lemma 7 is easier and can be found in Section SM2 of the supplementary materials.

In Theorem 3 the error is measured in the norm $\|\cdot\|_{C^k_{\mathrm{mix}}(\Gamma,X)}$, which involves multiple derivatives with respect to y. For this reason, multivariate versions of the product rule and

the chain rule will play an important role in the proof. In order to formulate these auxiliary results, the following notation is introduced.

7.1. Notation. Let $k \in \mathbb{N}_0$ be the integer from Theorem 3, and set

$$\boldsymbol{\eta} = (\underbrace{1,\dots,1}_{k},\dots,\underbrace{d,\dots,d}_{k}). \tag{7.1}$$

Let $m = kd$ and $M = \{1,\dots,m\}$. For a subset $S \subseteq M$ with $|S|$ elements we define

$$\frac{\partial^{|S|}}{\partial y^S} = \frac{\partial^{|S|}}{\prod_{j\in S} \partial y_{\eta_j}}.$$

This notation is well-defined, because for sufficiently smooth functions the order of the derivatives can be interchanged. Note that by definition maximal number of partial derivatives in each spatial direction depends on $\boldsymbol{\eta}$ and hence on k. In the special case $S = M$ we have

$$\frac{\partial^m}{\partial y^M} = \frac{\partial^m}{\partial y_{\eta_1}\cdots\partial y_{\eta_m}} = \frac{\partial^k}{\partial y_1^k}\cdots\frac{\partial^k}{\partial y_d^k}.$$

The power set of a set $S \subseteq M$ is denoted by $\mathcal{P}^S$, the power set without the empty set by $\mathcal{P}^S_*$, and the set of partitions of S into non-empty subsets by $\Pi(S)$. The complement S^c of $S \subseteq M$ is always understood as the complement in M, i.e. $S^c = M \setminus S$.

Example 5. *Let $m = 3$ and $M = \{1,2,3\}$. Then the five elements of $\Pi(M)$ are the following.*

Partitions with one block: $\{\{1,2,3\}\}$
Partitions with two blocks: $\{\{1\},\{2,3\}\}$, $\{\{2\},\{1,3\}\}$, *and* $\{\{3\},\{1,2\}\}$
Partitions with three blocks: $\{\{1\},\{2\},\{3\}\}$

Note that the empty set $\emptyset$ also has exactly one partition, namely $\emptyset$ itself.

The multivariate product rule may now be stated in the form

$$\frac{\partial^{|S|}}{\partial y^S}(fg) = \sum_{T\in\mathcal{P}^S} \frac{\partial^{|T|} f}{\partial y^T}\frac{\partial^{|S\setminus T|} g}{\partial y^{S\setminus T}} \tag{7.2}$$

for a set $S \subseteq M$, whereas the multivariate chain rule (also known as *Faà di Bruno's formula*) is given by

$$\frac{\partial^{|S|}}{\partial y^S} f(g(y)) = \sum_{\pi\in\Pi(S)} f^{|\pi|}(g(y)) \prod_{B\in\pi} \frac{\partial^{|B|} g}{\partial y^B}, \tag{7.3}$$

where $|\pi|$ is the number of "blocks" in the partition π. Proofs of these equations together with examples can be found in [13].

Example 6. *The power set of* $S = \{1, 2, 3\}$ *is*

$$\mathcal{P}^S = \Big\{\emptyset, \{1\}, \{2\}, \{3\}, \{1,2\}, \{1,3\}, \{2,3\}, \{1,2,3\}\Big\}, \tag{7.4}$$

and hence the multivariate product rule (7.2) *reduces to*

$$\begin{aligned}\frac{\partial^3}{\partial y_1\,\partial y_2\,\partial y_3}(fg) = f\cdot\frac{\partial^3 g}{\partial y_1\,\partial y_2\,\partial y_3} + \frac{\partial f}{\partial y_1}\cdot\frac{\partial^2 g}{\partial y_2\,\partial y_3} + \frac{\partial f}{\partial y_2}\cdot\frac{\partial^2 g}{\partial y_1\,\partial y_3} + \frac{\partial f}{\partial y_3}\cdot\frac{\partial^2 g}{\partial y_1\,\partial y_2}\\ + \frac{\partial^2 f}{\partial y_1\,\partial y_2}\cdot\frac{\partial g}{\partial y_3} + \frac{\partial^2 f}{\partial y_1\,\partial y_3}\cdot\frac{\partial g}{\partial y_2} + \frac{\partial^2 f}{\partial y_2\,\partial y_3}\cdot\frac{\partial g}{\partial y_1} + \frac{\partial^3 f}{\partial y_1\,\partial y_2\,\partial y_3}\cdot g.\end{aligned}$$

Each term is related to one of the sets in (7.4). *The multivariate chain rule* (7.3) *yields*

$$\begin{aligned}\frac{\partial^3}{\partial y_1\,\partial y_2\,\partial y_3} f(g(y)) &= f'(g(y))\frac{\partial^3 g(y)}{\partial y_1\,\partial y_2\,\partial y_3}\\ &+ f''(g(y))\left(\frac{\partial g(y)}{\partial y_1}\cdot\frac{\partial^2 g(y)}{\partial y_2\,\partial y_3} + \frac{\partial g(y)}{\partial y_2}\cdot\frac{\partial^2 g(y)}{\partial y_1\,\partial y_3} + \frac{\partial g(y)}{\partial y_3}\cdot\frac{\partial^2 g(y)}{\partial y_1\,\partial y_2}\right)\\ &+ f'''(g(y))\frac{\partial g(y)}{\partial y_1}\cdot\frac{\partial g(y)}{\partial y_2}\cdot\frac{\partial g(y)}{\partial y_3}.\end{aligned}$$

Each term corresponds to one of the partitions from Example 5. *For example, the partition* $\pi = \{\{2\}, \{1,3\}\}$ *has two blocks, i.e.* $|\pi| = 2$, *and we obtain*

$$f^{|\pi|}(g(y)) = f''(g(y)), \qquad \prod_{B\in\pi}\frac{\partial^{|B|} g}{\partial y^B} = \frac{\partial g(y)}{\partial y_2}\cdot\frac{\partial^2 g(y)}{\partial y_1\,\partial y_3}.$$

With this notation the commutator bounds (4.8) and (4.9) read

$$\left\|\left[\tfrac{\partial^{|S|}V(y)}{\partial y^S}, \Delta\right] w_1\right\|_{C(\Gamma,X)} \le C\|w_1\|_{C(\Gamma,H^1(\mathbb{T}^D))}, \qquad S\in\mathcal{P}^M, \tag{7.5}$$

$$\left\|\left[\Delta, \left[\tfrac{\partial^{|S|}V(y)}{\partial y^S}, \Delta\right]\right] w_2\right\|_{C(\Gamma,X)} \le C\|w_2\|_{C(\Gamma,H^2(\mathbb{T}^D))}, \qquad S\in\mathcal{P}^M. \tag{7.6}$$

Assumption 6 and the relations (7.1) with $m = kd$ imply that (7.5) and (7.6) hold for all $w_1 \in C(\Gamma, H^1(\mathbb{T}^D))$ and $w_2 \in C(\Gamma, H^2(\mathbb{T}^D))$.

$V(y)$ is a multiplication operator and thus

$$[\partial_{y_j} V(y), V(y)] = 0, \qquad j = 1, \dots, d,\ y\in\Gamma. \tag{7.7}$$

The same is also true for higher derivatives of $V(Y)$.

7.2. Local error.

Lemma 7. *Let $v \in C^k_{\mathrm{mix}}(\Gamma, H^2(\mathbb{T}))$. Under the assumptions of Theorem 3 (i) the error after one time-step is bounded by*

$$\|\Phi_\tau v - \mathrm{e}^{\mathrm{i}\tau H(y)} v\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \leq C_{loc}\tau^2 \|v\|_{C^k_{\mathrm{mix}}(\Gamma,H^1(\mathbb{T}^D))}. \tag{7.8}$$

The constant C_{loc} depends only on the constants on the right-hand side of (4.7) and (4.8), but not on τ.

The proof of Lemma 7 is given in Section SM2 of the supplementary materials.

Lemma 8. *Let $v \in C^k_{\mathrm{mix}}(\Gamma, H^2(\mathbb{T}))$. Under the assumptions of Theorem 3 (ii) the error after one time-step is bounded by*

$$\|\Phi_\tau v - \mathrm{e}^{\mathrm{i}\tau H(y)} v\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \leq C_{loc}\tau^3 \|v\|_{C^k_{\mathrm{mix}}(\Gamma,H^2(\mathbb{T}^D))}. \tag{7.9}$$

The constant C_{loc} depends only on the constants on the right-hand side of (7.5) and (7.6), but not on τ.

Proof of Lemma 8. Throughout we abbreviate

$$\mathcal{D} = \frac{\partial^m}{\partial y^M} = \frac{\partial^k}{\partial y_1^k} \cdots \frac{\partial^k}{\partial y_d^k}.$$

We only prove that

$$\|\mathcal{D}(\Phi_\tau v) - \mathcal{D}(\mathrm{e}^{\mathrm{i}\tau H(y)} v)\|_{C(\Gamma,X)} \leq C_{\mathrm{loc}}\tau^3 \|v\|_{C^k_{\mathrm{mix}}(\Gamma,H^2(\mathbb{T}^D))}$$

since the procedure for differential operators with lower order than $\mathcal{D}$ is completely analogous.

In Step 1 of the proof an expansion of $\mathcal{D}u(t,y) = \mathcal{D}\mathrm{e}^{\mathrm{i}tH(y)}v(y)$ in powers of τ is derived. Its representation is modified in Step 2. In Step 3 a corresponding expansion of $\mathcal{D}(\Phi_\tau v)$ is obtained. The Step 4, the difference between the two expansions is analyzed, and it is shown that all terms of $\mathcal{O}(\tau)$ and $\mathcal{O}(\tau^2)$ cancel.

Step 1. For the exact solution $u(t,y) = \mathrm{e}^{\mathrm{i}tH(y)}v(y)$, we have

$$\partial_t \mathcal{D}u(t,y) = \mathrm{i}H(y)\mathcal{D}u(t,y) + \mathrm{i}\sum_{S\in\mathcal{P}^M_*} \frac{\partial^{|S|}V(y)}{\partial y^S} \cdot \frac{\partial^{|S^c|}u(t,y)}{\partial y^{S^c}}$$

and the variation-of-constants formula yields

$$\mathcal{D}u(\tau,y) = \mathrm{e}^{\tau\mathrm{i}H(y)}\mathcal{D}v(y) + \mathrm{i}\int_0^\tau \mathrm{e}^{(\tau-r)\mathrm{i}H(y)} \sum_{S\in\mathcal{P}^M_*} \frac{\partial^{|S|}V(y)}{\partial y^S} \cdot \frac{\partial^{|S^c|}u(r,y)}{\partial y^{S^c}} \mathrm{d}r.$$

Using this expression again for the term with $u(r,y)$ in the integrand, this yields

$$\mathcal{D}u(\tau,y) = \mathrm{e}^{\tau\mathrm{i}H(y)}\mathcal{D}v(y) + \sum_{S\in\mathcal{P}^M_*} \left(I_1(S) + \sum_{T\in\mathcal{P}^{S^c}_*} I_2(S,T) \right) \tag{7.10}$$

with

$$I_1(S) = \mathrm{i}\int_0^\tau \mathrm{e}^{(\tau-r)\mathrm{i}H(y)}\frac{\partial^{|S|}V(y)}{\partial y^S}\mathrm{e}^{r\mathrm{i}H(y)}\frac{\partial^{|S^c|}v(y)}{\partial y^{S^c}}\mathrm{d}r, \tag{7.11}$$

$$I_2(S,T) = \mathrm{i}^2\int_0^\tau\int_0^r \mathrm{e}^{(\tau-r)\mathrm{i}H(y)}\frac{\partial^{|S|}V(y)}{\partial y^S}\mathrm{e}^{(r-\nu)\mathrm{i}H(y)}\frac{\partial^{|T|}V(y)}{\partial y^T}\frac{\partial^{|S^c\setminus T|}u(\nu,y)}{\partial y^{S^c\setminus T}}\mathrm{d}\nu\mathrm{d}r. \tag{7.12}$$

Note that formally $I_1(S) = \mathcal{O}(\tau)$ and that $I_2(S,T) = \mathcal{O}(\tau^2)$.

Step 2. In order to compare (7.10) with a corresponding representation of $\mathcal{D}(\Phi_\tau v)$ in Step 4, the integrals $I_1(S)$ and $I_2(S,T)$ have to be approximated by suitable quadrature formulas. The integral $I_1(S)$ is approximated by the trapezoidal rule, i.e.

$$\begin{aligned} I_1(S) &= \mathrm{i}\int_0^\tau \mathrm{e}^{(\tau-r)\mathrm{i}H(y)}\frac{\partial^{|S|}V(y)}{\partial y^S}\mathrm{e}^{r\mathrm{i}H(y)}\frac{\partial^{|S^c|}v(y)}{\partial y^{S^c}}\mathrm{d}r \\ &\approx \frac{\mathrm{i}\tau}{2}\left(\mathrm{e}^{\tau\mathrm{i}H(y)}\frac{\partial^{|S|}V(y)}{\partial y^S}\frac{\partial^{|S^c|}v(y)}{\partial y^{S^c}} + \frac{\partial^{|S|}V(y)}{\partial y^S}\mathrm{e}^{\tau\mathrm{i}H(y)}\frac{\partial^{|S^c|}v(y)}{\partial y^{S^c}}\right) =: I_1^{\square}(S). \end{aligned} \tag{7.13}$$

Abbreviating the integrand inside $I_1(S)$ by $h(r)$, the error of the trapezoidal rule can be expressed in Peano form as

$$E = \frac{\mathrm{i}\tau}{2}\Big(h(0)+h(\tau)\Big) - \mathrm{i}\int_0^\tau h(s)\mathrm{d}s = -\frac{\mathrm{i}\tau^3}{2}\int_0^1 \theta(1-\theta)h''(\theta\tau)\mathrm{d}\theta.$$

Hence, to obtain an error of order τ^3, it has to be shown that h is twice continuously differentiable with bounded second derivative. To check the required regularity of the integrand, we compute

$$\begin{aligned} \frac{\partial h}{\partial r} &= \mathrm{i}\mathrm{e}^{(\tau-r)\mathrm{i}H(y)}\left[\frac{\partial^{|S|}V(y)}{\partial y^S}, H(y)\right]\mathrm{e}^{r\mathrm{i}H(y)}\frac{\partial^{|S^c|}v(y)}{\partial y^{S^c}}, \\ \frac{\partial^2 h}{\partial r^2} &= \mathrm{e}^{(\tau-r)\mathrm{i}H(y)}\left[H(y),\left[\frac{\partial^{|S|}V(y)}{\partial y^S}, H(y)\right]\right]\mathrm{e}^{r\mathrm{i}H(y)}\frac{\partial^{|S^c|}v(y)}{\partial y^{S^c}}. \end{aligned}$$

These terms are bounded by (7.5), (7.6), and (7.7). The approximation (7.13) is of accuracy $\mathcal{O}(\tau^3)$, and hence we may replace $I_1(S)$ by $I_1^{\square}(S)$ in the following.

Now consider the second integral, $I_2(S,T)$. After setting

$$g(r,\nu) = \mathrm{e}^{(\tau-r)\mathrm{i}H(y)}\frac{\partial^{|S|}V(y)}{\partial y^S}\mathrm{e}^{(r-\nu)\mathrm{i}H(y)}\frac{\partial^{|T|}V(y)}{\partial y^T}\frac{\partial^{|S^c\setminus T|}u(\nu,y)}{\partial y^{S^c\setminus T}}$$

we obtain

$$
\begin{aligned}
I_2(S,T) &= \mathrm{i}^2 \int_0^\tau \int_0^r g(r,\nu)\mathrm{d}\nu\mathrm{d}r \\
&\approx \frac{1}{2}\left(\frac{\mathrm{i}\tau}{2}\right)^2 \cdot (g(0,0) + 2g(\tau,0) + g(\tau,\tau)) \\
&= \frac{1}{2}\left(\frac{\mathrm{i}\tau}{2}\right)^2 \cdot \mathrm{e}^{\tau \mathrm{i} H(y)} \frac{\partial^{|S|} V(y)}{\partial y^S} \frac{\partial^{|T|} V(y)}{\partial y^T} \frac{\partial^{|S^c\setminus T|} v(y)}{\partial y^{S^c\setminus T}} \\
&\quad + \left(\frac{\mathrm{i}\tau}{2}\right)^2 \cdot \frac{\partial^{|S|} V(y)}{\partial y^S} \mathrm{e}^{\tau \mathrm{i} H(y)} \frac{\partial^{|T|} V(y)}{\partial y^T} \frac{\partial^{|S^c\setminus T|} v(y)}{\partial y^{S^c\setminus T}} \\
&\quad + \frac{1}{2}\left(\frac{\mathrm{i}\tau}{2}\right)^2 \cdot \frac{\partial^{|S|} V(y)}{\partial y^S} \frac{\partial^{|T|} V(y)}{\partial y^T} \frac{\partial^{|S^c\setminus T|} u(\tau,y)}{\partial y^{S^c\setminus T}} \qquad (7.14) \\
&=: I_2^{\square}(S,T). \qquad (7.15)
\end{aligned}
$$

The very last term in (7.14) will be treated by yet another variation-of-constants formula to replace

$$
\frac{\partial^{|S^c\setminus T|} u(\tau,y)}{\partial y^{S^c\setminus T}} \qquad \text{by} \qquad \mathrm{e}^{\tau \mathrm{i} H(y)} \frac{\partial^{|S^c\setminus T|} v(y)}{\partial y^{S^c\setminus T}} + \mathcal{O}(\tau), \tag{7.16}
$$

at least if $S \cup T \neq M$ (or equivalently $|S| + |T| \neq m$). The quadrature formula $I_2^{\square}(S,T)$ for the triangle $\{(r,\nu)\colon\ 0 \le r \le \tau,\ 0 \le \nu \le r\}$ integrates constant functions exactly, and since it can be checked that the integrand has the required regularity, it follows that $I_2(S,T) = I_2^{\square}(S,T) + \mathcal{O}(\tau^3)$. Combining the above observations, we arrive at

$$
\mathcal{D}u(\tau,y) = \mathrm{e}^{\tau \mathrm{i} H(y)} \mathcal{D}v(y) + \sum_{S\in\mathcal{P}_*^M} \left(I_1^{\square}(S) + \sum_{T\in\mathcal{P}_*^{S^c}} I_2^{\square}(S,T) \right) + \mathcal{O}(\tau^3). \tag{7.17}
$$

Step 3. Now a corresponding expansion has to be derived for the numerical solution. We have

$$
\mathcal{D}(\Phi_\tau v) = \sum_{S\in\mathcal{P}^M} \frac{\partial^{|S|}\Phi_\tau(y)}{\partial y^S} \cdot \frac{\partial^{|S^c|} v(y)}{\partial y^{S^c}} = \Phi_\tau(y)\mathcal{D}v(y) + \sum_{S\in\mathcal{P}_*^M} \frac{\partial^{|S|}\Phi_\tau(y)}{\partial y^S} \cdot \frac{\partial^{|S^c|} v(y)}{\partial y^{S^c}} \tag{7.18}
$$

and, utilizing (7.2) and (7.3),

$$
\begin{aligned}
\frac{\partial^{|S|}\Phi_\tau}{\partial y^S} &= \sum_{T\in\mathcal{P}^S} \frac{\partial^{|T|} \mathrm{e}^{\frac{\mathrm{i}\tau}{2}V(y)}}{\partial y^T} \mathrm{e}^{\mathrm{i}\tau\Delta} \frac{\partial^{|S\setminus T|} \mathrm{e}^{\frac{\mathrm{i}\tau}{2}V(y)}}{\partial y^{S\setminus T}} \\
&= \sum_{T\in\mathcal{P}^S} \sum_{\pi\in\Pi(T)} \sum_{\sigma\in\Pi(S\setminus T)} \left(\tfrac{\mathrm{i}\tau}{2}\right)^{|\pi|+|\sigma|} \prod_{B\in\pi} \frac{\partial^{|B|} V(y)}{\partial y^B} \Phi_\tau \prod_{C\in\sigma} \frac{\partial^{|C|} V(y)}{\partial y^C}. \qquad (7.19)
\end{aligned}
$$

The crucial terms are those of $\mathcal{O}(\tau)$ and $\mathcal{O}(\tau^2)$, whereas higher-order terms can be neglected. In order to identify the terms with $|\pi| + |\sigma| \le 2$, we define the set $\mathcal{P}_{**}^S$ as the set $\mathcal{P}_*^S$ without

S. Separating the terms with $T = \emptyset$ and $T = S$ yields

$$\begin{aligned}\frac{\partial^{|S|}\Phi_\tau}{\partial y^S} &= \sum_{T\in\mathcal{P}^S_{**}} \left(\tfrac{\mathrm{i}\tau}{2}\right)^2 \frac{\partial^{|T|}V(y)}{\partial y^T}\Phi_\tau\frac{\partial^{|S\setminus T|}V(y)}{\partial y^{S\setminus T}} \\ &\quad + \sum_{\substack{\sigma\in\Pi(S)\\ |\sigma|\le 2}} \left(\tfrac{\mathrm{i}\tau}{2}\right)^{|\sigma|}\left[\Phi_\tau\prod_{C\in\sigma}\frac{\partial^{|C|}V(y)}{\partial y^C} + \prod_{C\in\sigma}\frac{\partial^{|C|}V(y)}{\partial y^C}\Phi_\tau\right] + \mathcal{O}(\tau^3) \\ &= \sum_{T\in\mathcal{P}^S_{**}} \left(\tfrac{\mathrm{i}\tau}{2}\right)^2 f(S,T) + \left(\tfrac{\mathrm{i}\tau}{2}\right)\left[\Phi_\tau\frac{\partial^{|S|}V(y)}{\partial y^S} + \frac{\partial^{|S|}V(y)}{\partial y^S}\Phi_\tau\right] + \mathcal{O}(\tau^3) \qquad (7.20)\end{aligned}$$

with

$$f(S,T) = \frac{\partial^{|T|}V(y)}{\partial y^T}\Phi_\tau\frac{\partial^{|S\setminus T|}V(y)}{\partial y^{S\setminus T}} + \frac{1}{2}\Phi_\tau\frac{\partial^{|T|}V(y)}{\partial y^T}\frac{\partial^{|S\setminus T|}V(y)}{\partial y^{S\setminus T}} + \frac{1}{2}\frac{\partial^{|T|}V(y)}{\partial y^T}\frac{\partial^{|S\setminus T|}V(y)}{\partial y^{S\setminus T}}\Phi_\tau.$$

The equality (7.20) follows from the fact that every partition $\sigma \in \Pi(S)$ with $|\sigma| = 2$ consists of an arbitrary subset $\emptyset \subsetneq T \subsetneq S$ and its complement in S. If we go through all such subsets T and notice that T is also the complement of $S\setminus T$, we have counted each partition $\sigma \in \Pi(S)$ with $|\sigma| = 2$ twice. Hence the factor $1/2$ appears in the second and third term in the definition of $f(S,T)$.

Before we substitute (7.20) into (7.18), we have to deal with some set-theoretic considerations. In fact, $S \in \mathcal{P}^M_*$ and $T \in \mathcal{P}^S_{**}$ is equivalent to saying that $T \in \mathcal{P}^M_*$ and $M \supseteq S \supsetneq T$. A set $S \supsetneq T$ can be written in a unique way as $S = S' \cup T$ with $S' \in \mathcal{P}^{T^c}_*$. Hence, for any function f, we have the identity

$$\sum_{S\in\mathcal{P}^M_*}\sum_{T\in\mathcal{P}^S_{**}} f(S,T) = \sum_{T\in\mathcal{P}^M_*}\sum_{S'\in\mathcal{P}^{T^c}_*} f(S'\cup T,T) = \sum_{S\in\mathcal{P}^M_*}\sum_{T\in\mathcal{P}^{S^c}_*} f(T\cup S,S).$$

The last step is changing the names of T and S' to S and T. In our case, we have

$$f(T\cup S,S) = \left[\frac{\partial^{|S|}V(y)}{\partial y^S}\Phi_\tau\frac{\partial^{|T|}V(y)}{\partial y^T} + \frac{1}{2}\Phi_\tau\frac{\partial^{|S|}V(y)}{\partial y^S}\frac{\partial^{|T|}V(y)}{\partial y^T} + \frac{1}{2}\frac{\partial^{|S|}V(y)}{\partial y^S}\frac{\partial^{|T|}V(y)}{\partial y^T}\Phi_\tau\right]. \qquad (7.21)$$

By substituting these formulas into (7.18), we obtain the expansion

$$\begin{aligned}\mathcal{D}(\Phi_\tau v) &= \Phi_\tau(y)\mathcal{D}v(y) + \sum_{S\in\mathcal{P}^M_*}\sum_{T\in\mathcal{P}^{S^c}_*}\left(\tfrac{\mathrm{i}\tau}{2}\right)^2 f(T\cup S,S)\cdot\frac{\partial^{|S^c\setminus T|}v(y)}{\partial y^{S^c\setminus T}} \\ &\quad + \sum_{S\in\mathcal{P}^M_*}\left(\tfrac{\mathrm{i}\tau}{2}\right)\left[\Phi_\tau\frac{\partial^{|S|}V(y)}{\partial y^S} + \frac{\partial^{|S|}V(y)}{\partial y^S}\Phi_\tau\right]\cdot\frac{\partial^{|S^c|}v(y)}{\partial y^{S^c}} + \mathcal{O}(\tau^3). \qquad (7.22)\end{aligned}$$

Step 4. Now we subtract (7.17) from (7.22). The local error bound (3.6) implies

$$\|\Phi_\tau v_0 - \mathrm{e}^{\mathrm{i}\tau H(y)} v_0\|_{C(\Gamma,X)} \le C\tau^3 \|v_0\|_{C(\Gamma,H^2(\mathbb{T}^D))}$$

for $v_0 \in C(\Gamma, H^2(\mathbb{T}^D))$. Hence, replacing the numerical flow Φ_τ by the exact flow $\mathrm{e}^{\tau \mathrm{i} H(y)}$ does not spoil the accuracy. By carefully comparing the terms in (7.22) and (7.21) with the ones in (7.17), (7.13) and (7.15), we obtain

$$\|\mathcal{D}(\Phi_\tau v) - \mathcal{D}(\mathrm{e}^{\mathrm{i}\tau H(y)} v)\|_{C(\Gamma,X)} \le C\tau^3 \tag{7.23}$$

for a constant C which depends only on the constants on the right-hand side of (4.7) and (4.8), but is independent of τ. All the $\mathcal{O}(\tau^3)$-terms and hence also in the constant C contain $\|v\|_{C^k_{\mathrm{mix}}(\Gamma,H^2(\mathbb{T}^D))}$ as a factor. ∎

7.3. Stability and global error. In order to pass from the local error to the global error, the following stability result is required.

Lemma 9. *Let $v \in C^k_{\mathrm{mix}}(\Gamma, X)$. Under the assumptions of Theorem 3 (i) the estimate*

$$\|\Phi_\tau v\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \le (1 + C_{stab}\tau)\|v\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \le \exp(C_{stab}\tau)\|v\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \tag{7.24}$$

holds for all step-sizes $\tau \in (0, 2]$. The constant C_{stab} is independent of τ, but depends on k and on $\|V\|_{C^k_{\mathrm{mix}}(\Gamma,L^\infty(\mathbb{T}^D))}$.

Proof. First, we observe that

$$\begin{aligned}\|\mathcal{D}(\Phi_\tau v)\|_{C(\Gamma,X)} &\le \sum_{S\in\mathcal{P}^M} \left\| \frac{\partial^{|S|}\Phi_\tau(y)}{\partial y^S} \right\| \left\| \frac{\partial^{m-|S|} v(y)}{\partial y^{S^c}} \right\|_{C(\Gamma,X)} \\ &\le \|\Phi_\tau\| \left\| \frac{\partial^m v(y)}{\partial y^M} \right\|_{C(\Gamma,X)} + \sum_{S\in\mathcal{P}^M_*} \left\| \frac{\partial^{|S|}\Phi_\tau(y)}{\partial y^S} \right\| \cdot \|v\|_{C^k_{\mathrm{mix}}(\Gamma,X)}, \end{aligned} \tag{7.25}$$

with $\|\cdot\| = \|\cdot\|_{C(\Gamma,\mathcal{B}(X))}$. For $S \neq \emptyset$, (7.19) yields

$$\left\| \frac{\partial^{|S|}\Phi_\tau}{\partial y^S} \right\| \le \sum_{T\in\mathcal{P}^S} \sum_{\pi\in\Pi(T)} \sum_{\sigma\in\Pi(S\setminus T)} \left(\tfrac{\mathrm{i}\tau}{2}\right)^{|\pi|+|\sigma|} \left\| \prod_{B\in\pi} \frac{\partial^{|B|}V(y)}{\partial y^B} \Phi_\tau \prod_{C\in\sigma} \frac{\partial^{|C|}V(y)}{\partial y^C} \right\|.$$

Since $V \in C^k_{\mathrm{mix}}(\Gamma, L^\infty(\mathbb{T}^D))$ and $\|\Phi_\tau\| \le 1$, the norm on the right-hand side can be bounded by some constant C which only depends on $\|V\|_{C^k_{\mathrm{mix}}(\Gamma,L^\infty(\mathbb{T}^D))}$. Thus, sorting after powers of τ, we obtain

$$\left\| \frac{\partial^{|S|}\Phi_\tau}{\partial y^S} \right\| \le C\Big(\tfrac{\tau}{2} + \big(\tfrac{\tau}{2}\big)^2 + \cdots + \big(\tfrac{\tau}{2}\big)^{|S|}\Big),$$

which is bounded by $C|S|\tau/2$ as long as $\tau \le 2$. Thus, by (7.25),

$$\|\mathcal{D}(\Phi_\tau v)\|_{C(\Gamma,X)} \le \left\| \frac{\partial^m v(y)}{\partial y^M} \right\|_{C(\Gamma,X)} + C_k\tau\|v\|_{C^k_{\mathrm{mix}}(\Gamma,X)}$$

for all $\tau \leq 2$ with a constant C_k. Of course, the procedure is similar if one considers derivatives of lower order than k. Hence, we arrive at

$$\|\Phi_\tau v\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \leq (1 + C_k\tau)\|v\|_{C^k_{\mathrm{mix}}(\Gamma,X)}$$

as long as $\tau \leq 2$. ∎

Proof of Theorem 3. In order to prove part (i) we combine the local error bound (7.8) and the stability estimate (7.24) to derive the global error bound. This is a typical "Lady Windermere's fan" argument. We have

$$\begin{aligned}
\|\Phi_\tau^n u_0 - \mathrm{e}^{\mathrm{i}t_n H(y)}u_0\|_{C^k_{\mathrm{mix}}(\Gamma,X)} &\leq \sum_{j=0}^{n-1} \|\Phi_\tau^j(\Phi_\tau \mathrm{e}^{\mathrm{i}H(y)t_{n-j-1}}u_0) - \Phi_\tau^j(\mathrm{e}^{\mathrm{i}t_{n-j}H(y)}u_0)\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \\
&\leq \sum_{j=0}^{n-1} \exp(C_{\mathrm{stab}}\tau j)\|\Phi_\tau \mathrm{e}^{\mathrm{i}H(y)t_{n-j-1}}u_0 - \mathrm{e}^{\mathrm{i}t_{n-j}H(y)}u_0\|_{C^k_{\mathrm{mix}}(\Gamma,X)} \\
&\leq \sum_{j=0}^{n-1} \exp(C_{\mathrm{stab}}\tau j)C_{\mathrm{loc}}\tau^2\|\mathrm{e}^{\mathrm{i}t_{n-j-1}H(y)}u_0\|_{C^k_{\mathrm{mix}}(\Gamma,H^1(\mathbb{T}^D))} \\
&\leq \frac{\exp(C_{\mathrm{stab}}\tau)^n - 1}{\exp(C_{\mathrm{stab}}\tau) - 1} C_{\mathrm{loc}}\tau^2 \max_{t\in[0,t_n]} \|u(t,\cdot)\|_{C^k_{\mathrm{mix}}(\Gamma,H^1(\mathbb{T}^D))} \\
&\leq \exp(C_{\mathrm{stab}}t_n)\frac{C_{\mathrm{loc}}}{C_{\mathrm{stab}}}\tau M_k^{(1)}.
\end{aligned}$$

Note that C_{stab} and C_{loc} are exactly the constants from the stability and local error estimates (7.24) and (7.8). Replacing (7.8) by (7.9) proves part (ii) of Theorem 3. ∎

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REFERENCES

[1] W. Auzinger, O. Koch, and M. Thalhammer, *Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part II. Higher-order methods for linear problems*, J. Comput. Appl. Math., 255 (2014), pp. 384–403, https://doi.org/10.1016/j.cam.2013.04.043, https://doi.org/10.1016/j.cam.2013.04.043.

[2] I. Babuška, F. Nobile, and R. Tempone, *A stochastic collocation method for elliptic partial differential equations with random input data*, SIAM Rev., 52 (2010), pp. 317–355, https://doi.org/10.1137/100786356.

[3] V. Barthelmann, E. Novak, and K. Ritter, *High dimensional polynomial interpolation on sparse grids*, Adv. Comput. Math., 12 (2000), pp. 273–288, https://doi.org/10.1023/A:1018977404843, https://doi.org/10.1023/A:1018977404843.

[4] A. Chertock, S. Jin, and A. Kurganov, *An operator splitting based stochastic Galerkin method for the one-dimensional compressible Euler equations with uncertainty.* Preprint, 2015, http://www.math.wisc.edu/~jin/publications.html (accessed 2018-10-12).

[5] S. Descombes and M. Thalhammer, *An exact local error representation of exponential operator splitting methods for evolutionary problems and applications to linear Schrödinger equations in the semi-classical regime*, BIT, 50 (2010), pp. 729–749, https://doi.org/10.1007/s10543-010-0282-4, https://doi.org/10.1007/s10543-010-0282-4.

[6] M. B. Giles, *Improved multilevel Monte Carlo convergence using the Milstein scheme*, In: Monte Carlo and quasi-Monte Carlo methods 2006. Selected papers based on the presentations at the 7th international conference 'Monte Carlo and quasi-Monte Carlo methods in scientific computing', Ulm, Germany, August 14–18, 2006., Springer, Berlin, 2008, pp. 343–358.

[7] M. B. Giles, *Multilevel Monte Carlo path simulation*, Operations Research, 56 (2008), pp. 607–617.

[8] M. B. Giles, *Multilevel Monte Carlo methods*, Acta Numer., 24 (2015), pp. 259–328, https://doi.org/10.1017/S096249291500001X, https://doi.org/10.1017/S096249291500001X.

[9] A.-L. Haji-Ali, F. Nobile, L. Tamellini, and R. Tempone, *Multi-index stochastic collocation convergence rates for random PDEs with parametric regularity*, Found. Comput. Math., 16 (2016), pp. 1555–1605, https://doi.org/10.1007/s10208-016-9327-7, https://doi.org/10.1007/s10208-016-9327-7.

[10] A.-L. Haji-Ali, F. Nobile, L. Tamellini, and R. Tempone, *Multi-index stochastic collocation for random PDEs*, Comput. Methods Appl. Mech. Engrg., 306 (2016), pp. 95–122, https://doi.org/10.1016/j.cma.2016.03.029, https://doi.org/10.1016/j.cma.2016.03.029.

[11] E. Hansen and A. Ostermann, *Exponential splitting for unbounded operators*, Math. Comp., 78 (2009), pp. 1485–1496, https://doi.org/10.1090/S0025-5718-09-02213-3, https://doi.org/10.1090/S0025-5718-09-02213-3.

[12] H. Harbrecht, M. Peters, and M. Siebenmorgen, *On multilevel quadrature for elliptic stochastic partial differential equations*, in Sparse grids and applications, vol. 88 of Lect. Notes Comput. Sci. Eng., Springer, Heidelberg, 2013, pp. 161–179, https://doi.org/10.1007/978-3-642-31703-3, https://doi.org/10.1007/978-3-642-31703-3.

[13] M. Hardy, *Combinatorics of partial derivatives*, Electron. J. Combin., 13 (2006), pp. Research Paper 1, 13, http://www.combinatorics.org/Volume_13/Abstracts/v13i1r1.html.

[14] T. Jahnke and C. Lubich, *Error bounds for exponential operator splittings*, BIT, 40 (2000), pp. 735–744, https://doi.org/10.1023/A:1022396519656, https://doi.org/10.1023/A:1022396519656.

[15] T. Kato, *Perturbation theory for linear operators*, Classics in Mathematics, Springer-Verlag, Berlin, 1995. Reprint of the 1980 edition.

[16] A. Kofler, T. Levajković, H. Mena, and A. Ostermann, *A splitting/polynomial chaos expansion approach for stochastic evolution equations*, J. Evol. Equ., 21 (2021), pp. 1345–1381, https://doi.org/10.1007/s00028-020-00627-5, https://doi.org/10.1007/s00028-020-00627-5.

[17] J. Lang, R. Scheichl, and D. Silvester, *A fully adaptive multilevel stochastic collocation strategy for solving elliptic PDEs with random data*, J. Comput. Phys., 419 (2020), pp. 109692, 17, https://doi.org/10.1016/j.jcp.2020.109692, https://doi.org/10.1016/j.jcp.2020.109692.

[18] C. Lasser and C. Lubich, *Computing quantum dynamics in the semiclassical regime*, Acta Numer., 29 (2020), pp. 229–401, https://doi.org/10.1017/s0962492920000033, https://doi.org/10.1017/s0962492920000033.

[19] C. Lubich, *From quantum to classical molecular dynamics: reduced models and numerical analysis*, Zurich Lectures in Advanced Mathematics, European Mathematical Society (EMS), Zürich, 2008, https://doi.org/10.4171/067, https://doi.org/10.4171/067.

[20] M. Motamed, F. Nobile, and R. Tempone, *A stochastic collocation method for the second order wave equation with a discontinuous random speed*, Numer. Math., 123 (2013), pp. 493–536, https://doi.org/10.1007/s00211-012-0493-5.

[21] C. Neuhauser and M. Thalhammer, *On the convergence of splitting methods for linear evolutionary Schrödinger equations involving an unbounded potential*, BIT, 49 (2009), pp. 199–215, https://doi.org/10.1007/s10543-009-0215-2, https://doi.org/10.1007/s10543-009-0215-2.

[22] F. Nobile, R. Tempone, and C. G. Webster, *A sparse grid stochastic collocation method for partial differential equations with random input data*, SIAM J. Numer. Anal., 46 (2008), pp. 2309–2345, https://doi.org/10.1137/060663660.

[23] F. Nobile, R. Tempone, and C. G. Webster, *A sparse grid stochastic collocation method for partial differential equations with random input data*, SIAM J. Numer. Anal., 46 (2008), pp. 2309–2345, https://doi.org/10.1137/060663660, https://doi.org/10.1137/060663660.

[24] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, vol. 44 of Applied Mathematical Sciences, Springer-Verlag, New York, 1983, https://doi.org/10.1007/978-1-4612-5561-1, https://doi.org/10.1007/978-1-4612-5561-1.

[25] A. L. Teckentrup, P. Jantsch, C. G. Webster, and M. Gunzburger, *A multilevel stochastic*

collocation method for partial differential equations with random input data, SIAM/ASA J. Uncertain. Quantif., 3 (2015), pp. 1046–1074, https://doi.org/10.1137/140969002, https://doi.org/10.1137/140969002.

[26] H.-W. van Wyk, *Multilevel sparse grid methods for elliptic partial differential equations with random coefficients*. Preprint, 2014, https://arxiv.org/abs/1404.0963.

[27] K. Wu, H. Tang, and D. Xiu, *A stochastic Galerkin method for first-order quasilinear hyperbolic systems with uncertainty*, J. Comput. Phys., 345 (2017), pp. 224–244, https://doi.org/10.1016/j.jcp.2017.05.027.

[28] D. Xiu and J. S. Hesthaven, *High-order collocation methods for differential equations with random inputs*, SIAM J. Sci. Comput., 27 (2005), pp. 1118–1139, https://doi.org/10.1137/040615201.