Supplementary Information: Digital Quantum Simulation, Trotter Errors, and Quantum Chaos of the Kicked Top

Lukas M. Sieberer,[1,2,*] Tobias Olsacher,[1] Andreas Elben,[1,2]
Markus Heyl,[3] Philipp Hauke,[4,5] Fritz Haake,[6] and Peter Zoller[1,2]

[1] *Center for Quantum Physics, University of Innsbruck, 6020 Innsbruck, Austria*
[2] *Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria*
[3] *Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany*
[4] *Kirchhoff-Institute for Physics, Heidelberg University, 69120 Heidelberg, Germany*
[5] *Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany*
[6] *Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany*

(Dated: August 15, 2019)

I. PERTURBATION THEORY

In the regular regime of Trotter step sizes below τ_*, corrections to the ideal long-time averages of observables due to Trotterization can be obtained by treating the difference between the effective Hamiltonian H_τ obtained from the FM expansion and the target Hamiltonian H in time-dependent perturbation theory as described in Ref. [1]. Here, we generalize the discussion of Ref. [1], which assumed a fixed initial state $|\psi_0\rangle$ polarized along the z-axis, to an arbitrary choice of $|\psi_0\rangle$.

The starting point is the FM expansion of the effective Hamiltonian H_τ up to second order in τ (see Ref. [2] in the context of the kicked top)

$$H_\tau = H + \tau C_1 + \tau^2 C_2 = H + \frac{\mathrm{i}\tau}{2}[H_x, H_z] - \frac{\tau^2}{12^2}[H_x - H_z, [H_x, H_z]], \tag{1}$$

where the operator $V = \tau C_1 + \tau^2 C_2$ acts as a time-independent correction to the target Hamiltonian $H = H_x + H_z$. The effective Hamiltonian gives rise to a time evolution according to the Schrödinger equation

$$\mathrm{i}\partial_t |\psi\rangle = H_\tau |\psi\rangle \tag{2}$$

which we transform into an interaction picture according to

$$|\psi_I(t)\rangle = \mathrm{e}^{\mathrm{i}Ht}|\psi\rangle, \qquad V_I = \mathrm{e}^{\mathrm{i}Ht} V \mathrm{e}^{-\mathrm{i}Ht}. \tag{3}$$

We obtain the time-evolution operator from time t_0 to t as

$$W(t, t_0) = \mathsf{T}\mathrm{e}^{-\mathrm{i}\int_{t_0}^{t} V_I(s)\,\mathrm{d}s} \tag{4}$$

where T denotes a time-ordered exponential. We determine $W(t) = W(t, 0)$ ($t_0 = 0$) up to second order in the Trotter step τ.

A. Corrections to the energy

We are interested in an expansion of the quantity

$$\begin{aligned}\Delta E(t) &= \langle H(t)\rangle_\tau - E_0 = \langle\psi_0|\mathrm{e}^{\mathrm{i}H_\tau t} H \mathrm{e}^{-\mathrm{i}H_\tau t}|\psi_0\rangle - \langle\psi_0|H|\psi_0\rangle \\ &= \tau\left(\langle\psi_0|C_1|\psi_0\rangle - \langle\psi_0|\mathrm{e}^{\mathrm{i}H_\tau t} C_1 \mathrm{e}^{-\mathrm{i}H_\tau t}|\psi_0\rangle\right) + \tau^2\left(\langle\psi_0|C_2|\psi_0\rangle - \langle\psi_0|\mathrm{e}^{\mathrm{i}H_\tau t} C_2 \mathrm{e}^{-\mathrm{i}H_\tau t}|\psi_0\rangle\right),\end{aligned} \tag{5}$$

* lukas.sieberer@uibk.ac.at

where we used Eq. (1), in the Trotter step τ for an arbitrary initial state $|\psi_0\rangle$. To this end, we replace $\mathrm{e}^{-\mathrm{i}H_\tau t}$ by $W(t)$ which yields the time dependent correction up to second order in the Trotter step τ:

$$\Delta E(t) = \tau\langle\psi_0|C_1 - C_{1,I}(t)|\psi_0\rangle + \frac{\tau^2}{4}\langle\psi_0|\mathrm{e}^{\mathrm{i}Ht}\,[H_z,[H_x,H_z]]\,\mathrm{e}^{-\mathrm{i}Ht}|\psi_0\rangle + \frac{\mathrm{i}\tau^2}{2}\langle\psi_0|[H_z, C_{1,I}(t)]|\psi_0\rangle + \tau^2\langle\psi_0|C_2 - C_{2,I}(t)|\psi_0\rangle + O(\tau^3). \quad (6)$$

The long-time averages of the above expectation values are determined in the diagonal ensemble [3],

$$\overline{\langle\psi_0|O|\psi_0\rangle} = \lim_{t\to\infty}\frac{1}{t}\int_0^t \langle\psi_0|O(t)|\psi_0\rangle\,dt = \sum_{\lambda\in\sigma(H)} |\langle\psi_0|\lambda\rangle|^2\langle\lambda|O|\lambda\rangle \quad (7)$$

where the states $|\lambda\rangle$ form a basis of eigenstates of the target Hamiltonian, $H\,|\lambda\rangle = \lambda\,|\lambda\rangle$. This simplifies the correction to

$$\overline{\Delta E} = \tau\langle\psi_0|C_1|\psi_0\rangle + +\tau^2\langle\psi_0|C_2|\psi_0\rangle - \frac{\tau^2}{4}\sum_{\lambda\in\sigma(H)}|\langle\psi_0|\lambda\rangle|^2\langle\lambda|\,[H_z,[H_x,H_z]]\,|\lambda\rangle - \tau^2\sum_{\lambda\in\sigma(H)}\mathrm{Im}\left(\langle\lambda|\psi_0\rangle\langle\psi_0|H_z|\lambda\rangle\langle\lambda|C_1|\lambda\rangle\right) - \frac{\tau^2}{12}\sum_{\lambda\in\sigma(H)}|\langle\psi_0|\lambda\rangle|^2\langle\lambda|\,[H_x - H_z,[H_x,H_z]]\,|\lambda\rangle + O(\tau^3). \quad (8)$$

This expression yields the dotted lines in Fig. 1**e** of the main text (MT).

B. Corrections to arbitrary observables

In the same way as before we derive an expansion up to second order in the Trotter step τ for the correction to an arbitrary observable A starting from an initial state $|\psi_0\rangle$. After taking long-time averages in the diagonal ensemble we obtain the result

$$\begin{aligned}\overline{A} = &\sum_{\lambda\in\sigma(H)}|\langle\psi_0|\lambda\rangle|^2\langle\lambda|A|\lambda\rangle - \tau\,\mathrm{Im}\left(\sum_{\lambda\in\sigma(H)}|\langle\lambda|\psi_0\rangle|^2\langle\lambda|H_zA|\lambda\rangle - \sum_{\lambda\in\sigma(H)}\langle\lambda|\psi_0\rangle\langle\psi_0|H_z|\lambda\rangle\langle\lambda|A|\lambda\rangle\right)\\
&+\frac{\tau^2}{4}\left(\sum_{\lambda\in\sigma(H)}|\langle\lambda|\psi_0\rangle|^2\langle\lambda|H_zAH_z|\lambda\rangle + \sum_{\lambda\in\sigma(H)}|\langle\psi_0|H_z|\lambda\rangle|^2\langle\lambda|A|\lambda\rangle\right) - \frac{\tau^2}{2}\mathrm{Re}\left(\sum_{\lambda\in\sigma(H)}\langle\lambda|H_z|\psi_0\rangle\langle\psi_0|\lambda\rangle\langle\lambda|H_zA|\lambda\rangle\right)\\
&+\frac{\tau^2}{6}\mathrm{Re}\left(\sum_{\lambda_1\neq\lambda_2}\Big(\langle\psi_0|\lambda_2\rangle\langle\lambda_2|A|\lambda_1\rangle - \langle\psi_0|\lambda_1\rangle\langle\lambda_1|A|\lambda_1\rangle\Big)\langle\lambda_2|\psi_0\rangle\langle\lambda_1|\,[H_x - H_z,[H_x,H_z]]\,|\lambda_2\rangle\frac{1}{\lambda_1-\lambda_2}\right)\\
&-\frac{\tau^2}{2}\mathrm{Re}\left(\sum_{\lambda_1\neq\lambda_2}\Big(\langle\psi_0|\lambda_2\rangle\langle\lambda_2|A|\lambda_1\rangle - \langle\psi_0|\lambda_1\rangle\langle\lambda_1|A|\lambda_1\rangle\Big)\langle\lambda_2|\psi_0\rangle\langle\lambda_1|[H_x,H_z]H_z|\lambda_2\rangle\frac{1}{\lambda_1-\lambda_2}\right)\\
&+\frac{\tau^2}{2}\mathrm{Re}\left(\sum_{\lambda\in\sigma(H)}\langle\psi_0|\lambda\rangle\langle\lambda|H_z|\psi_0\rangle\langle\lambda|AH_z|\lambda\rangle\right) - \frac{\tau^2}{2}\mathrm{Re}\left(\sum_{\lambda\in\sigma(H)}\langle\psi_0|\lambda\rangle\langle\lambda|A|\lambda\rangle\langle\lambda|H_z^2|\psi_0\rangle\right) + O(\tau^3). \quad (9)\end{aligned}$$

II. MEASUREMENT OF OTOCS USING STATISTICAL CORRELATIONS OF RANDOMIZED MEASUREMENTS

The onset of chaos and thus the breakdown of DQS is diagnosed by the OTOC defined in Eq. (17) of MT. In the following, we describe here how the OTOC can be measured in experiments.

The measurement of the OTOC is very challenging due to the alternation between operators at time zero and a finite time t. Protocols to measure $C(t)$ (or $F(t)$ defined in Eq. (24) of MT) that have been proposed in the literature thus involve backward time evolution [4–8] or the coupling to auxiliary quantum systems [9], and the first measurements have been implemented only recently [10–12]. Here we propose to measure the OTOC by adapting a recently developed measurement protocol [13] which does not require the above ingredients. Instead, it is an example of measurement protocols which are based on statistical correlations between randomized measurements. This concept was first devised for Rényi entropies [14–16], and was recently demonstrated in a trapped-ion quantum simulator [17] and in NMR [18]. The crucial ingredient in this class of measurement protocols are random unitary transformations which form (approximate) unitary two-designs. Thus, we first comment on the generation of such random unitaries in collective spin models and subsequently discuss how to use them to measure the OTOC.

A. Generation of random unitaries

In systems realizing collective spin models, the same tools that are used to engineer Hamiltonians of the form given in Eq. (7) of MT can be applied to generate random unitaries from approximate unitary two-designs. Unitary two-designs are ensembles that approximate the circular unitary ensemble (CUE) up to 2nd order correlations [19]. We adapt ideas from Ref. [15, 16] to create such random unitaries from a series of random quenches as a random time evolution operator u,

$$u = u_\eta \cdots u_1 \qquad \text{with} \qquad u_\alpha = \mathrm{e}^{-\mathrm{i}H_z^\alpha \tau}\mathrm{e}^{-\mathrm{i}H_x^\alpha \tau} \tag{10}$$

where the Hamlitonians H_μ^α take the same form as in Eq. (7) of MT,

$$H_\mu^\alpha = h_\mu^\alpha S_\mu + J_\mu S_\mu^2/(2S+1). \tag{11}$$

For each quench, parameters h_μ^α and J_μ^α are chosen independently from uniform distributions $h_\mu^\alpha \in [0.5/\tau, 1.5/\tau]$, $J_\mu^\alpha \in [5.5/\tau, 6.5/\tau]$ such that the kicked top which would be realized by periodic repetition of any of the u_α is deep in the chaotic regime [20].

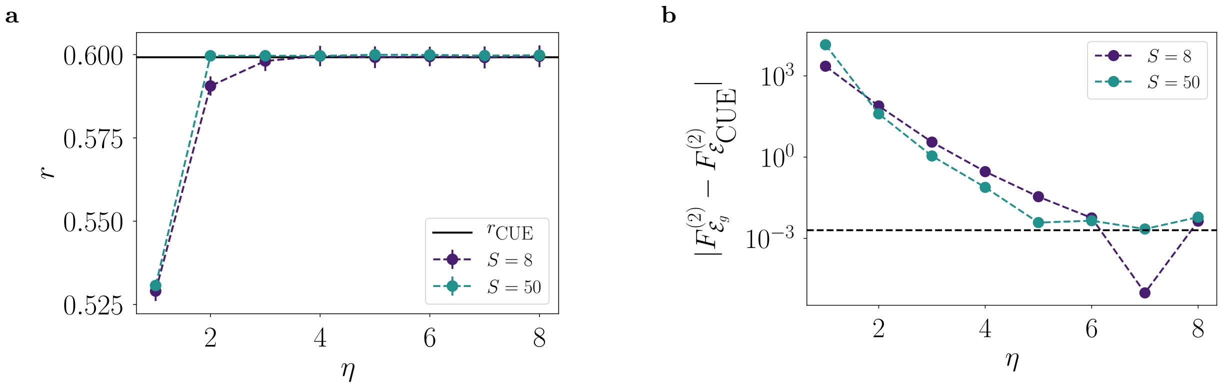
To test whether the ensemble of thusly created random unitaries indeed forms a unitary two-design, we consider first their phase spacing statistics as characterized by the ratios of adjacent phase spacing [21]. As displayed in Fig. 1, we observe a very rapid convergence of the mean value $\langle r\rangle$ with the number of quenches η towards the CUE value $r_{\mathrm{CUE}} = 0.5996(1)$. Second, to test not only eigenvalues but also the eigenvectors of the created unitaries, we consider the second frame potential [19], which is defined as

$$F_{\mathcal{E}}^{(2)} = \frac{1}{|\mathcal{E}|}\sum_{U,V\in\mathcal{E}} \left|\mathrm{tr}(U^\dagger V)\right|^4 \tag{12}$$

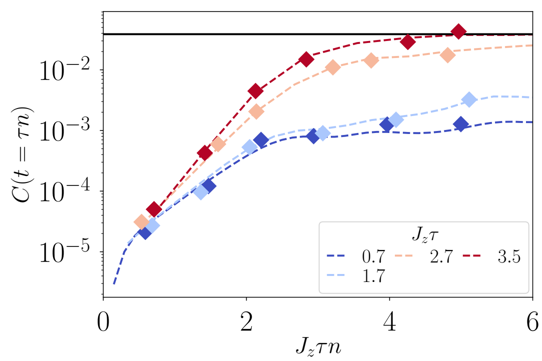
where $\mathcal{E}$ is an ensemble of unitary matrices. As shown in Ref. [19], for $\mathcal{E}$ being a unitary two-design, the frame potential takes a minimal value $F_{\mathrm{CUE}}^{(2)} = 2!$, and $F_{\mathcal{E}}^{(2)} - F_{\mathrm{CUE}}^{(2)}$ represents a fine-grained measure of distance between an ensemble $\mathcal{E}$ and a unitary two-design. However, we note that for small ensembles $|\mathcal{E}| \ll \mathcal{D}^4$, the diagonal contribution $\mathcal{D}^4/|\mathcal{E}|$ in the sum Eq. (12) dominates, irrespective of the properties of $\mathcal{E}$. Thus, to test numerically using a finite sample size whether the generated random unitaries are sampled from an approximate unitary two-design, we consider the quantity $F_{\mathcal{E}}^{(2)} - F_{\mathcal{E}_{\mathrm{CUE}}}^{(2)}$. Here, $F_{\mathcal{E}_{\mathrm{CUE}}}^{(2)} = 2! + \mathcal{D}^4/|\mathcal{E}_{\mathrm{CUE}}|$ is the average frame potential of a finite number $|\mathcal{E}_{\mathrm{CUE}}|$ of unitaries sampled from the CUE (see also Ref. [22]). In Fig. 1, $F_{\mathcal{E}}^{(2)} - F_{\mathcal{E}_{\mathrm{CUE}}}^{(2)}$ is displayed as function of number of quenches η, for a sample size $|\mathcal{E}_{\mathrm{CUE}}| = |\mathcal{E}_g| = 500$. We observe rapid convergence of $F_{\mathcal{E}_g}^{(2)} - F_{\mathrm{CUE}}^{(2)}$ towards the statistical error threshold $\sim 1/|\mathcal{E}_g|$, signaling that the generated random unitaries are indeed sampled from an (approximate) unitary two-design.

B. Protocol to measure the OTOC

The generated random unitaries, sampled from an approximate unitary two-design, can be used to measure the OTOC according to the following recipe [13]: (i) To an arbitrary pure state $|\psi_0\rangle$, apply a random unitary u generated via random quenches (see Appendix II A), to prepare the state $|\psi_u\rangle = u\,|\psi_0\rangle$. This randomized state serves as the input for two independent experiments. (ii.a) Evolve the state in time with $U(t)$ and measure the expectation value $\langle W(t)\rangle_u = \langle\psi_u|U^\dagger(t)WU(t)|\psi_u\rangle$ of the operator W. (ii.b) The state ψ_u is perturbed by the operator V, evolved in time and W is measured, to obtain $\langle V^\dagger W(t)V\rangle_u = \langle\psi_u|V^\dagger U^\dagger(t)WU(t)V|\psi_u\rangle$. (iii) Repeat steps (i) and (ii) for a sample of random unitaries u to estimate the statistical correlations of the two expectation values obtained in (ii.a)



Supplementary Figure 1. Generation of approximate two-designs. Convergence of $N_U = 500$ generated random unitaries to an approximate two-design as a function of the number of random quenches η for different spin sizes S. **a** Average adjacent phase spacing ratio. The black line corresponds to the CUE value. **b** Difference of the frame potential $F_{\mathcal{E}_g}$ of the generated unitaries to the frame potential $F_{\mathcal{E}_{\mathrm{CUE}}} = k! + d^4/N_U$ of an ensemble of same size $|\mathcal{E}_g| = |\mathcal{E}_{\mathrm{CUE}}| = 500$ which is drawn from the CUE. The black dashed line is the statistical error threshold $\sim 1/|\mathcal{E}_g|$.



Supplementary Figure 2. *Measurement of the OTOC.* Time evolution of the exact (solid lines) and "measured" (dots) squared commutator $C(t) = 2\,(S\,(S+1)/3 - \mathrm{Re}(F(t))$ for a system with collective spin $S = 64$. Parameters are the same as in Fig. 2 of the main text. The "measurements" are simulated using $N_U = 100$ random unitaries generated with $\eta = 5$ random quenches (same parameters as in Fig. 1). Projection noise is not included. The black line is the COE value.

and (ii.b) across the unitary ensemble. As shown in Ref. [13], the OTOC can be expressed in terms of these statistical correlations as

$$F(t)/F(0) = \frac{\overline{\langle W(t)\rangle_u \langle V^\dagger W(t) V\rangle_u}}{\left(\overline{\langle W(t)\rangle_u^2}\;\overline{\langle V^\dagger W(t) V\rangle_u^2}\right)^{1/2}}, \tag{13}$$

where $\overline{\cdots}$ denotes the ensemble average over random unitaries u. This expression underpins the interpretation of $F(t)$ as a measure of the butterfly effect in a quantum system: In analogy to rapidly diverging classical chaotic trajectories, the expectation values in the numerator can become decorrelated due to the perturbation V of the initial state. This is diagnosed by the decay of $F(t)$. In Fig. 2, data points correspond to simulated experiments using 100 generated random unitaries. The data demonstrates that the protocol outlined above can serve as another experimental probe to delimit the region of applicability of DQS and the onset of quantum chaos.

[1] Heyl, M., Hauke, P. & Zoller, P. Quantum localization bounds Trotter errors in digital quantum simulation. *Sci. Adv.* **5**, eaau8342 (2019).

[2] Bandyopadhyay, J. N. & Guha Sarkar, T. Effective time-independent analysis for quantum kicked systems. *Phys. Rev. E* **91**, 032923 (2015).

[3] Rigol, M., Dunjko, V. & Olshanii, M. Thermalization and its mechanism for generic isolated quantum systems. *Nature* **452**, 854–858 (2008).
[4] Swingle, B., Bentsen, G., Schleier-Smith, M. & Hayden, P. Measuring the scrambling of quantum information. *Phys. Rev. A* **94**, 040302 (2016).
[5] Zhu, G., Hafezi, M. & Grover, T. Measurement of many-body chaos using a quantum clock. *Phys. Rev. A* **94**, 062329 (2016).
[6] Bohrdt, A., Mendl, C. B., Endres, M. & Knap, M. Scrambling and thermalization in a diffusive quantum many-body system. *New J. Phys.* **19**, 063001 (2017).
[7] Shen, H., Zhang, P., Fan, R. & Zhai, H. Out-of-time-order correlation at a quantum phase transition. *Phys. Rev. B* **96**, 054503 (2017).
[8] Yoshida, B. & Yao, N. Y. Disentangling Scrambling and Decoherence via Quantum Teleportation. *Phys. Rev. X* **9**, 11006 (2019).
[9] Yao, N. Y. *et al.* Interferometric Approach to Probing Fast Scrambling. Preprint at: arXiv:1607.01801 (2016).
[10] Li, J. *et al.* Measuring Out-of-Time-Order Correlators on a Nuclear Magnetic Resonance Quantum Simulator. *Phys. Rev. X* **7**, 031011 (2017).
[11] Gärttner, M. *et al.* Measuring out-of-time-order correlations and multiple quantum spectra in a trapped-ion quantum magnet. *Nat. Phys.* **13**, 781–786 (2017).
[12] Landsman, K. A. *et al.* Verified quantum information scrambling. *Nature* **567**, 61–65 (2019).
[13] Vermersch, B., Elben, A., Sieberer, L. M., Yao, N. Y. & Zoller, P. Probing Scrambling Using Statistical Correlations between Randomized Measurements. *Phys. Rev. X* **9**, 021061 (2019).
[14] van Enk, S. J. & Beenakker, C. W. J. Measuring Tr ρ^n on Single Copies of ρ Using Random Measurements. *Phys. Rev. Lett.* **108**, 110503 (2012).
[15] Elben, A., Vermersch, B., Dalmonte, M., Cirac, J. I. & Zoller, P. Rényi Entropies from Random Quenches in Atomic Hubbard and Spin Models. *Phys. Rev. Lett.* **120**, 050406 (2018).
[16] Vermersch, B., Elben, A., Dalmonte, M., Cirac, J. I. & Zoller, P. Unitary n -designs via random quenches in atomic Hubbard and spin models: Application to the measurement of Rényi entropies. *Phys. Rev. A* **97**, 1–10 (2018).
[17] Brydges, T. *et al.* Probing Rényi entanglement entropy via randomized measurements. *Science* **364**, 260–263 (2019).
[18] Nie, X. *et al.* Detecting scrambling via statistical correlations between randomized measurements on an NMR quantum simulator. Preprint at arXiv:1903.12237 (2019).
[19] Roberts, D. A. & Yoshida, B. Chaos and complexity by design. *J. High Energy Phys.* **2017**, 121 (2017).
[20] Haake, F., Kuś, M. & Scharf, R. Classical and quantum chaos for a kicked top. *Zeitschrift für Phys. B Condens. Matter* **65**, 381–395 (1987).
[21] D'Alessio, L. & Polkovnikov, A. Many-body energy localization transition in periodically driven systems. *Ann. Phys. (N. Y).* **333**, 19–33 (2013).
[22] Cotler, J., Hunter-Jones, N., Liu, J. & Yoshida, B. Chaos, Complexity, and Random Matrices **11** (2017).