

Quantum Chaos and Universality in Trotterised Digital Quantum Simulations

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Digital quantum simulation (DQS) is one of the most promising paths for achieving first useful real-world applications for industry-scale quantum processors. Yet even assuming continued rapid progress in device engineering and successful development of fault-tolerant quantum processors, extensive algorithmic resource optimisation will long remain crucial to exploit their full computational power. Currently, among leading DQS algorithms, Trotterisation provides state-of-the-art resource scaling. Moreover, recent theoretical studies of Trotterised Ising models suggest that it also offers feasible performance for unexpectedly large step sizes up to a sharp breakdown threshold, but demonstrations and characterisation have been limited, and the question of whether this behaviour applies as a general principle has remained open. Here, we study a set of paradigmatic DQS models with experimentally realisable Trotterisations, and show that a range of Trotterisation performance behaviours, including the existence of a sharp threshold, are remarkably universal. Carrying out a detailed characterisation of a range of performance signatures, we demonstrate that it is the onset of digitisation-induced quantum chaos at this threshold that underlies the breakdown of Trotterisation. Specifically, combining analysis of detailed system dynamics with conclusive, global static signatures based on random matrix theory, we observe clear signatures of regular behaviour before the threshold, and conclusive, initial-state-independent evidence for the onset of quantum chaotic dynamics beyond the threshold. We also show how this behaviour consistently emerges as a function of system size for sizes and times already relevant for current experimental DQS platforms. Finally, introducing new error metrics, we show that the Trotter errors are an analytic function for large regions in step size below the threshold, and can be bounded even at long simulation times. The advances in this work open up many important questions about the algorithm performance and general shared features of sufficiently complex Trotterisation-based DQS. Answering these will be crucial for extracting the maximum simulation power from future quantum processors.

I. INTRODUCTION

Quantum simulation offers exciting opportunities for quantum processors to tackle the “in-silico” modelling of complex quantum systems that is often intractable for even the most advanced classical computing technology [1]. In analogue quantum simulation (AQS), a controllable, specialised surrogate is engineered to directly emulate the dynamical properties of the full target system, with rapid scaling of NISQ-era processors being achieved for models in condensed-matter physics [2–6] and lattice gauge theories [7–9]. In digital quantum simulation (DQS) [10], complex target dynamics is instead constructed in discrete steps from a sequence of simpler interaction primitives (gates) on a more generic processor. This versatile approach offers universal programmability that is not limited to models which can be mapped *in toto* onto systems re-

alisable naturally in a laboratory environment, and has been used to simulate highly varied target models across quantum chemistry [11–14], ultrastrong coupling [15–17], condensed-matter [18–22] and high-energy [23] physics.

A digital gate-based approach offers compatibility with future universal quantum computers [10] and the capacity for error correction to overcome the noise and decoherence limiting the power of noisy intermediate-scale quantum (NISQ) devices [24]. Yet it also introduces digitisation errors intrinsic to the algorithm which are reduced through finer and more sophisticated discretisation [10, 25–35]. Typically, this increases the required experimental resources (in terms of gates, qubits or runtime) and the exposure to noise, thus creating a trade-off between sufficient discretisation (algorithmic errors) and acceptable hardware noise (gates, decoherence, etc). In medium-term NISQ applications, DQS resource requirements can be somewhat reduced by combining the discretisation that increases versatility and accessible complexity, with analogue toolbox primitives to maximally exploit architecture-specific efficiencies [15–20, 22]. Ultimately, however, for

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both NISQ devices and even fully error-corrected quantum processors, simulation power will for a long time be limited by such resource constraints. It is therefore an essential open problem to improve our fundamental understanding of digitisation error and how much can be tolerated for a given application, and if possible, how to compensate or correct them.

The most common, and arguably still best-performing approach to DQS, known as Trotterisation [10, 35], is to approximate the target dynamics with small discrete time steps (Trotter steps) composed of primitive gate sequences determined by Trotter-Suzuki product formulas [25–29]. Coarser discretisation of time leads to larger Trotter errors, and two recent works studying Trotterised Ising models [36, 37], observed a performance threshold, where the Trotter approximation breaks down rapidly and completely, and the digitised dynamics beyond showed signatures of quantum chaotic behaviour. Another work [38] shows similar threshold behaviour for heating in a Trotterised spin chain with nearest-neighbour exchange interactions. References [36, 37] also showed that the errors in observables can be explained in terms of perturbative corrections quantified by the Floquet-Magnus expansion (see also [39]), showing that finer digitisation is not necessarily needed for improved accuracy. In order to exploit the possibilities these ideas open up, it is crucial to develop a deeper understanding of the Trotterisation threshold and how universally these systems behave. Creating the tools to characterise this threshold, and studying how close to it we can operate effectively will not only be important for optimising the power of future DQs, but could also be essential for bringing forward the time frame on which future quantum processors can be used to solve useful applications.

In this paper, we study a set of paradigmatic, Trotterised model systems, from which we develop new insights into the Trotterisation threshold, its universality and its connection with the onset of quantum chaotic dynamics. Using new techniques, we carry out an improved, detailed characterisation of the threshold for experimentally realisable Trotterisations of the Heisenberg [19, 20], Rabi-Dicke [15–17], and all-to-all Ising (A2A-Ising) [37] models. This allows us to target a set of important questions in the context of the Trotterisation threshold, such as the influence of symmetries, simulation with non-qubit components, and systems with infinite-dimensional Hilbert spaces. Across highly varied models, signatures and parameter regimes, we demonstrate strongly qualitatively similar performance behaviour, identifying distinctive regions in step size and simulation time that share surprisingly universal features. In each model, we observe a sharp Trotterisation threshold that marks an abrupt onset of quantum chaotic dynamics breaking down the periodic and quasiperiodic behaviour observed at small step sizes. We also observe a series of regular (non-quantum chaotic) regions beyond the threshold which we call stable islands. Our static analyses provide initial-state-independent signatures derived solely from the Trot-

terised unitary, supporting and extending the dynamical observations. By choosing system parameters giving integrable target dynamics, our results show that the observed quantum chaotic dynamics in the Trotterised evolution arises solely from digitisation.

In each model, we analyse the full system dynamics to reveal new detailed insight into the threshold behaviour. We show that the same threshold is shared among all signatures studied, including the simulation fidelity, which was previously thought not to exhibit a sharp threshold based on analysis exploring time averages [37]. Trotterised dynamics display clear signatures of (quasi)periodicity and quantum chaos [22, 40–46], and localisation and delocalisation [47, 48], respectively, before and after the threshold. We study how the threshold and onset of quantum chaos scale over several orders of magnitude in Hilbert-space dimension, starting from the smallest cases, and investigate the minimum sizes required to observe the threshold and quantum chaos. Specifically, using temporal averages (and evolutions) of the same dynamical signatures, we consistently observe indicators of quantum chaotic dynamics once the system becomes large enough. After this size, the positions of the threshold, which are in all cases respectable fractions of the relevant coupling strengths, show no significant dependence on dimension.

While these dynamical signatures provide useful insight, they also have some limitations, providing only indicative evidence of quantum chaos and for a particular initial state. To extend our dynamical observations, we therefore use the random matrix theory (RMT) [49] properties of quantum chaotic systems, specifically the eigenvector statistics [50, 51], to conclusively demonstrate the onset of quantum chaos at a sharp threshold in step size. We introduce a reduced chi-squared goodness-of-fit test statistic X_{RMT}^2 to quantify agreement or disagreement with the characteristic RMT statistics, and we again show for all models the existence of a sharp threshold for large enough systems at a step size that does not depend significantly on Hilbert-space dimension. Contrary to dynamical signatures, the eigenvector statistics reflect (initial state independent) properties of the Trotterised unitary. The fact that these signatures still conclusively exhibit quantum chaotic dynamics, illustrates that the threshold behaviour also does not depend significantly on initial state. Our dynamical analysis also finds that threshold behaviours and dynamical signatures of quantum chaos can arise even at the smallest system sizes. However, while X_{RMT}^2 still shows a noticeable change at the threshold at these sizes, we have so far only observed conclusive agreement with RMT for sufficiently large, if still modest, sizes.

Finally, we introduce time-averaged error measures that can distinguish Trotter errors from discrete sampling errors (which are observed even in the ideal system dynamics), and we show that the same threshold appears in each. These analyses also provide insight into the relationship of the errors with Trotter step size, total simulation time, and system size. We find that the pre-threshold er-

rors are generally much smaller than the errors in chaotic regions, with varying dependence on system size and total simulation times. Significantly, we observe that, when correctly defined, the error measures are an analytic function of step size before the threshold, which suggests that it may be possible to at least partially correct these errors using a perturbative approach like the Floquet-Magnus expansion [36, 37].

The paper is organized as follows. In Sec. II, we provide key background information about Trotterisation, its Floquet interpretation, and quantum chaos (with a more detailed background on quantum chaos in appendix A). Sec. III describes the physical models and their experimentally accessible Trotterisations. Our detailed findings are presented in the main part of the paper in Sec. IV, and we discuss our conclusions and the outlook in Sec. V.

II. BACKGROUND

This section summarises the relevant concepts from Trotterisation and quantum chaos, introducing the notations and definitions that are used in the rest of the manuscript. In all the equations here, we take $\hbar = 1$.

A. Trotter Errors

In Trotterisation, the target model Hamiltonian $H_M = \sum_{l=1}^L H_l$ is decomposed into a sum of experimentally accessible Hamiltonians $\{H_l\}$. Then, the desired time evolution $U_M(t) = e^{-iH_M t}$ is approximated by a sequence of discrete time evolution operators $U_l(\tau) = e^{-iH_l \tau}$ for corresponding Hamiltonians H_l , according to [10]

$$U_M(t) \approx \underbrace{\left[\prod_l U_l(\tau) \right]}_{:=U_\tau^r}, \quad (1)$$

where we define the (Trotter) step size $\tau = t/r$ as the ratio of total simulated time t and number of (Trotter) steps r . Defining the unitary operators U_τ and U_τ^r for a single and r Trotter steps, respectively, the approximation errors ϵ can be defined using a Taylor series expansion [10]

$$U_M(t) - U_\tau^r = \frac{t^2}{r} \sum_{l>m} [H_l, H_m] + \mathcal{O}\left(\frac{t^3}{r^2}\right), \quad (2)$$

where $\mathcal{O}(t^3/r^2)$ subsumes the higher-order corrections. Eq. (1) is a generic example of first-order Trotterisation, but in general the unitary operations in a Trotter step U_τ are determined also by a Trotterisation order. The approximation errors $\|U_M(t) - U_\tau^r\| \rightarrow 0$ for $r \rightarrow \infty$ (i.e. $\tau \rightarrow 0$) for fixed t , and the rate of convergence to continuum depends on the order of the Trotterisation [26–29]. Trotter-Suzuki approximations (at any order) become exact when all the summands $\{H_l\}$ commute, but this

is commonly not satisfied. Additionally, in practice, τ is always finite, so we target a maximum error ϵ (for fixed simulated time t) and try to determine the Trotter step size (for a particular Trotterisation order) required to achieve the desired accuracy.

The usual assumption in Eq. (2) is that the first-order error term dominates (and consequently bounds) the errors, but this intuition does not always hold [35]. A more concrete bound on the error can be obtained by using a tail bound of the Taylor expansion [52]. This worst-case bound scales, at best, linearly with simulation time t [52], and can be expressed in terms of the required number of steps r_{2k} that ensures an error $\|U_M(t) - U_\tau^r\| \leq \epsilon$ for a $2k$ (th)-order Trotterisation [52, 53]:

$$r_{2k} = \mathcal{O}\left(\frac{(\max_l \|H_l\| Lt)^{1+\frac{1}{2k}}}{\epsilon^{\frac{1}{2k}}}\right), \quad (3)$$

where the $\|\cdot\|$ is the spectral-norm, L is the number of summands, and k is any positive integer.

Though Trotterisations provide convenient implementations of direct Hamiltonian decompositions, the scaling of the gate estimate in Eq. (3) with time, system size, and other parameters draws a pessimistic picture for the product formulas. Consequently, alternative, so-called post-Trotter DQS algorithms [30–33], with different overheads such as requirements for auxiliary qubits, have been developed to overcome the apparent inefficiency of Trotterisation. But while the generic estimates of gate complexities, such as Eq. (3), provide sufficient conditions for the desired accuracy [52], empirical analyses of Trotterisation algorithms show that such rigorous estimates are often loose, and the desired accuracy is typically already achieved for orders of magnitude fewer steps than the estimates [35, 53–58]. Additionally, recent rigorous theory results [35], providing improved bounds on Trotter errors, showed that Trotterisation can match or even outperform the state-of-the-art post-Trotter algorithms, suggesting that Trotterisation may even be the optimal algorithm. Also note that the performance of Trotterisation algorithms might be improved even further by exploiting commutations between summands [34, 54] and/or by randomised ordering of unitary evolutions in each Trotter step [53, 59, 60].

Since we focus on Trotterisation algorithms in this paper, we may, unless otherwise specified, use DQS to refer specifically to Trotterisation.

B. Trotterisation Sequences as Floquet Systems

In addition to gate complexities, it is equally important to know the nature of the errors and the minimum r (maximum τ) at which the approximation is still valid. For example, before the complete breakdown point of the approximation due to coarse digitisation [36, 37], it may still be possible to correct the errors. Alternatively, it may also be possible to predict the $r \rightarrow \infty$ (i.e. $\tau \rightarrow 0$)

value for a particular choice of observable from a smaller number of steps.

An alternative approach to Trotter error analyses [36, 37] is to interpret the Trotterised evolution as the stroboscopic dynamics under a Floquet Hamiltonian H_F ,

$$U_\tau = \prod_l U_l(\tau) = e^{-iH_F\tau}. \quad (4)$$

The digitisation error in the effective Floquet Hamiltonian is then quantified by the Floquet-Magnus (FM) expansion,

$$H_F = H_M + i\frac{\tau}{2} \sum_{l>m} [H_l, H_m] + \mathcal{O}(\tau^2), \quad (5)$$

where $\mathcal{O}(\tau^2)$ subsumes any higher-order corrections. The Floquet-Magnus expansion has a finite radius of convergence τ^* , beyond which the approximation breaks down. Theoretically, this represents the largest step size for which Trotterisation will realise a meaningful approximate simulation. Taking the Floquet-Magnus expansion as a special case of a more general Magnus expansion for a periodically time-dependent Hamiltonian, a rigorous sufficient condition of convergence can be derived that suggests that the radius of convergence should scale in inverse proportion to system size [61–63]. If this lower bound on τ^* were tight, its scaling with inverse system size would suggest that realising large system sizes should be very challenging.

As discussed in the introduction, two recent numerical works studying DQS of the Ising model by some of the authors [36, 37] identified a performance threshold in Trotter step size (a threshold τ) separating a region of controllable errors from a quantum chaotic regime. A work investigating where the Floquet-Magnus expansion diverges saw a similar threshold in Floquet heating [38]. Moreover, by interpreting the Trotterised evolution as a periodically time-dependent quantum system, Refs [36, 37] considered the errors in dynamical quantities, such as expectation values, rather than errors in the full time evolution operator ($\|U_M(t) - U_\tau^t\|$), and they showed that the pre-threshold Trotter errors in the Ising DQS agree with the perturbative corrections predicted by the Floquet-Magnus expansion [36]. Another very recent result [39] shows that structural deviations can arise in the Floquet Hamiltonian that cause localised regions of high Trotter errors even at step sizes in the perturbative region. Nevertheless, the findings of Refs [36, 37] open up interesting potential avenues for achieving better practical results with accessible performance, even for NISQ-era DQS. For example, perturbative treatments could enable extrapolation of ideal dynamics (i.e. $\tau \rightarrow 0$) from the simulations with finite Trotter step sizes τ . This would effectively circumvent the impact of Trotter errors by allowing accurate simulation results to be calculated from simulations run over a range of comparatively large Trotter step sizes, and would simultaneously also help minimise the impact of errors extrinsic to the algorithm, such as decoherence and imperfect gates. Our results here dramatically extend the scope

of these findings and help elevate the observations (that were mainly limited to Ising models) from Refs [36, 37] to the status of a universal DQS principle [39].

C. Quantum Chaos

In contrast to classical chaos, where infinitesimal differences in initial states diverge exponentially in time, the unitarity of dynamics in quantum mechanics ensures that the overlap between two arbitrary initial states stays the same for all times t ,

$$\begin{aligned} \mathcal{F}(\psi_1(0), \psi_2(0)) &= |\langle \psi_1(0) | \overbrace{U^\dagger(t)U(t)}{=1} | \psi_2(0) \rangle|^2 \\ &= \mathcal{F}(\psi_1(t), \psi_2(t)), \end{aligned} \quad (6)$$

where $\mathcal{F}(\psi_1, \psi_2) := |\langle \psi_1 | \psi_2 \rangle|^2$ is the fidelity between the states $|\psi_1\rangle$ and $|\psi_2\rangle$. But while the notion of quantum chaos does not naively follow popular concepts of classical chaos, similar intuitive signatures can still be found in quantum dynamics. For example, the perturbation fidelity between two states evolved from the same initial state $|\psi\rangle$ under two slightly different unitaries $U(t)$ and a perturbed $U_p(t)$, $\mathcal{F}(\psi_p(t), \psi(t)) := |\langle \psi | U_p^\dagger(t)U(t) | \psi \rangle|^2$, decays exponentially for quantum chaotic systems [40]. Unfortunately, although this interpretation is intuitive, this fidelity decay signature is reliable only for appropriate perturbations [42].

There are many other dynamical signatures of quantum chaos [46], and all of them (including the reliability of a perturbation for fidelity decay [42]) derive from certain features governing the eigenvectors of either a unitary evolution operator, or equivalently its corresponding Hamiltonian. For quantum chaotic systems, the eigenvectors show certain random matrix properties, namely that the distribution of their components in another basis follow specific distributions from random matrix theory (RMT) [49–51]. This type of analysis, known as eigenvector statistics, underlies the study of quantum chaos that will be described in this work. A more detailed overview of quantum chaos, its relation with RMT, and technical subtleties in calculating the signatures of quantum chaos are provided in appendix A.

Throughout this paper, we use (quasi)periodic, regular or stable interchangeably to mean *non-quantum chaotic*.

III. PHYSICAL MODELS AND THEIR TROTTERISATIONS

To obtain a more comprehensive understanding of the Trotterisation threshold observed in Refs [36, 37], we consider a set of paradigmatic model systems, which share the feature that their Trotterised dynamics could be realisable experimentally in the near future: the (i) Ising (in all-to-all interactions limit), (ii) Heisenberg, and (iii) Rabi-Dicke models. In this section, we provide descriptions

of the model Hamiltonians H_M and their experimentally realisable Trotter-Suzuki decompositions. Since our goal is to investigate the threshold behaviour of Trotter errors, we do not provide either an extensive or a complete summary (or references) of these models. They are extensively studied fundamental quantum models describing magnetism (Ising and Heisenberg [64]) and light-matter interactions (Rabi-Dicke [65–69]), and they and their various generalisations and modifications offer rich physical phenomena and practical applications, such as quantum phase transitions (in Ising [70–72], Heisenberg [73], and Dicke and Rabi models [66, 74]), and even mappings to NP problems [75].

A. Spin Models

The general spin-spin interaction Hamiltonian [64]

$$H = \sum_{k,l} g_{k,l} [\alpha (\sigma_x^k \sigma_x^l + \sigma_y^k \sigma_y^l) + \beta \sigma_z^k \sigma_z^l] \quad (7)$$

defines the Heisenberg interaction for $\alpha = \beta = 1$, Ising interaction for $\alpha = 0$ & $\beta = 1$, and the exchange (or XY-) interaction for $\alpha = 1$ & $\beta = 0$, where σ_μ are the Pauli spin operators with $\mu \in \{x, y, z\}$. Example Trotterisations of these models are considered in Refs [19, 20], [36, 37, 39], and [38], respectively. The structure of the coefficients $g_{k,l}$ defines further variations in each case [64]. Here, we consider all-to-all ($g_{k,l} \neq 0 \forall k, l$) and one-dimensional nearest-neighbour ($g_{k,l} \neq 0$ iff $|k - l| = 1$) interactions for the Ising and Heisenberg models, respectively.

1. The Ising Model

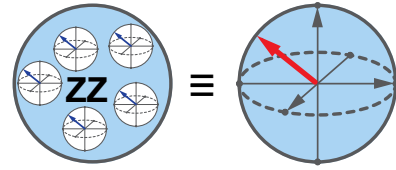
Trotterisation thresholds in Ising-model DQS have been considered for various regimes of power-law interactions in Refs [36, 37]. Here, we revisit the all-to-all (A2A) case, and reveal new insight into the threshold behaviour. In this limit, the DQS model maps to the quantum kicked top [37], and reduces to a collective spin system with total spin j , as depicted in Fig. 1 (a), facilitating the study of threshold behaviours up to relatively large system sizes. Here, we describe the corresponding quantum kicked-top model and the effective target Hamiltonian, and refer to Ref. [37] for further details of the model. Specifically, the corresponding Trotter-Suzuki decomposition is given by the kicked-top Floquet operator

$$U_I(t) = e^{-iH_I t} \approx \left(e^{-iH_z t/n} e^{-iH_x t/n} \right)^r = U_\tau^r, \quad (8)$$

where $H_I = H_z + H_x$ is the effective target-model Hamiltonian. The individual summand Hamiltonians are

$$H_\mu = \omega_\mu J_\mu + g_\mu J_\mu^2 / (2j + 1), \quad (9)$$

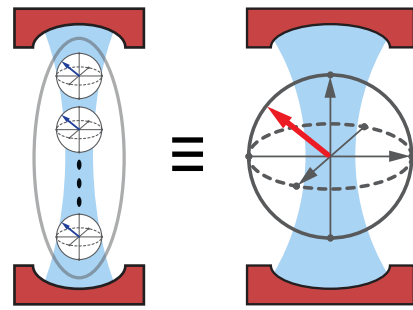
for $\mu \in \{x, z\}$, with standard angular momentum operators J_μ of a spin $j = N/2$ system, corresponding to the



(a) DQS of all-to-all (A2A) Ising system of N qubits maps to the quantum kicked top of a single spin with spin number $j = N/2$. Here, ZZ represents the Ising interaction.



(b) The nearest-neighbour Heisenberg model is a chain of N qubits with XYZ coupling between each neighbouring qubits.



(c) The collective behaviour of the qubit ensemble inside a cavity is represented as a large spin for the Dicke model.

Figure 1. Pictorial schematics of the physical models analysed in this paper.

(maximal) collective spin of $N = 2j$ spin-1/2 systems in an A2A-Ising system [37]. The quantum kicked-top models have already been implemented in various platforms, including in a single Caesium atom with $j = 3$ [76], the collective spin of an ensemble of three superconducting qubits [22] corresponding to $j = 3/2$, and others (including novel proposals [77]) discussed in Ref. [37].

For ease of comparison and consistency, we show our results for the same simulation parameters as in Ref. [37], that is $g_z := g$ (with time measured in units of $2\pi/g$ for all models), $\omega_x = 0.1g_z$, $g_x = 0.7g_z$, and $\omega_z = 0.3g_z$, and the initial state is $|\theta = 0, \phi = 0\rangle = |j, j\rangle$, where $|\theta, \phi\rangle = \exp(i\theta(J_x \sin(\phi) - J_y \cos(\phi))) |j, m = j\rangle$ is the spin coherent state. The qualitative behaviour of our results does not depend on the precise values of these parameters [37].

2. The Heisenberg Model

The Heisenberg model is an extensively studied model in the quantum theory of magnetism [64], and, in addition

to its fundamental importance, the random-field version of this model is proposed to allow demonstrations of quantum speed-up in quantum simulations [34]. Here, we consider the uniform-field case with parameters and system sizes readily available in current experiments [20].

Specifically, we consider a nearest-neighbour interacting spin chain version of the Heisenberg model with open boundary conditions, homogenous couplings, and a longitudinal external field (as depicted in Fig. 1 (b)):

$$H_H = \underbrace{\frac{\omega}{2} \sum_{k=1}^N \sigma_z^k}_{H_z} + g \sum_{k=1}^{N-1} (\sigma_x^k \sigma_x^{k+1} + \sigma_y^k \sigma_y^{k+1} + \sigma_z^k \sigma_z^{k+1}), \quad (10)$$

where g is the nearest-neighbour coupling strength, and ω is the Zeeman splitting due to the homogenous magnetic field applied in the z -direction. All our results, including the existence of stable islands, qualitatively hold also for the cases with a transverse (i.e. σ_y or σ_x term) or no external field (data available, but not shown). The Heisenberg interaction is rotationally symmetric, and the distinction between longitudinal and transverse fields is not strictly relevant for it. However, the rotational symmetry is broken by the chosen Trotterisation, and this distinction is relevant for analysing the Trotterised unitary and is reflected in its eigenvector statistics (see appendix C1).

The Heisenberg model Hamiltonian in Eq. (10) can be decomposed into $H_H = H_z + H_{xy} + H_{xz} + H_{yz}$ [19, 20], where the exchange interaction

$$H_{xy} = g' \sum_{k=1}^{N-1} (\sigma_x^k \sigma_x^{k+1} + \sigma_y^k \sigma_y^{k+1}), \quad (11)$$

with interaction strength $g' = g/2$, is the workhorse interaction for many experimental platforms. H_z is just the free-evolution, and the other two terms of the decomposition are obtained from the exchange interaction by applying local transformations:

$$H_{xz} = \mathcal{R}_{x, \frac{\pi}{2}}^{\vee k} H_{xy} \mathcal{R}_{x, \frac{\pi}{2}}^{\vee k \dagger} = g' \sum_{k=1}^{N-1} (\sigma_x^k \sigma_x^{k+1} + \sigma_z^k \sigma_z^{k+1}), \quad (12)$$

and

$$H_{yz} = \mathcal{R}_{y, \frac{\pi}{2}}^{\vee k} H_{xy} \mathcal{R}_{y, \frac{\pi}{2}}^{\vee k \dagger} = g' \sum_{k=1}^{N-1} (\sigma_y^k \sigma_y^{k+1} + \sigma_z^k \sigma_z^{k+1}), \quad (13)$$

where $\mathcal{R}_{x(y), \theta}^{\vee k} = \prod_{k=1}^N e^{-i\theta J_{x(y)}^k}$ are locally applied, single-qubit ($j = 0.5$) rotations by an angle $\theta = \pi/2$ along the $J_{x(y)} = j \times \sigma_{x(y)}$.

This decomposition, without the Zeeman term, was proposed [19] and experimentally realised in circuit-QED [20]. The generalisation we introduce here can be implemented in any platform [20, 78] with the exchange interaction and

single-qubit rotations, via the following Trotterisation

$$U_\tau = U_z(\tau) \prod_{k=1}^{N-1} U_{xy}^{k, k+1}(\tau) \prod_{k=1}^{N-1} U_{xz}^{k, k+1}(\tau) \prod_{k=1}^{N-1} U_{yz}^{k, k+1}(\tau), \quad (14)$$

where the $U_{ab}^{k, k+1}(t) = \exp(-iH_{ab}^{k, k+1}t)$ are unitary operators $\forall ab \in \{xy, xz, yz\}$, $U_z = \exp(-iH_z t)$, and the qubit rotations are implicit.

In our numerical simulations, we choose the highly symmetric parameters of $\omega = g$, and the initial state for the results presented in the main text of the paper is $|1\rangle_{i=1} \otimes |0\rangle_{i>1}$, with all qubits in the ground state except for a single excitation in the first qubit. We explored the Heisenberg DQS for a range of different parameters, and the threshold behaviour does not depend on the precise choice of these parameters, but the (quasi)periodic dynamics before the threshold may show variations depending on the initial state. We discuss initial-state effects further in our results (Sec. IV), and support these discussions in appendix C3 by analysing the results for spin coherent, product, and random initial states.

B. The Rabi-Dicke Model

The quantum Rabi (QR) model [65] describes the fundamental interaction between a two-level system (i.e., a qubit) and a single mode of the quantised electromagnetic field

$$H_R = \omega_c a^\dagger a + \frac{\omega_q}{2} \sigma_z + g(a^\dagger + a)\sigma_x, \quad (15)$$

where a^\dagger and a are the creation and annihilation operators for the field mode, and ω_c , ω_q , and g are the cavity-field, qubit, and coupling frequencies. Both natural and typical experimental systems typically satisfy $g \ll \omega_c, \omega_q$, where a rotating-wave approximation (RWA) applies, reducing the QR model to the Jaynes-Cummings (JC) model [67]

$$H_{JC} = \omega_c a^\dagger a + \frac{\omega_q}{2} \sigma_z + g(a^\dagger \sigma_- + a \sigma_+), \quad (16)$$

where $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$ are raising/lowering operators for a two-level system. However, DQS provides a flexible platform to explore the full QR model without the need for challenging, direct experimental implementations. This was recently demonstrated in circuit QED [16], and can easily be generalised.

One important generalisation is the N -qubit case described by the Dicke model [66]:

$$H_D = \omega_c a^\dagger a + \frac{\omega_q}{2} \sum_{k=1}^N \sigma_z^k + \frac{g}{\sqrt{N}} \sum_{k=1}^N (a^\dagger + a)(\sigma_+^k + \sigma_-^k). \quad (17)$$

By exploiting the collective spin behaviour of the atomic ensemble (as depicted in Fig. 1 (c)), it can be written in terms of angular momentum operators [69]

$$H_D = \omega_c a^\dagger a + \omega_j J_z + \frac{g}{\sqrt{2j}} (a^\dagger + a)(J_+ + J_-), \quad (18)$$

where $j = N/2$ is the total collective spin, the frequency $\omega_j = \omega_q$, and $J_{\pm} = (J_x \pm iJ_y)/2$ are raising/lowering operators of an angular momentum with total spin j . Under the RWA, the Dicke model reduces to the Tavis-Cummings (TC) model [68],

$$H_{TC} = \omega_c a^\dagger a + \omega_j J_z + \frac{g}{\sqrt{2j}} (a^\dagger J_- + a J_+). \quad (19)$$

In systems with access to TC coupling and single-qubit rotations, digital quantum simulation of the Dicke Hamiltonian (including the Rabi Hamiltonian) can be achieved via the decomposition

$$H_D = H_{TC}(g, \Delta_c, \Delta_j^{TC}) + H_{ATC}(g, \Delta_c, \Delta_j^{ATC}), \quad (20)$$

where the anti-Tavis-Cummings (anti-TC) Hamiltonian

$$\begin{aligned} H_{ATC} &= \mathcal{R}_{x,\pi}^{\vee k} H_{TC} \mathcal{R}_{x,\pi}^{\vee k \dagger} \\ &= \Delta_c a^\dagger a - \Delta_j^{ATC} J_z + \frac{g}{\sqrt{2j}} (a^\dagger J_+ + a J_-) \end{aligned} \quad (21)$$

contains only the counter-rotating terms and is obtained from the TC interaction by locally applied qubit rotations of an angle π . The effective simulation frequencies are $\omega_c^{\text{eff}} = 2\Delta_c$ and $\omega_j^{\text{eff}} = \Delta_j^{TC} - \Delta_j^{ATC}$, where $\Delta_\mu = \omega_\mu - \omega_{\text{RF}}$ are defined relative to a nearby rotating frame (RF), giving precise control of simulated frequencies (see Ref. [16] for details on the RF and its experimental implementation in circuit QED). The first-order Trotterisation

$$U_\tau = U_{TC}(\tau) U_{ATC}(\tau), \quad (23)$$

where $U_{A/TC}(t) = \exp(-iH_{A/TC}t)$, is proposed in Ref. [15]. Both this and the 2nd-order Trotterisations are experimentally realised for $j = 0.5$, i.e., the Rabi model, in circuit QED [16].

The Dicke model is known to be quantum chaotic for g values around the critical coupling strength $g_c = \sqrt{\omega_c \omega_j}/2$ of the superradiant phase transition [79, 80]. In order to study digitisation-induced quantum chaos, we specifically choose cavity and spin frequencies far enough from its quantum chaotic regime, in its normal phase, but still staying in the ultra-strong coupling regime (so that RWA does not apply). Our results (on the existence and the qualitative properties of the threshold) hold for both the quantum chaotic and regular parameter regimes of the Dicke model, and, in the appendix D 4, we discuss our choice of parameters and also provide example results for the Dicke DQS in its quantum chaotic regime. In our numerical simulations, the system parameters are $\omega_j = \omega_c = 3.5g$ (giving $g_c = 1.75g$, which is sufficiently larger than g for the model to be non-quantum chaotic), and the initial state is $|0\rangle \otimes |j, j\rangle$: that is, with zero photons in the cavity and the qubit ensemble in the spin coherent state $|j, j\rangle = |\theta = 0, \phi = 0\rangle$, where $|\theta, \phi\rangle = \exp(i\theta(J_x \sin(\phi) - J_y \cos(\phi))) |j, m = j\rangle$. In our descriptions, we will sometimes refer to the Rabi-Dicke model to emphasise our results encompass both cases.

IV. TROTTERISATION THRESHOLD AND ONSET OF QUANTUM CHAOS

In this section, we present the main results of this work, demonstrating a clear Trotterisation threshold shared across a range of physical signatures, and conclusive evidence for the onset of quantum chaos beyond the threshold. As described in Sec. II A, when all the terms in a Trotter-Suzuki decomposition commute, the digitised dynamics perfectly matches the target dynamics for any Trotter step size. In such a situation, Trotterised dynamics cannot exhibit any sort of step-size related threshold behaviour. On the other hand, when there are non-commuting terms in the decomposition that give rise to Trotter errors, it was recently shown in the context of Trotterised Ising models [36, 37] that there can be a performance threshold, and it is possible for the Trotterised dynamics beyond the threshold to be quantum chaotic, even when the target dynamics is regular. Here, to characterise this threshold behaviour in depth and study how generically it arises in Trotterised DQS, we carry out a broader and more comprehensive analysis of Trotterisation performance thresholds across a range of experimentally achievable physical models and system sizes, using new and expanded characterisation techniques. In the models we study, we conclusively show that this breakdown in Trotterisation results from the onset of digitisation-induced quantum chaos beyond the threshold. Therefore, our results suggest there may be a generic, intrinsic connection between the onset of quantum chaos and the breakdown of Trotterisation, both of which stem from the non-commutations of the Trotter decomposition.

For each model, we analyse various dynamical, time-averaged, and static quantities together with error measures, to show that the Trotterisation has a performance threshold in (Trotter) step size without a significant dependence on system size. We first analyse the time evolution of various quantities at one system size, providing new insights into the threshold behaviour. We then compare the time averages of these dynamical quantities for system sizes across multiple orders of magnitude in Hilbert-space dimension, starting from the smallest and scaling up. In every model, the Trotterised dynamics show signatures of quantum chaos beyond the threshold with additional model-dependent characteristics, such as the structure of stable islands observed inside the quantum chaotic regions. Following this, we then combine powerful static signatures based on RMT, namely eigenvector statistics, with a chi-squared goodness-of-fit test, and we conclusively demonstrate the transition from regular to quantum chaotic dynamics at this threshold, show its system-size and initial-state independence, and identify the existence of stable islands beyond the threshold. With these powerful but experimentally less accessible static analyses, we provide further support to the analyses using dynamical signatures that are easier to characterise and measure experimentally. Finally, using various error measures, we analyse the relationship of the errors with the system size,

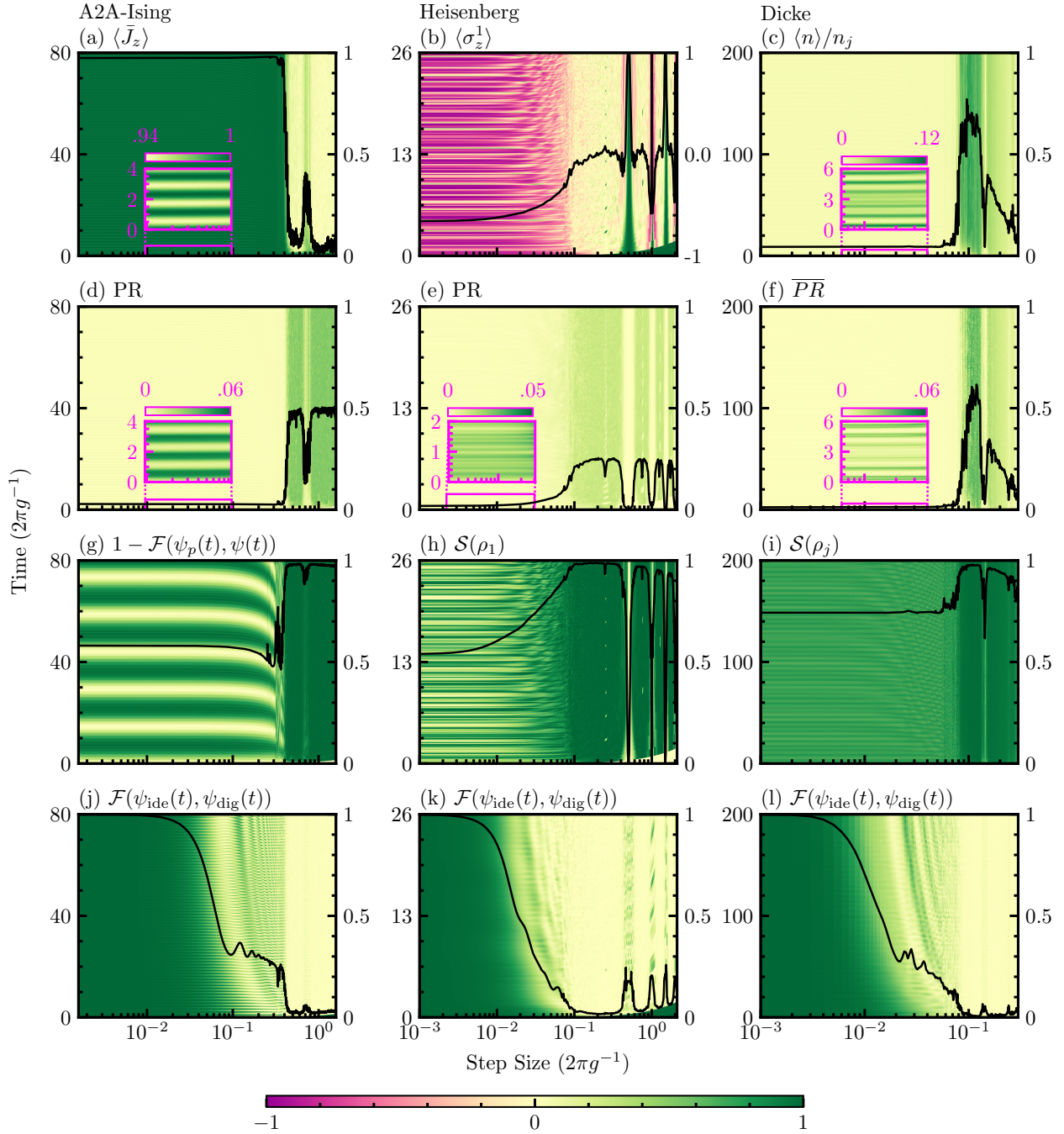


Figure 2. Full dynamics for each model system, showing (a–c) local observables, (d–f) delocalisation, (g–i) further complementary dynamical signatures of quantum chaos, and (j–l) simulation fidelity. Left to right, columns show results for A2A-Ising (with $j = 64$), Heisenberg (chain of $N = 8$ qubits), and Dicke (with $j = 6$) models, respectively, with x-axes common to each column showing step sizes. The y-axes of the colour plots (left axes) are the simulation times. The black lines (right y-axes) are the time averages of the colour plots. In each model, dynamical quantities share a common Trotterisation threshold at a critical step size separating (quasi)periodic from quantum chaotic regimes. (a–c) (Quasi)periodicity in expectation values of example local observables is clearly observed prior to the threshold, and destroyed after it: shown for (a) magnetisation $\langle \bar{J}_z \rangle = \frac{1}{j} \langle J_z \rangle$, (b) polarization of qubit one $\langle \sigma_z^1 \rangle$, and (c) normalised photon number $\langle n \rangle / n_j$ (with $n_j = 7 \times \dim_j$). (d–f) Localised initial states rapidly delocalise beyond the threshold, quantified by participation ratios (PR, Eq. (24)). (g–i) further complementary dynamical signatures of quantum chaos exhibit the same threshold: e.g., infidelity under perturbation $1 - \mathcal{F}(\psi_p(t), \psi(t))$ (see Eq. (25)) for Ising, and normalised sub-system entropies $\mathcal{S}(\rho_i)$ (Eq. (26)) for Heisenberg (first qubit) and Dicke (spin), are all rapidly maximised beyond the threshold. (j–l) Simulation fidelity $\mathcal{F}(\psi_{\text{dig}}(t), \psi_{\text{ide}}(t))$ decays rapidly beyond the same threshold, showing surprisingly universal behaviour across the different models. Clear quasiperiodic oscillations in the near pre-threshold region explaining why the time-averaged simulation fidelity does *not* show the same sharp threshold. In each model, the dynamical signatures of quantum chaos (a–i) disappear in certain regimes beyond the threshold, referred to as stable islands, showing revival of regular dynamics, without a corresponding return of accurate target system simulation (j–l).

total simulation time, and step size.

A. Threshold in Dynamical Quantities

Here, we show that studying time evolutions, rather than time averages, provides clear signatures both for the regular and quantum chaotic dynamics revealing improved insight into the threshold behaviour. We study the time evolutions of expectation values, localisation measures, quantum chaos signatures, and simulation fidelities as a function of step size. In particular, regular/quantum chaotic dynamics before/after the threshold, such as observation/destruction of (quasi)periodicity in expectation values, enable identification of Trotterisation thresholds, even when they are not always clear from the time averages of dynamical quantities, especially for the simulation fidelities. Finally, we note that the dynamical quantities exhibit islands of non-chaotic behaviour (stable islands) inside the quantum chaotic regime, which we discuss in more detail in Sec. IV A 4.

Colour plots in Fig. 2, with the time on (the left) y-axes and the step size on x-axes, show our results for the dynamical quantities given in the titles of each sub-figure. The black lines on the colour plots are the time average of the same quantities (averaged over the full time-axis), with their y-axes given on the right side of the figures (matching the corresponding colour bar axes).

1. Destruction of (Quasi)periodicity in the Dynamics of Physical Observables

In quantum simulations, we are mostly interested in expectation values of some physical observables, which are often periodic or quasiperiodic for regular quantum dynamics, and the destruction of (quasi)periodicity is a characteristic signature of quantum chaotic dynamics. Here, we show the onset of this destruction in Trotterised dynamics as the step size is increased beyond a threshold. Figures 2 (a-c) illustrate this effect for A2A-Ising (with $j = 64$), Heisenberg (chain of $N = 8$ qubits), and Dicke (with $j = 6$) models in the time evolutions of the observables, (a) magnetisation, i.e. the normalised expectation value $\langle J_z \rangle = \frac{1}{j} \langle J_z \rangle$ of the J_z angular momentum operator, (b) first qubit polarization, i.e. expectation value of Pauli z-operator $\langle \sigma_z^1 \rangle$, and (c) normalised photon number $\langle n \rangle / n_j$ (with $n_j = 7 \times \dim_j := 7 \times (2 \times j + 1)$) based on the numerical observations discussed in the Sec. IV B), respectively. Because the total simulation time of each model in Fig. 2 is chosen to reveal long time details of the dynamics, especially for simulation fidelities discussed in Sec. IV A 3, some of the fast lower contrast dynamics in (quasi)periodic regimes are only revealed when zoomed in. The insets in Fig. 2 show the (quasi)periodic behaviour present in each model by magnifying both the temporal features and the colour contrasts. We have observed this behaviour over a wide range of time scales and show both

short- and long-time examples as part of the Trotter error analysis in Sec. IV D.

The threshold position is clear from both the destruction of (quasi)periodicity and the time averages (shown in black lines) in Fig. 2 for (a) Ising and (c) Dicke models. For the Heisenberg model, however, while the time averages do not exhibit a clear threshold, the reason for this is immediately apparent from the full time evolution. Specifically, while a changing oscillation frequency prior to the threshold affects the time averages and obscures the threshold, the full dynamics show a clear sharp threshold between (quasi)periodic and quantum chaotic dynamics. Here, the pre-threshold behaviour is connected with the observation of larger Trotter errors for different initial states. We show this by analysing the Heisenberg DQS for various classes of initial states in appendix C 3 and show that all the states ultimately converge to the same threshold but show significantly varying Trotter errors prior to the threshold. Note, our results do not depend on the specific choice of operator for the expectation values or the sub-system. The first qubit of the Heisenberg chain is used only for numerical convenience, see appendix C 2 for the other qubits in the Heisenberg chain. These *local* results (i.e. dynamics for a particular initial state) are confirmed and supported also by the eigenvector statistics analyses in Sec. IV C, which provide a *global* property of the Trotter step unitary, that is necessarily independent of other factors like initial state and the choice of the sub-system, and it shows a clear transition from regular to quantum chaos beyond the threshold.

2. Dynamical Signatures of Quantum Chaos

In the previous section, we used our observation of clear qualitative destruction of (quasi)periodicity to illustrate a transition to quantum chaotic dynamics as a function of step size. In this section, we conduct a more quantitative study of this transition using a number of dynamical signatures underpinned by the connection of quantum chaos to ergodic dynamics and thermalisation.

For a closed system with a pure initial state, a concept of thermalisation can only be achieved in a context where the ergodic hypothesis holds, namely for dynamics where the time and state-space averages match for any macroscopic observable. Quantum chaotic dynamics provide a natural mechanism to achieve this condition for quantum systems [22, 45, 81, 82]. Specifically, quantum chaos drives a thermalisation-like process by dynamically delocalising the system state to span a large portion of the Hilbert space. This process, which relates to the simple intuitive description of quantum chaotic dynamics as being exponentially sensitive to perturbations in system parameters, is reflected for composite quantum systems in an increase of sub-system entropy. To study these concepts, in the following sections, we discuss example measures quantifying de-localisation, perturbation sensitivity, and entropy.

a. Delocalisation We first quantify the delocalisation of the time-evolved state $|\psi(t)\rangle$ in a given basis $\mathcal{B} = \{|j\rangle\}$ by means of the participation ratio (PR) [36, 37],

$$\text{PR} := \frac{1}{\mathcal{D}} \left(\sum_{j=1}^{\mathcal{D}} |\langle \psi(t) | j \rangle|^4 \right)^{-1}, \quad (24)$$

where \mathcal{D} is the dimension of the Hilbert space. Quantum chaotic dynamics acts to create delocalisation, but to see this effect, it is important to choose an initial state and basis such that the state is initially localised. In this definition, the normalisation factor ensures the PR lies between \mathcal{D}^{-1} for a fully localised state and 1 for a fully delocalised state. In the Dicke model, the cavity is infinite dimensional, and the choice of \mathcal{D} is non-trivial. We here choose a finite $\mathcal{D} = (2 \dim_j)^2$ (labelled \overline{PR}) and justify this choice in Sec. IV B.

Figures 2 (d–f) show that the temporal evolutions of PRs for A2A-Ising, Heisenberg, and Dicke models, and their time averages, are all clearly separated into localised and delocalised regions at the same step sizes as other quantities in Fig. 2. In A2A-Ising and Heisenberg Trotterisations, the PR beyond the threshold saturates to maximum values that can be well understood in terms of RMT symmetries and choice of the initial state. The maximum PR value is related to the RMT class and the choice of basis $\mathcal{B} = \{|j\rangle\}$, and it is limited to 0.5, as observed in Fig. 2 (d) for A2A-Ising DQS, for further details see the discussions in Ref. [37]. The fact that the PR for the Heisenberg DQS saturates here to ~ 0.25 (Fig. 2 (e)) results from the choice of initial state. The results in appendix C 3 studying the digital Heisenberg dynamics for various initial states show that the PR saturates to 0.5 for most states.

The maximum PR values in the Dicke model are more difficult to interpret due to our observation that the finite spin-ensemble dimension appears to limit how far the state can delocalise in the infinite dimensional cavity space (discussed further in later sections). Nevertheless, it is clear that the system shows larger delocalisation beyond the threshold. We also observe that the \overline{PR} follows the same decaying trend beyond the stable island seen in the photon number. Our numerical analyses do not provide an explanation for this behaviour, which we leave as an open question.

b. Fidelity decay Sensitivity to small perturbations in the system parameters is one of the most widely appreciated characteristics of quantum chaotic dynamics. This concept can be quantified via a variety of related signatures such as fidelity decay, Loschmidt amplitude and echo, and out-of-time order correlators (OTOCs) [40, 42, 72, 83, 84], which are also useful in other contexts like quantum phase transitions and systems with broken time-reversal symmetries [72, 83, 84]. However, a drawback is that such signatures are reliable only if the perturbation itself does not show RMT distribution in its eigenvector statistics [42].

Here, we look at the perturbation fidelity, defined as the overlap

$$\mathcal{F}(\psi_p(t), \psi(t)) := |\langle \psi(0) | U_p^\dagger(t) U(t) | \psi(0) \rangle|^2 \quad (25)$$

between two states evolved from the same initial state $|\psi(0)\rangle$ under a unitary $U(t)$ and a perturbed unitary $U_p(t)$ [40]. In the case of quantum kicked top pertaining to the A2A-Ising model, we identify a reliable perturbation by applying $\exp(-iH_z 0.05\tau)$ to the Trotter step unitary U_τ (see also appendix A 4). Figure 2 (g) shows that the fidelity decay, or rather, here, the complementary perturbation error (infidelity under perturbation) $1 - \mathcal{F}(\psi_p(t), \psi(t))$, displays a regular oscillating signature before the threshold, and a characteristic exponential decay after, providing further strong evidence of the digitisation-induced transition to quantum chaotic dynamics. This trend is observed for arbitrarily small perturbations, with the perturbation strength only affecting the oscillation and decay rates in the two regimes.

c. Sub-system Entropy For the Heisenberg and Dicke models, we illustrate an alternative signature of quantum chaotic dynamics that does not require perturbative comparisons, namely the increase of entanglement between subsystems, as characterised by the sub-system entropy [22, 41, 43, 44].

Here, we consider a normalised von Neumann entropy,

$$\mathcal{S}(\rho_i) = -\frac{1}{\ln(\mathcal{D}_i)} \text{Tr}(\rho_i \ln(\rho_i)), \quad (26)$$

where $\rho_i := \text{Tr}_{\text{not}[i]}(\rho_{\text{system}})$ is the reduced state of sub-system i with dimension \mathcal{D}_i . The normalisation factor $\frac{1}{\ln(\mathcal{D}_i)}$ rescales the usual entropy to be in $[0, 1]$ for any sub-system dimension, simplifying comparisons between different systems. This signature can be calculated via tomography of the sub-system state, but importantly does not require access to the full system state [22]. Figures 2 (h) & (i) show that sub-system entropies jump to much larger values beyond the digitisation threshold for both qubit 1 in the Heisenberg model and the spin- j sub-system in the Dicke model. In Sec. IV B, we show that this entropy approaches the maximum value asymptotically with system size.

The observations of delocalisation, fidelity decay, and increased sub-system entropies beyond the threshold provide strong evidence for the quantum chaotic dynamics, and we show strong evidence for the onset of quantum chaos using random matrix theory in Sec. IV C. Combined with the observation that time averages of expectation values saturate to the relevant Hilbert-space means for each model and observable, for $\langle \bar{J}_z \rangle$ in A2A-Ising (Fig. 2 (a)), $\langle \sigma_z^1 \rangle$ for Heisenberg (Fig. 2 (b)), and cavity and qubit parity in the Dicke model (not shown), they also provide evidence for the idea that the digitisation-induced quantum chaos is driving the ergodic dynamics beyond the threshold.

In this section, we study the overall simulation performance as characterised by the simulation fidelity with the target state. In previous work [37], where simulation performance was characterised through the use of time-averaged quantities, the simulation fidelity seemed to exhibit no persistent threshold behaviour. Here, however, by studying full time evolutions, we demonstrate that a clear breakdown threshold also appears at the same location in the simulation fidelity, and can explain the apparently inconsistent behaviour observed in Ref. [37].

The simulation fidelity, defined as the overlap between the states $\psi_{\text{dig}}(t)$ and $\psi_{\text{ide}}(t)$ obtained, respectively, from Trotterised and ideal dynamics,

$$\mathcal{F}(\psi_{\text{dig}}(t), \psi_{\text{ide}}(t)) := |\langle \psi_{\text{dig}}(t) | \psi_{\text{ide}}(t) \rangle|^2, \quad (27)$$

directly characterises simulation performance via the error in the simulated output state. Figures 2 (j–l) respectively for A2A-Ising, Heisenberg, and Dicke models, show that the simulation fidelity is oscillatory in time before the threshold and quickly decays beyond it. This sharp change in the dynamical characteristics of simulation fidelity identifies the threshold.

Studying the simulation fidelity dynamics from Figures 2 (j–l) in more detail, we can identify three qualitatively distinctive regions of dynamical behaviour. In the first region of each model, at short enough times and small enough step sizes, the simulation fidelity shows a clear fast oscillation with a period that is approximately step-size independent, but an amplitude that gets deeper with increasing step size. At larger step sizes and times, the slower and larger excursions in simulation fidelity with step-size-dependent (quasi)periodicity start to dominate. Finally, at the same step-size threshold as observed in other signatures, we see a sharp (simulation-time-independent) transition from (quasi)periodic fidelity evolution to the sudden collapse in simulation fidelity, an effect which becomes increasingly stark with increasing system size.

These dynamical results provide clear explanations for the trends observed in the time-averaged values in Ref. [37]. Namely, while the same sharp threshold can be observed in simulation fidelity as in other signatures, significant pre-threshold reductions in time-averaged simulation fidelity result from the increasing amplitude and complexity of (quasi)periodic oscillations with both step and system sizes, to the extent that the breakdown threshold in time-averaged fidelity can even be completely obscured at larger system sizes (see also Sec. IV B). They furthermore show that the fidelity does not irrevocably break down until after the sharp threshold, hinting that pre-threshold errors could be significantly correctable with perturbative treatments, such as Floquet-Magnus expansion used in Refs [36, 37] for observable expectations. This implies that, before the threshold, the states might differ only up to perturbative corrections in the Floquet-Magnus expansion for the specific Trotterisation.

While not in the scope of this paper, our results highlight that a detailed study of full simulation fidelity dynamics and possible connections to perturbative error correction terms may reveal valuable new insights into the nature of Trotter errors.

Perhaps the most surprising feature of our results is that the dynamics of Trotterised simulation fidelity across such different model systems should exhibit such strikingly similar qualitative behaviour, that is remarkably robust to specific model and parameter choices. Our three models cover different systems, system parameters and symmetries. Yet in terms of both the nature of the Trotterisation threshold and the nature of error perturbations in the (quasi)periodic regimes, the observation and behaviour of simulation fidelity in the three qualitatively different regions shown here, is remarkably robust to specific model and parameter choices (including across rather wide-ranging exploratory numerical analyses not reproduced here).

4. *Stable Islands*

In each model, we see a clear sharp threshold between (quasi)periodic and quantum chaotic dynamics at the same step size for all physical signatures. Beyond the threshold, however, we also observe clear localised regions, as seen in Fig. 2, where the quantum chaotic dynamics are partially or strongly interrupted, which we call “stable islands”. These islands are localised at resonant step sizes where the digitisation matches a certain periodicity in the system dynamics, and are more or less pronounced depending on the strength of the underlying symmetries in both the system Hilbert space and the specific choice of Trotterisation recipe. For example, very strong stable islands are observed in the Heisenberg model at step sizes where the two-body exchange interactions *freeze out*: that is, for our model parameters, at every $\tau_{\text{stable}} = 0.5 n (2\pi g^{-1})$ for integer n , where $U_{xy}(\tau_{\text{stable}}) = \mathbb{1}$. This effect is much less prominent in the simulation fidelity, because the digitisation-induced regular dynamical behaviour does not generally match the underlying, non-digitised target dynamics. We will explore these effects in more detail in future work.

B. *System Size Dependence of the Threshold*

In this section, we explore how the threshold behaves as a function of system size by analysing the time averages of the dynamical quantities. In the previous section, we show that the threshold is always clear from the time evolution of dynamical quantities, while time averaging these quantities may hinder the identification of the threshold in certain cases. However, using the full dynamics would be impractical for studying the dependence of the threshold on system size. In this part, with the help of our understanding of the full dynamics from the previous

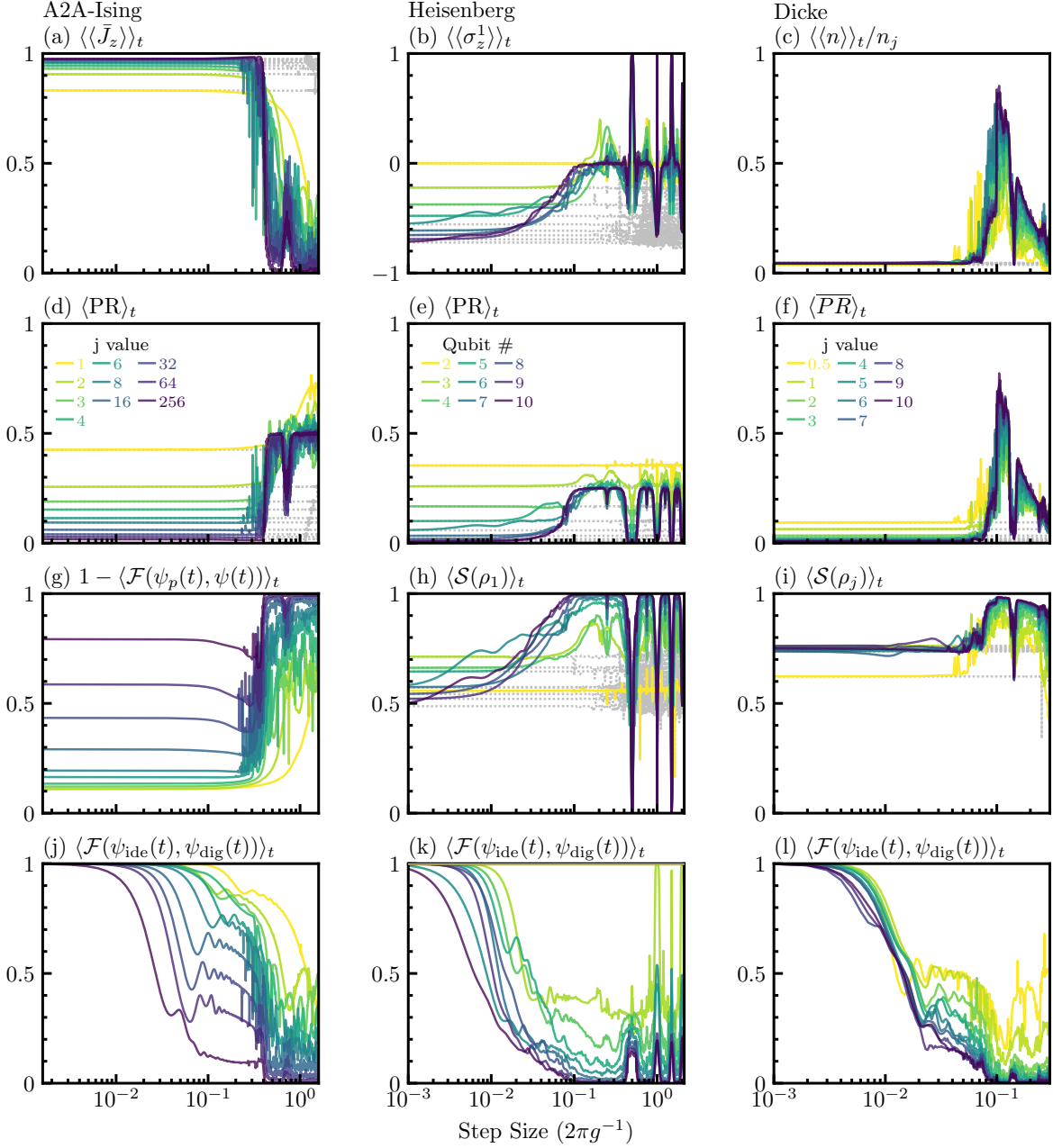


Figure 3. Time-averages of dynamical signatures for each model compared across system size: (a–c) local observables, (d–f) delocalisation, (g–i) further complementary dynamical signatures of quantum chaos, and (j–l) simulation fidelity. Left to right, columns show results for A2A-Ising, Heisenberg, and Rabi-Dicke models, respectively, with line colours corresponding to system sizes given in legends in (d–f), and x-axes common to each column showing step sizes. $\langle \cdot \rangle_t$ represents time averaging over periods $t = 200 (2\pi g^{-1})$ (A2A-Ising), $t = 50 (2\pi g^{-1})$ (Heisenberg), and $t = 200 (2\pi g^{-1})$ (Rabi-Dicke). (a–c) Expectation values of example local observables: (a) magnetisation $\langle \langle \bar{J}_z \rangle \rangle_t$, (b) polarization of qubit one $\langle \langle \sigma_z^1 \rangle \rangle_t$, and (c) normalised photon number $\langle \langle n \rangle \rangle_t / n_j$. Dotted silver lines are time averages of sampled ideal dynamics, sampled at intervals of τ , to illustrate the emergence of sampling errors at large step sizes, even in the absence of digitisation errors. (d–f) Time-averaged participation ratios $\langle \text{PR} \rangle_t$ show clear delocalisation beyond the threshold. (g–i) Beyond the threshold, infidelity under perturbation $\langle 1 - \mathcal{F}(\psi_p(t), \psi(t)) \rangle_t$ for Ising in (g), and normalised sub-system entropies $\langle \mathcal{S}(\rho_i) \rangle_t$ for Heisenberg (first qubit) (h) and Dicke (spin) (i), rapidly approach maximum values for increasing system size. (j–l) While time-averaged simulation fidelities $\langle \mathcal{F}(\psi_{\text{dig}}(t), \psi_{\text{ide}}(t)) \rangle_t$ do not show the same sharp threshold because of pre-threshold quasiperiodic oscillations, they show a secondary drop at the threshold. Where they occur (e.g., for large enough j values in the A2A-Ising and Rabi-Dicke models), stable islands are readily observed in time-averaged signatures, and are observed at the same position independent of size.

section, we analyse the temporal averages of the dynamical quantities for system sizes, starting from the smallest examples and increasing in each case by multiple orders of magnitude in Hilbert space size. Figure 3 shows the temporal averages of the same dynamical quantities as Fig. 2 for various system sizes (in different line colours), and it shows that the threshold is largely independent of system size across a rather large range of Hilbert-space dimension, here limited mainly by numerics. Note that this conclusion can be expected to continue to hold at very large system sizes, because the target systems considered here are integrable (and therefore non-quantum chaotic). In non-integrable target systems, the Trotterisation threshold can still exist and be observable even when the target dynamics are themselves quantum chaotic irrespective of step size. (In App. D 4 b, we show an example in the $j=6$ Dicke model where the Trotterised dynamics show stronger signatures of quantum chaos after the threshold than the ideal dynamics, even when the ideal dynamics are already in the quantum chaotic regime of the model.) As discussed in Ref. [36], however, the threshold position may move to smaller step sizes in these cases for very large system sizes and run times, due to generic Floquet heating effects (see Discussion for more details).

It is important to note that subtle issues can arise when calculating time averages from discretely sampled time series. The light grey lines in Fig. 3 show the temporal averages for the ideal evolution sampled at equal time intervals τ , showing that undersampling at large step sizes can cause averaging errors even in ideal dynamics. This also highlights there is a key distinction between discrete sampling errors and the Trotterisation errors, which we discuss further in Sec. IV D. Here, we focus on the temporal averages of the Trotterised dynamics and discuss the characteristics of their deviations from the ideal averages in each model.

a. A2A-Ising model Top to bottom, the first column of Fig. 3 shows the time averages of (a) $\langle \bar{J}_z \rangle$ values, (d) PRs, (g) perturbation fidelities, and (j) simulation fidelities for a selection of system sizes between $j = 1$ and $j = 256$ (labelled in Fig. 3 (d)), averaged over $t = 200$ ($2\pi g^{-1}$). Thresholds in the first three of these quantities clearly appear around the same position for any system size considered, and at the same location as a secondary drop in the simulation fidelities which marks its transition from oscillatory to decaying behaviour. At the smallest sizes ($j \in \{1, 2, 3\}$), however, we observe neither a sharp secondary drop in simulation fidelity, nor sharp thresholds in the other quantities, although noticeable, smooth deviations from the ideal dynamics do occur starting around the same threshold position. In appendix B 1, we provide the dynamical evolutions of $\langle \bar{J}_z \rangle$ expectation values for $j \in \{1, 2, 3, 4, 6, 8\}$ and observe that (quasi)periodicity is destroyed once $j \geq 4$, consistent with the eigenvector statistics analyses in Sec. IV C. The threshold does not move appreciably in position with system size, and becomes sharper once the system is large enough to show quantum chaotic dynamics (in this case

$j \geq 4$). These results suggest that quantum chaotic dynamics beyond the threshold may be necessary for the system to exhibit a sharp threshold.

b. Heisenberg model Top to bottom, the second column of Fig. 3 shows the time averages of (b) $\langle \sigma_z^1 \rangle$ values, (e) PRs, (h) sub-system entropies for the first qubits, and simulation fidelities for the system sizes given in the Fig. 3 (e) and for $t = 50$ ($2\pi g^{-1}$). The threshold position is still largely independent of system size, but identification of the threshold from these time-averaged quantities is more subtle, due to initial-state effects discussed in Sec. IV A 1. In appendix C 3, we provide the time averaging and error analyses for various types of initial states, and they show that the significant pre-threshold deviation here reflects the fact that some initial state choices result in large Trotter errors before the threshold. In connection with this point, for the same system sizes considered here, we also carry out eigenvector statistics analyses in Sec. IV C, which show that *global* signatures (i.e., independent of initial state) of the Trotter step unitaries still show the same sharp threshold. An additional note here is that the two-qubit case does not have any Trotter errors, so it exactly follows the ideal dynamics, resulting in a unit simulation fidelity (yellow line in Fig. 3 (k)), even though the other time-averaged quantities still suffer from sampling effects at large steps.

c. Dicke model Top to bottom, the third column of Fig. 3 shows the time averages of (b) scaled $\langle n \rangle / n_j$ values, (e) normalised PRs, (h) sub-system entropies for the spin components, and (l) simulation fidelities for the system sizes labelled in Fig. 3 (f) and for $t = 200$ ($2\pi g^{-1}$). Here, we observe a sharp threshold even at the smallest size $j = 0.5$, the Rabi model. In the appendix D 1, we include the dynamical evolutions of $\langle n \rangle / n_j$, sub-system entropy, and simulation fidelity for the Rabi model, which already show dynamical signatures of quantum chaos, such as the destruction of (quasi)periodicity. Thus, we still see a sharp threshold whenever we also observe dynamical signatures of quantum chaos beyond the threshold. Surprisingly, however, in the next section, we show that the eigenvector statistics in the Sec. IV C do *not* agree with the RMT distributions for the Rabi model, with RMT agreement once again obtained only when the spin component is large enough, see Sec. IV C for the details.

The Trotterisation threshold (and quantum chaos beyond it) exists only when there are non-commuting terms in the Trotter decomposition, which, otherwise, would be an exact equation and show regular dynamics for any τ (since we have chosen integrable target model parameters). In the Trotterised Dicke model, the non-commutation between the TC and anti-TC component unitaries in each Trotter step is introduced primarily by single-qubit gates, with no similar effect arising from cavity operators. This suggests that the quantum chaotic dynamics in this model is mainly driven by the spin- j component Hilbert space. This intuition is supported by our numerical observations: for example, the entropy in the spin- j component is maximised, and, as shown in appendix D 2,

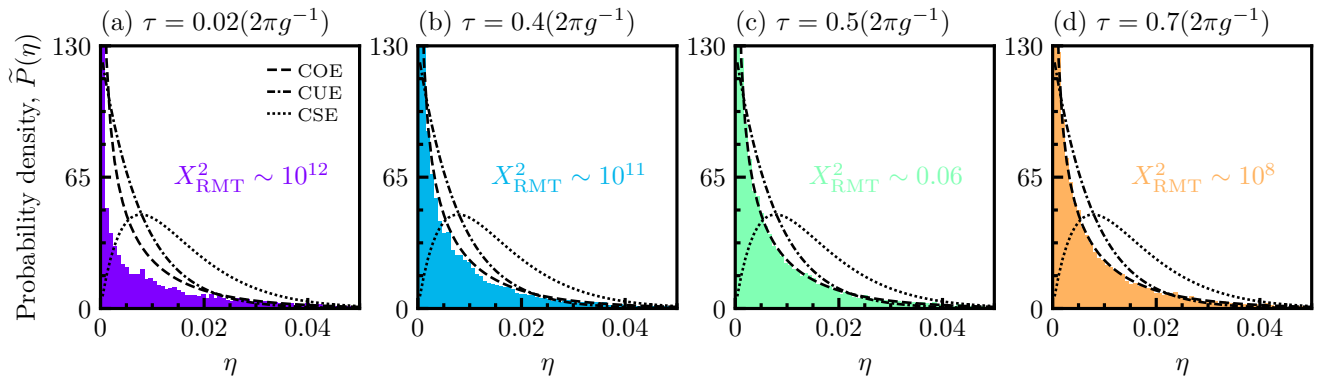


Figure 4. Histograms showing eigenvector statistics of the $j = 64$ A2A-Ising Trotter step unitary (TSU) for representative step sizes in different regimes: (a) $\tau = 0.02 (2\pi g^{-1})$ (before the threshold), (b) $\tau = 0.4 (2\pi g^{-1})$ (on the threshold), (c) $\tau = 0.5 (2\pi g^{-1})$ (quantum chaotic regime beyond the threshold), and (d) $\tau = 0.7 (2\pi g^{-1})$ (stable island in the quantum chaotic regime). Agreement with random matrix theory (RMT) distributions, shown for different time-reversal symmetries by black dashed and dotted lines in each plot, provides conclusive evidence of quantum chaotic dynamics. While the agreement/disagreement in (a) and (c) are visually clear, the apparent visual *agreement* in (d) is misleading as it corresponds to a stable island, and even (b) shows apparently reasonable agreement at a purely visual level. The reduced chi-squared goodness-of-fit test statistic X^2_{RMT} is used to quantify these agreements in each model: values calculated against the closest (COE) distribution (labelled in colour on each figure) provide quantitative and objective conclusions for agreement/disagreement with RMT, for example showing clear *disagreement* in (b) and successfully distinguishing stable islands (such as in (d)) from quantum chaotic regimes.

the maximum photon numbers and PR values beyond the threshold are, respectively, linear and quadratic in the dimension of the spin- j component $\dim_j = 2j + 1$. In our results, we normalise the photon numbers and PR values by $n_j = 7 \times \dim_j$ and $(2 \times \dim_j)^2$, respectively, where the coefficients 7 and 2 are identified numerically (see appendix D 2). The question of how to normalise the Hilbert-space dimensionality also arises in the context of the eigenvector statistics analysis we discuss in Sec. IV C, where the results are consistent with the somewhat empirical approach taken here.

C. Eigenvector Statistics

In this section, we analyse the static properties of the Trotterised evolution, namely the eigenvector statistics of the Trotter step unitary, to support and extend our dynamical analyses. In the previous sections, time evolutions and averages of dynamical quantities are employed to show the Trotterisation threshold, its insignificant system size dependence, and the dynamical signatures of quantum chaos beyond the threshold. These dynamical analyses, however, while strongly indicative, do not provide rigorous evidence of quantum chaos in the Trotterised unitary evolution without relying on additional random matrix theory (RMT) analysis, nor do they allow strong conclusions about the initial-state dependence (or independence) of the threshold. That is, they are generally neither conclusive nor global. By contrast, using eigenvector statistics, we conclusively demonstrate the onset of quantum chaotic dynamics beyond the threshold, and since this approach probes global properties of the Trotterised unitary, we simultaneously show that this

threshold does not depend significantly on the initial-state choice. This means that the onset of quantum chaos in the system dynamics might arise at slightly different step sizes for different initial states, but any variation is confined to a finite but very small range of step sizes. We, therefore, leave how to objectively quantify a precise position for (otherwise visually clear) thresholds as an open question.

1. Eigenvector Statistics

Dynamical signatures of quantum chaos are fundamentally consequences of random matrix theory (RMT) properties of the eigenvectors and eigenvalues of a quantum chaotic system [46], respectively, known as eigenvector [50, 51] and level-spacing statistics [85, 86] (see appendix A for further details). Here, we calculate the eigenvector statistics of the Trotter step unitary (TSU) U_τ by expanding its eigenvectors $|\phi_i\rangle_\tau = \sum_{k=1}^{\mathcal{D}} c_{ik} |k\rangle$ in a basis $\{|k\rangle\}$, defined by the eigenvectors of the free Hamiltonian (i.e., without the coupling terms $\propto g$) in each model. The squared moduli of complex coefficients $\eta = |c_{ik}|^2$ then show certain distributions for quantum chaotic systems [50, 51, 87]. Depending on the time-reversal symmetry of the system, there arise three (main) physically relevant random matrix ensembles [88], known as circular-orthogonal ensemble (COE), circular-unitary ensemble (CUE), and circular-symplectic ensemble (CSE) for unitary random matrices [49]. Their corresponding

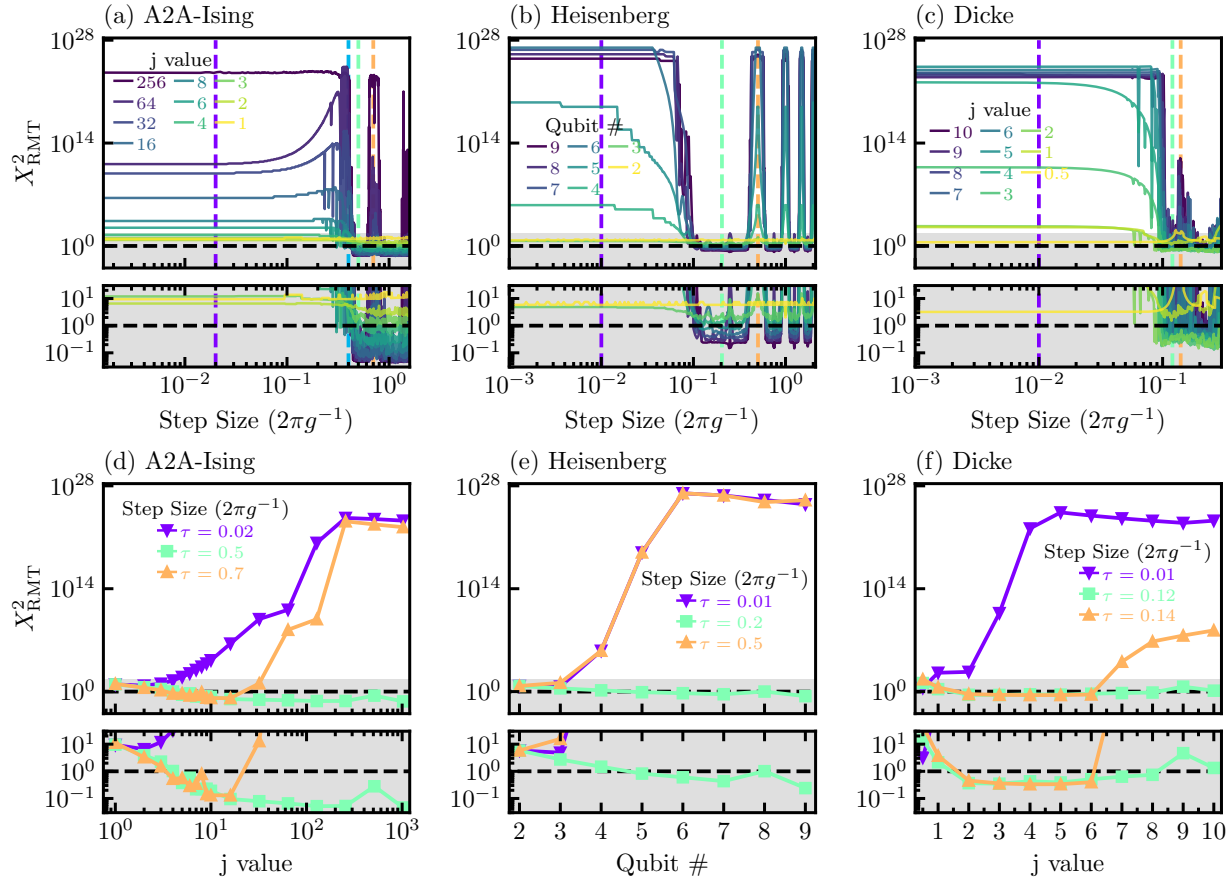


Figure 5. The reduced chi-squared goodness-of-fit test statistic X_{RMT}^2 , calculated from the Trotter step unitary (TSU) U_τ , quantifying each model's agreement with RMT eigenvector statistics. (a–c) X_{RMT}^2 versus step size (x-axes) for the system sizes given in the legends for A2A-Ising TSU, Heisenberg TSU, and Dicke TSU, respectively. (d–f) X_{RMT}^2 versus system size (x-axes) for representative step sizes chosen in the regular and quantum chaotic regimes, and on the stable islands, with extra panels below showing expanded views highlighting the grey areas, where $X_{\text{RMT}}^2 \lesssim 1$. The step sizes, recorded in the legends, are marked as vertical dashed lines in (a–c). The colours are also chosen to correspond to the histograms plotted in Figs 4 (a–d) (for the A2A-Ising TSU). From (a–c), the goodness-of-fit test statistic not only shows the sharp threshold observed in dynamical quantities but also identifies stable islands. Figures (d–f) show how these features emerge at modest sizes as system sizes increase. In the A2A-Ising and Dicke models, we observe that (quasi)periodic dynamics for the stable islands does not emerge from the surrounding quantum chaotic regime until larger system sizes, and that X_{RMT}^2 is able to track this behaviour successfully. In the A2A-Ising and Heisenberg models, the (quasi)periodicity of the stable islands is sufficiently marked that X_{RMT}^2 is comparable on the stable islands to the pre-threshold non-quantum chaotic regime.

reduced probability densities are:

$$\tilde{P}_{\text{COE}}(\eta) = \frac{\Gamma\left(\frac{\mathcal{D}}{2}\right)}{\Gamma\left(\frac{\mathcal{D}-1}{2}\right)} \frac{(1-\eta)^{(\mathcal{D}-3)/2}}{\sqrt{\pi\eta}}, \quad (28)$$

$$\tilde{P}_{\text{CUE}}(\eta) = (\mathcal{D}-1)(1-\eta)^{\mathcal{D}-2}, \quad \text{and} \quad (29)$$

$$\tilde{P}_{\text{CSE}}(\eta) = (\mathcal{D}-1)(\mathcal{D}-2)\eta(1-\eta)^{\mathcal{D}-1}, \quad (30)$$

where \mathcal{D} is the dimension of the Hilbert space, and $\Gamma(x)$ is the Gamma function, or generalized factorial. We denote these distributions in our figures by the above three letter acronyms of the corresponding classes. Relevant details about these distributions, the choice of basis $\{|k\rangle\}$, the relation between RMT and quantum chaos, and other technical factors are summarised in the appendix A.

2. Goodness-of-Fit Test for Eigenvector Statistics

In this section, we demonstrate that the visual comparison of the eigenvector statistics against the above RMT distribution can be misleading. We overcome this problem by combining the eigenvector statistics with a reduced chi-squared goodness-of-fit test, and use a reduced chi-squared goodness-of-fit test statistic, X_{RMT}^2 , to clearly and objectively demonstrate the onset of quantum chaos in the Trotterised dynamics both as a function of step and system sizes.

a. Failure of visual comparisons versus X_{RMT}^2 Figure 4 shows the eigenvector statistics of the A2A-Ising TSU calculated in the J_z basis for $j = 64$. Figures 4 (a–

d) are, respectively, for the step sizes from (a) $\tau = 0.02$ ($2\pi g^{-1}$) before the threshold, (b) $\tau = 0.4$ ($2\pi g^{-1}$) on the threshold, (c) $\tau = 0.5$ ($2\pi g^{-1}$) in the quantum chaotic regime beyond the threshold, and (d) $\tau = 0.7$ ($2\pi g^{-1}$) on a stable island in the quantum chaotic regime. Note that collective spin behaviour in the A2A-Ising DQS restricts the system evolution into a total-spin conserved subspace $\mathcal{D}_j = 2j + 1$ of the full Hilbert space $\mathcal{D}_N = 2^N$ of N spin-1/2 systems. In this respect, it does not display many-body quantum chaos of N systems but quantum chaos of a single spin j , and the standard RMT distributions in Fig. 4 are for $\mathcal{D}_j = 2j + 1$. Because the A2A-Ising decomposition in Eq. (8) has only time-reversal symmetry, it should show COE statistics [37]. While Figure 4 (a/c) shows clear visual disagreement/agreement with the expected COE distribution, the apparent visual *agreement* in Fig. 4 (d) is highly misleading, as this corresponds to a stable island, where the quantum chaotic dynamics are definitely interrupted. To characterise this agreement in a more quantitative manner, we introduce a reduced-chi-squared goodness-of-fit test statistic X_{RMT}^2 to provide a generic quantitative signature for the agreement with the eigenvector statistics expected for random matrix theory (see appendix A 3 for the definition and more details). The values of X_{RMT}^2 comparing the histogram plots with the relevant COE distribution in Figs 4 (a–d) are, respectively, (a) $\sim 10^{12}$, (b) $\sim 10^{11}$, (c) ~ 0.06 , and (d) $\sim 10^8$, successfully identifying not only the agreement/disagreement in regular/quantum-chaotic regime, but also the significant disagreement on the stable island. For Figure 4 (b), which arguably also agrees reasonably well visually, the X_{RMT}^2 demonstrates even stronger disagreement with the target COE distribution.

The X_{RMT}^2 goodness-of-fit test statistic provides a single and (compared to visual inspection) meaningful value for a histogram plot, and therefore also allows us to analyse the eigenvector statistics as a function of some parameter. Below, we provide the analyses of eigenvector statistics for the Trotter step unitaries of each DQS as a function of step and system sizes. Full eigenvector statistics histograms for some relevant step and system sizes are shown in appendix B 2 for A2A-Ising, in appendix C 1 for Heisenberg, and in appendix D 3 for Dicke Trotterisations. Note that X_{RMT}^2 values for the Dicke DQS are obtained by setting the cavity truncation to $\text{dim}_c = \text{dim}_j$, and we discuss this further following a description of the results.

b. Onset of Quantum Chaos as the Trotter Step Size Increases Figure 5 (a–c) shows the X_{RMT}^2 test statistic as a function of step size, respectively, for (a) the A2A-Ising TSU (against COE), (b) the Heisenberg TSU (against CUE), and (c) the Dicke TSU (against COE). In each model, X_{RMT}^2 shows a sharp drop to ≤ 1 for system sizes larger than a certain value that depends on the model, indicating that the eigenvector statistics of these TSUs show good agreement with the corresponding RMT distribution. This provides conclusive evidence that we observe a sharp transition from regular to quantum chaotic dynamics at the same position as the threshold

identified by studying each model’s full system dynamics, and which sets in already at quite modest system sizes. Across all models and multiple orders of magnitude in Hilbert-space dimension, once the system reaches sufficient size, we do not observe any significant movement of the threshold position with system size.

c. Onset of Quantum Chaos as the System Size Increases Here, we examine X_{RMT}^2 as a function of system size for three indicative step sizes in the regular (pre-threshold), quantum-chaotic (beyond-threshold), and stable-island regions. Figures 5 (d–f) plot this dependence for (d) A2A-Ising TSU (against COE), (e) Heisenberg TSU (against CUE), and (f) Dicke TSU (against COE), respectively, for the step sizes given in each legend. Before the threshold, X_{RMT}^2 is much larger than 1 in every DQS and any system size considered. This means that, as expected, the eigenvectors do not show RMT properties before the threshold, and the DQS is (quasi)periodic (non-quantum chaotic) for these step sizes. By contrast, X_{RMT}^2 rapidly drops below 1 for the quantum chaotic regime of each model as the system size increases. The bottom panels showing a zoomed-in view of the grey shaded regions where $X_{\text{RMT}}^2 \lesssim 1$ show clearly at what size each system’s TSU starts to agree convincingly with RMT in the quantum chaotic regime: namely, for $j \geq 4$ in A2A-Ising, for $N \geq 4$ in Heisenberg, and for $j \geq 2$ in Dicke Trotterisations, respectively. Figures 5 (d–f) also show that X_{RMT}^2 rapidly increases to values much greater than 1 for step sizes in the stable islands, which appear at any system size in the Heisenberg DQS, and emerge at larger sizes in the A2A-Ising and Rabi-Dicke models.

d. Finite Truncation of the Cavity Dimension in the Rabi-Dicke DQS Similar to the A2A-Ising DQS, the Dicke DQS also consists of a mapping from N spin-1/2 systems to a single total spin $j = N/2$. Below, we argue that, as a result of the single-qubit gates in the Dicke Trotterisation, the effective total spin component j of the model is the main driver of quantum chaotic dynamics. However, there are additional complications in the eigenvector statistics analyses of the Dicke TSU that arise from numerically truncating the infinite-dimensional cavity at a finite value dim_c . It is non-trivial and is not in the scope of this paper to provide a rigorous, theoretical explanation of the effects of cavity Hilbert-space truncation on eigenvector statistics, but, in appendix D 3, we study it in some detail numerically. Complementing the eigenvector statistics with another strong signature of quantum chaos from RMT, the level-spacing statistics [45, 46, 85, 86], we observe that the beyond-threshold Dicke TSUs show agreement with RMT distributions only for $\text{dim}_c \sim \text{dim}_j$, both for eigenvector and level-spacing statistics. Any agreement is lost simultaneously in both of these statistics when $\text{dim}_c \gg \text{dim}_j$. Combined with the dynamical observations that maximum photon build-up is linear in dim_j , and the PR is quadratic in dim_j (and the fact that the reduced entropy of the spin j subsystem is nearly maximised), these results indicate that quantum chaotic dynamics and Trotterisation breakdown in

the Dicke model are primarily driven from effects arising within the Hilbert space of the spin component.

D. Trotter Error Analyses

In each model, by analysing the statistical properties of the Trotter step unitary and temporal evolutions (and averages) of various dynamical quantities, we have identified a threshold in Trotter step size beyond which the Trotterised dynamics become quantum chaotic. Here, we analyse the Trotterisation errors in state fidelities and expectation values, and we identify the same threshold in each error measure and also examine the behaviour of the errors before and beyond the threshold. We look at the Trotter errors for various system sizes and different time scales: The shorter time scales considered can be achieved within accessible coherence times for current experimental platforms, demonstrating that studies of Trotter-error scaling with step size are within reach of current experiments.

Figure 6 shows our error analysis for the A2A-Ising, Heisenberg, and Dicke models. We first analyse errors in the expectation values of local observables, using the same observables considered in previous sections. The results in Figs 6 (a-c) highlight an important subtlety: namely, even for ideal dynamics, sampling the time evolution at fixed times τ can lead to errors in time averages at large enough τ . These time averages also depend strongly on the averaging time, with more pronounced errors arising at smaller step sizes for short averaging times. Such undersampling errors obviously become more significant with a lower sampling rate. Here, we introduce appropriate error measures to distinguish trivial sampling errors from the approximation errors caused by Trotterisation.

We start by considering the absolute difference between the temporal averages (as previously studied in Ref. [37])

$$\Delta O := \left| \langle \langle O^{\text{dig}} \rangle \rangle_t - \langle \langle O^{\text{ide}} \rangle \rangle_t \right|, \quad (31)$$

where $\langle O \rangle$ is the expectation value of some operator O , with the superscripts (dig/ide) indicating expectation values obtained, respectively, from digital and ideal dynamics (sampled at every τ), and the second layer of brackets $\langle \cdot \rangle_t$ represent time averaging for total simulation time t . Figures 6 (d-f) show ΔO for each model. In each model, ΔO shows an approximately increasing trend with step size leading up to the previously identified threshold positions, before flattening out after the thresholds. (Note that the error values for the $\langle J_z \rangle$ expectations in Ising and $\langle n \rangle$ photon numbers in Dicke are not normalised with spin sizes to avoid removal of system size dependencies in the errors.) In the A2A-Ising model (Fig. 6 (d)), the errors reveal a reasonably clear threshold at the right position, although this is somewhat complicated by the appearance of additional noise prior to the threshold. In the Heisenberg and Rabi-Dicke models (Fig. 6 (e-f)), however, the situation becomes much less clear, with significant

extra noise before and after the threshold, and clear irregular behaviour even at small τ . Moreover, while ΔO still shows a generally increasing trend with step size, it does not show an obvious scaling dependence with system size and/or total simulation time across any of the models. So even though this measure does to some degree separate the sampling errors from the Trotter errors, it nevertheless does not provide a good error measure for the differences in time evolutions. For example, a small difference between the averages does not guarantee that the time evolutions are actually close.

We therefore introduce and analyse an alternative time-averaged error, namely the average, point-to-point absolute difference between expectation values

$$\delta O := \left| \langle \langle O^{\text{dig}} \rangle - \langle O^{\text{ide}} \rangle \rangle_t \right|, \quad (32)$$

where the notation is the same as in Eq. (31). Now, δO captures the absolute deviations of Trotterised evolution from the ideal dynamics at every sample, and therefore both separates the Trotter errors from sampling errors, and reliably measures how close the full dynamical evolutions are (not just their averages). Figures 6 (g-i) show δO , and, contrary to ΔO , we observe that δO is a simple analytic function of step size over a large range of step sizes (prior to a plateau region that appears at long time averages), suggesting that it can be perturbatively expanded (and corrected) in step size. Unlike ΔO , δO shows a clear increasing trend with both step size and total simulation time, and also, with some subtle variations, as a function of system size. From Figs 6 (g-i), we see that the average, point-to-point error also shows the thresholds much more clearly, especially in the A2A-Ising and Rabi-Dicke models, with the errors before the threshold being consistently smaller than the errors in the quantum chaotic regime. Even in the Heisenberg model, where the pre-threshold errors near to the threshold almost reach the error levels observed in the quantum chaotic regime, the errors still show a clear change in their scaling with step size beyond the threshold.

Another averaged, point-to-point error measure is the averaged simulation (state) infidelity (or simulation error) $1 - \langle \mathcal{F}(\psi_{\text{dig}}(t), \psi_{\text{ide}}(t)) \rangle_t$, shown in Figs 6 (j-l), and it shows the same behaviours observed in δO . The lack of a sharp threshold in average simulation fidelity (which approaches 0 already as it nears the threshold) has already been explained as the result of the extra oscillatory behaviour of simulation fidelity before the threshold. This effect is obviously also reflected in the simulation error. Consistent with our explanation, it affects the long time averages much more than the short, and we identify the threshold as the residual, secondary jump in simulation errors highlighted by the insets of Figs 6 (j-l).

Our point-to-point error measures (i.e. δO and simulation fidelity), in contrast to ΔO , provide reliable error measures that separate Trotter and sampling errors. Before the threshold, they increase with total simulation time and also generally with system size. They are also largely increasing smooth functions of Trotter step size

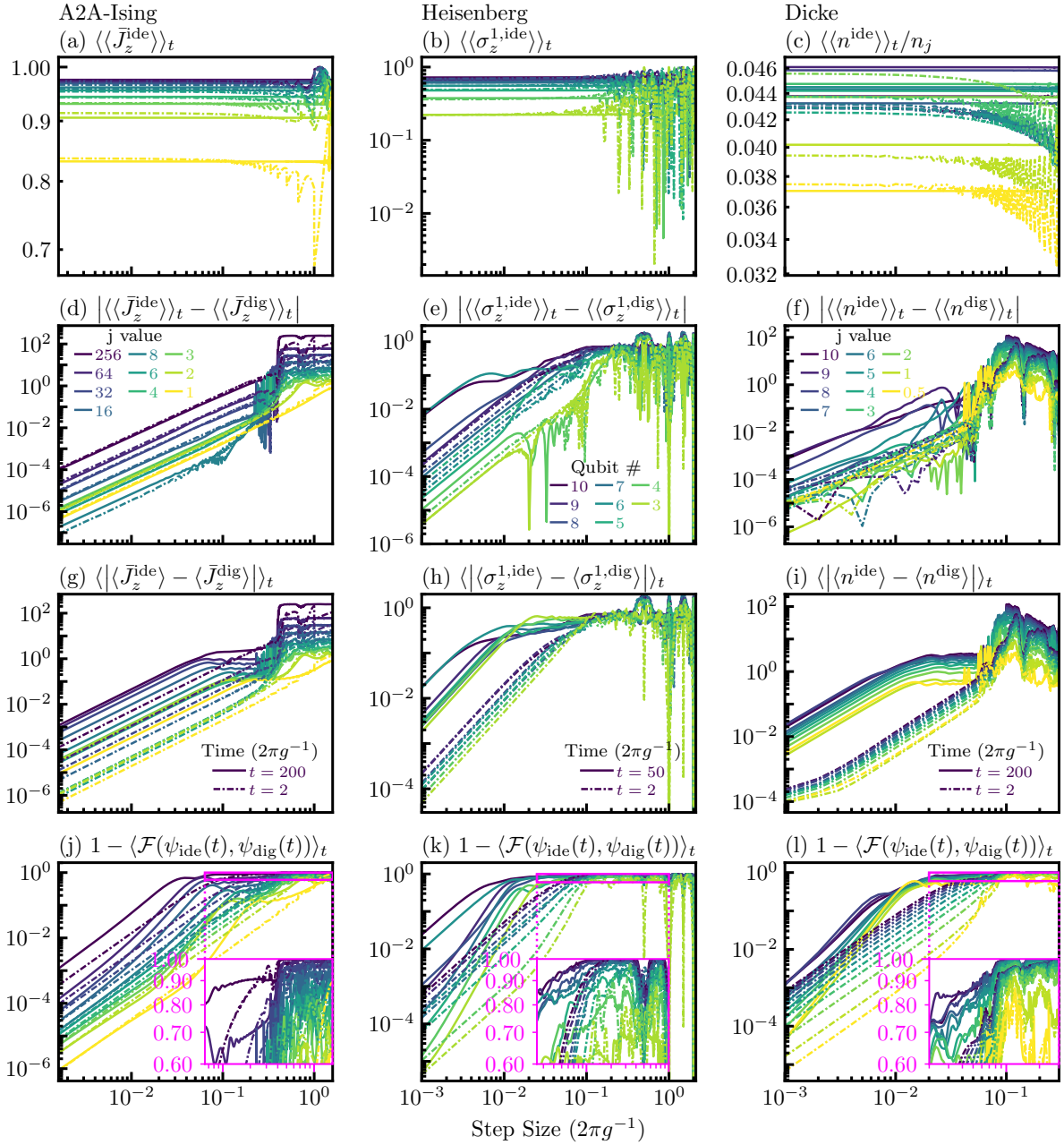


Figure 6. Trotterisation error analysis for (a–i) local-observable expectation values and (j–l) simulation fidelity for different system sizes and different time scales. Left to right, the columns show results for A2A-Ising, Heisenberg, and Rabi-Dicke models, respectively, with line colours corresponding to system sizes shown in the legends of (d–f), line styles indicating the averaging time (shown in the legend of (g–i)), and Trotter step sizes on the x-axes common to each column. The specific quantities plotted on the y-axes are given in the sub-figure titles, with $\langle \cdot \rangle_t$ representing time averaging. The sub/super-scripts *ide* and *dig* represent quantities obtained, respectively, from the ideal and digital simulations. Local-observable errors are calculated for expectation value of magnetisation \bar{J}_z (A2A-Ising), the first qubit polarization σ_z^1 (Heisenberg), and the photon number n (Rabi-Dicke). (a–c) Raw temporal averages for expectation values $\langle \langle O^{\text{ide}} \rangle \rangle_t$ for coarsely sampled ideal dynamics plotted against step-size sampling intervals, τ . Sampling errors for the ideal dynamics depend strongly on averaging time, but can be disentangled from Trotterisation errors by comparing the digital quantities $\langle O^{\text{dig}}(t) \rangle$ with coarsely sampled ideal $\langle O^{\text{ide}}(t) \rangle$. (d–i) The absolute difference between time-averaged expectation values for digital and ideal dynamics, $|\langle \langle O^{\text{ide}} \rangle \rangle_t - \langle \langle O^{\text{dig}} \rangle \rangle_t|$. (g–i) Time average of the absolute, point-to-point difference between digital and ideal dynamics at each time step, $\langle |\langle O^{\text{ide}} \rangle - \langle O^{\text{dig}} \rangle| \rangle_t$. (j–l) The simulation infidelity $1 - \langle \mathcal{F}(\psi_{\text{dig}}(t), \psi_{\text{ide}}(t)) \rangle_t$, is another point-to-point error metric. The quasiperiodic pre-threshold oscillations observed in the full simulation fidelity dynamics cause the threshold to be seen as a secondary jump in the time-averaged simulation infidelity, highlighted by the insets in (j–l).

before the threshold, and show simple, approximately analytic behaviour over a significant range of step sizes, to near the threshold for shorter averaging times, and up to the saturation values at longer averaging times. Thus, these errors have an approximate perturbative expansion in step size within this region, such as the Floquet-Magnus expansion [36]. For local observables, the errors seem to saturate at long averaging times to an upper bound which is smaller than the errors in the quantum chaotic regions.

V. DISCUSSION AND OUTLOOK

The power of a quantum simulator, as represented by the achievable complexity of tasks that it can solve, is typically limited by physical resources (e.g., fabrication costs or runnings costs per qubit, cooling budget per qubit), hardware performance (e.g., qubit noise and decoherence, gate errors, etc), and in the case of DQS, the intrinsic accuracy of the digitisation algorithm (e.g., Trotter errors). In large-scale quantum simulators, these resource costs will be to some degree fungible, and balancing them will become an engineering optimisation to maximise simulation power. For example, in fault-tolerant DQS, error correction will ultimately allow hardware performance limits to be surpassed by transferring the cost into increased consumption of physical resources. But because these costs snowball as the noise to be corrected approaches the fault-tolerant threshold, directly optimising hardware performance will still remain crucial. Similarly, methods for improving digitisation accuracy typically result in increased exposure to noise and decoherence. For example, in architectures where gate times operate reasonably close to the speed of the control electronics, the total run time (and hence decoherence effects) can be increased because the time spent on buffers between gates can be significant. Also, constructing complex interactions from simple primitive operations often requires additional transformation gates (e.g., as in the Heisenberg and Dicke models defined in Eqs 14 and 23, respectively), adding both run time and gate errors. Similarly, increasing the *order* in Trotterisation algorithms, which typically requires the addition of negative-time unitary evolutions (at least beyond second order), also increases the laboratory run time required to achieve a given simulation time. As a result, any improvements that can be achieved in terms of relaxing the digitisation requirements for a given simulation accuracy, will also directly decrease the decoherence and gate errors experienced by the processor.

1. On universality of the Trotterisation performance

In this work, we have focussed exclusively on digitisation errors, in particular Trotter errors, to study the ultimate performance limits that Trotterisation algorithms will face. We numerically investigate the performance of three experimentally realisable Trotterisation models:

the A2A-Ising, Heisenberg, and Dicke models. Our results demonstrate a striking similarity of behaviour in the performance of these simulations. The models themselves encompass widely distinct system types and symmetries (kicked tops, nearest-neighbour spin chains with longitudinal and transverse external fields, and coupled spin-cavity systems with infinite dimension), and as well as the specific parameters selected for the results in the main text and appendices, we saw qualitatively similar behaviour across different parameter choices. Using a range of dynamical and static signatures (derived from state evolutions and unitary operators, respectively), in each model, we have demonstrated the emergence of a performance threshold at modest system sizes that is shared across all signatures we studied.

Specifically, across a range of dynamical (Figs 2(a-i) and 3(a-i)) and static (Fig. 5) signatures of quantum chaos, once a sufficiently large system size is reached, all models studied exhibit regular, (quasi)periodic behaviour prior to, and quantum chaotic dynamics after the threshold. But more than this, by studying the full dynamics of the simulation fidelity, we see that even widely different models exhibit strikingly similar behaviours: a high-fidelity region at smaller steps and shorter times, with fast, but relatively stable oscillatory errors; a second region between that and the threshold exhibiting additional, slower large-amplitude oscillations; strong quantum chaotic behaviour after the threshold; and intermittently emerging stable islands where the quantum chaotic dynamics is interrupted and some degree of (quasi)periodicity reemerges. The surprising universality of these effects across varied models and different parameter choices suggests that there may exist underlying generic principles governing the behaviour of Trotterised DQS, which may help to predict features of large-scale simulations which are difficult to study classically. More work is required to identify and understand these underlying principles. Interesting open questions in this direction include, for example, finding out whether these generic behaviours persist for different digitisation techniques, even more varied simulation models (e.g., in quantum chemistry), and non-integrable target systems.

2. On interpretation of the Trotterisation threshold

Focussing now directly on the threshold transition to quantum chaos, combining what we learn from across all our results provides valuable insight into the underlying nature of the breakdown in simulation performance. From the full dynamics for each model (Fig. 2), we observe clear (quasi)periodic dynamics, consistent with the Trotterised system being non-quantum-chaotic, until immediately prior to the threshold (given in units of $2\pi/g$: $\tau_{\text{A2A-Ising}} \sim 0.4$, $\tau_{\text{Heisenberg}} \sim 0.09$ and $\tau_{\text{Rabi-Dicke}} \sim 0.08$). The pre-threshold oscillatory behaviour is particularly clear and sudden for the local observables (Fig. 2(a-c)) and participation ratio (Fig. 2(d-f)). For the perturbation

fidelity (Fig. 2(g)), entropy of entanglement (Fig. 2(h-i)) and simulation fidelity (Fig. 2(j-l)), the periodicity of the oscillations starts changing prior to the threshold, but clear oscillations continue until the threshold. This understanding is also backed up by Trotter error analysis shown in Fig. 6, and particularly the full quantum state error calculated from the simulation fidelities Fig. 6(j-l). Focussing on the plots with shorter time averaging, where the simulation-fidelity time averages are less complicated by the behaviour in the pre-threshold, quasiperiodic region, we observe that the full quantum state errors follow an analytic, increasing trend up until just prior to the threshold. In other words, the Trotter error grows steadily with step size, which matches the intuition derived from considering the Trotterised (Floquet) Hamiltonian as a convergent Floquet-Magnus expansion, with the zeroth-order solution reproducing the target dynamics and perturbatively increasing correction terms [36, 37]. And while the errors may still become significant in this region, they are in some sense still well behaved: from a given step size, you can expect to improve performance by reducing the step size, and worsen performance by increasing it.

Beyond the threshold, the static X_{RMT}^2 signatures based on eigenvector statistics (Fig. 5) demonstrate that, once the system is large enough, the Trotter step unitary shows strong quantitative agreement with RMT distributions, providing conclusive and quantitatively rigorous evidence that the Trotterised dynamics very rapidly become quantum chaotic beyond the threshold. And since we chose target systems and parameters corresponding to integrable dynamics, we know that it is not the target dynamics (H_M in Eq. (5)), but the increasingly dominant Trotter errors that give rise to the observed quantum chaos. But if the Trotter step unitary becomes a *completely random matrix*, the rather intuitive picture of the Trotterised DQS as an approximate simulation of some underlying target model breaks down entirely. These results suggest we can make a direct connection between the onset of digitisation-induced quantum chaotic behaviour in DQS and the empirical breakdown in meaningful simulation performance. While we do not make any rigorous connection between this threshold and the formal radius of convergence in the corresponding Floquet-Magnus expansion, it seems reasonable to identify the quantum chaotic threshold as an *emergent* radius of convergence for simulation performance.

As a note, we wish to emphasise at this point the importance of introducing the X_{RMT}^2 goodness-of-fit test statistic as an objective, quantitative measure of similarity of the Trotter step unitary with an appropriate random unitary matrix. As discussed in Sec. IV C and illustrated in Fig. 4, the visual comparisons usually applied to determine agreement with RMT are completely inadequate to reliably and accurately identify whether genuine agreement is present.

3. On size dependence of the threshold

From the time-averaged dynamical signatures studied in Figs 3 and 6, we see that neither the threshold nor the characteristics of quantum chaotic dynamics are observed at the smallest system sizes for the A2A-Ising and Heisenberg models. These only emerge once the system is large enough ($j \gtrsim 4$ for A2A-Ising, see also Appendix Fig. 9, and $N \gtrsim 5$ for Heisenberg), and the same size is observed for the onset of quantum chaos as identified by quantitatively rigorous agreement with RMT (Fig. 5, see also Appendix Figs 10 and 11). For the Rabi-Dicke model, however, the threshold and *dynamical* signatures of quantum chaos are visible even at the smallest system sizes (one qubit and one cavity, see Appendix Fig. 14), yet conclusive proof of quantum chaotic behaviour consistent with RMT is still only observed for large enough spin dimensions. While the exact reason for this different behaviour is still an open question, we speculate that this may arise from the presence of the infinite-dimensional cavity in the Rabi-Dicke system.

As discussed in Section II, the Floquet-Magnus approximation in the general case breaks down beyond a formal radius of convergence τ^* , and the inverse scaling of a rigorous sufficient condition for convergence with system size [61–63] (if tight) would imply that realising accurate simulations for very large systems could require vanishingly small Trotter step sizes. This could have significant, fundamental implications for the practicality of future large-scale DQS. Yet results from recent works [36–38] do not appear to conform to these expectations. We have significantly extended the previous work on this issue, in terms of both the range of models and characterisation tools, and have seen minimal if any movement of the threshold, certainly much less than the almost 3 orders of magnitude variation in Hilbert space size studied. Indeed, the threshold arguably becomes more fixed in position as size increases, with the main potential movement observed at low system sizes where the thresholds are less sharp and harder to locate precisely. These observations seem to contradict the expectation that $\tau^* \propto N^{-1}$ for the radius of convergence of the Floquet-Magnus expansion.

Recent asymptotic results in the field of Floquet physics [89–92] suggest that any sufficiently generic, fixed, interacting quantum many-body system, when subjected to periodic driving, will heat up indefinitely, which is a signature of quantum chaotic dynamics. They are asymptotic in the sense that they hold under asymptotic limits on system size and run time. In the context of DQS [36, 37], Trotterisation can be interpreted as implementing a periodically driven, time-dependent Hamiltonian, and the digitised dynamics understood in terms of an effective Floquet Hamiltonian. In the thermodynamic limit and asymptotically long times, generic Trotterised DQS may therefore also exhibit quantum-chaos-driven heating, which suggests the breakdown threshold may eventually shift to smaller Trotter steps. But this heating takes place exponentially slowly in the fast driving regime

which usually characterises a DQS operating in the pre-threshold regime, emerging (in the worst case) only over time scales $t \gtrsim \tau_0 e^{\tau_0/\tau}$ (if not even longer). Indeed, while τ_0 in this lower bound denotes a microscopic time scale related to natural system frequency scales, in practice heating seems to occur only for very large systems at very long times, and has not been observed in numerical simulations except in very specific exceptions [93, 94]. It therefore seems likely that the apparent size-independent scaling of the Trotterisation threshold observed here, will continue for sizes and times applicable to NISQ-era and early fault-tolerant processors, where error mitigation and resource optimisation will be so critical. It is not yet understood what system sizes will bring these heating effects into play. But even for systems and run times that do eventually reach large enough scales, they can still be exponentially suppressed by increased digitisation. That is, for specific, long, yet finite simulation times, the Trotterisation threshold can persist even in the thermodynamic limit, because heating will only become effective for large enough τ . (We show an example in App. D 4 b in the quantum chaotic region of the Dicke model, where digitisation-induced quantum chaos still creates a threshold.)

Our work also raises a number of interesting open questions in this area of asymptotic heating and Trotterisation thresholds. For example, the Hamiltonian of the Trotter-Floquet system divides naturally into a time-independent (DC) term, H_0 , and a purely “AC” time-dependent term, $V(t)$, satisfying the usual assumption [92] $\int_0^\tau V(t) dt = 0$, under which the reference Hamiltonian reduces to the target model Hamiltonian, $H_0 = H_M$. In the context of quantum many-body physics, sufficiently generic systems are, with vanishingly infrequent exceptions, non-integrable (or quantum chaotic). For integrable systems, however, which occur with measure zero and arise from fine-tuning of system parameters and symmetries, the asymptotic heating results [89–92] do not necessarily hold [38]. In this work, to focus on digitisation-induced quantum chaos, we specifically consider systems and parameters which remain integrable even for very large system sizes. Such systems may support a full performance threshold for Trotter errors even in the thermodynamic limit. This obviously needs to be studied in more detail, but such a result, even if it does not hold completely universally, would provide valuable evidence that DQS can be carried out reliably, even at very large scales, which will be critical, if future large-scale quantum computers are to realise the promising applications of most interest. Another very important point is that these asymptotic heating results have only been studied in the context of systems with bound energy spectra, like networks of spins or fermions. It is a completely open question what might happen for systems involving bosonic degrees of freedom, which give rise to very different phenomena under periodic driving, such as parametric resonance. Systems like the Rabi-Dicke model considered here could provide interesting testbeds for exploring these questions, with potential implications

for both fundamental physics and quantum processors utilising bosonic degrees of freedom.

Finally, at a more practical level, while the threshold behaviours studied in this work are visually quite clear, an important open challenge for understanding the size dependence of the threshold is to develop an objective quantitative description of where the threshold sits. Our X_{RMT}^2 test statistic provides a promising way to attack this problem, since it captures a direct quantitative measure of agreement with RMT in a single number, but a number of subtleties in how to identify the threshold make this an important open question for future work. For example, while the thresholds observed in X_{RMT}^2 in Fig. 5 are quite sharp, and get sharper with increasing system size, they nevertheless appear to consistently span a small finite region in step size, broader than is observed in the full dynamics. Further study of these effects are required, but we speculate this may arise because X_{RMT}^2 is defined from the global unitary. That is, it would be consistent with the notion of mixed-phase regions in phase space, well known in the context of the kicked top [22, 37], for the position of the chaotic threshold to show some dependence on system initial state. Indeed, it would not be surprising for such an effect to be quite significant, although our initial exploration of this possibility in App. Fig. 12 suggested the threshold is actually rather stable. Also, while a goodness-of-fit test statistic value of $X_{\text{RMT}}^2 \sim 1$ is known to indicate good agreement with the target probability distribution, further study is required to understand how the test statistic is expected to behave in the non-quantum-chaotic regions, and in particular whether there is a way to identify the smallest step sizes where the threshold starts. Finally, we observe that X_{RMT}^2 appears to exhibit some strong sensitivity to step size near (and to some extent beyond) the Trotterisation threshold, which would be intuitively consistent with the known sensitivity of quantum chaotic dynamics to Hamiltonian perturbations. This effect looks particularly pronounced during the narrow threshold transition, which also creates some ambiguity in identifying a single, precise threshold. We leave finding an objective way to precisely describe the threshold position, in either the dynamical or static (X_{RMT}^2) signatures, as a topic for future research.

4. On scaling of Trotter errors with step size

A key motivation for our work and the previous work in Refs [36, 37] is that a better understanding of the detailed behaviour of Trotter errors in DQS may allow a more nuanced use of Trotterisation to better balance the Trotter errors against the effects of decoherence and gate noise. For example, Refs [36, 37] show, at least for specific cases in the Ising model, that the pre-threshold errors of example observables agree with the values predicted by a perturbative Floquet-Magnus expansion of the system dynamics. In Figures 6 (g–l), we extend these observations and show that well-defined, point-to-point errors show

clear analytic scaling across a wide span of Trotter step sizes, even up to near the quantum chaotic threshold for shorter simulation times, across a wide range of models and parameter regimes, and even for the simulation error, which is a property of the global quantum state. As suggested first in [36], this means that measuring results for a range of larger step sizes can potentially allow more accurate values to be predicted by extrapolating the observations back to smaller step sizes, which then don't need to be measured explicitly. Furthermore, provided these errors can be explained perturbatively, calculating the correction terms in a perturbative expansion like the Floquet-Magnus expansion may provide insight into how to *correct* these errors at an algorithmic level, to further compensate and reduce the observed Trotter errors without moving to smaller Trotter step sizes. Critical to demonstrating the universality of this behaviour was the introduction of more nuanced time-averaged errors that distinguished reliably between sampling errors and Trotter errors and eliminated spurious fluctuations in the error scaling curves which obscured the true underlying trends in the data.

Other key questions about the Trotter error scaling that still require further investigation, include: a more detailed investigation of how the error scaling depends on system size and simulation time; and why the longer-time Trotter errors appear to saturate to a finite error below the threshold that remains considerably below the value saturated by quantum chaotic dynamics beyond the threshold.

5. Towards experiments and potential applications

In future work, and especially in the design of future experiments, it will also be important to study the interplay between Trotter errors and noise. At the simplest level, to be able to experimentally observe the onset of quantum chaotic dynamics at the Trotterisation threshold, the decay and dephasing times will need to be significantly longer than the quantum chaotic collapse time. For the strongly quantum chaotic systems demonstrated here (Fig. 2), this occurs already after very few Trotter steps, but to distinguish this reliably from (quasi)periodic dynamics in the regular (pre-threshold) regime, it will obviously be necessary to observe coherent dynamics over a longer duration. In this context, decoherence can be modelled straightforwardly using a traditional master equation in the “lab frame” of the simulator system, and simple initialisation and measurement errors can be modelled heuristically via appropriate choices of starting states and measurements POVMs. By contrast, simple gate errors such as calibration errors and parameter drift errors can be modelled using random noise parameters and Monte-Carlo techniques. The effects of gate errors, however, can be expected to raise more subtle questions for future study, since hardware errors such as gate errors and residual couplings can already lead to quantum chaotic dy-

namics [95–100], even in analogue quantum systems. Note that, based on our work in this paper, some experimental results previously observed in Ref. [16] for the quantum Rabi model, can be interpreted as providing preliminary experimental verifications of our new results, indicating that the performance required to investigate these effects is already within reach of current experiments.

In this work, use of random matrix theory has been crucial in conclusively establishing quantum chaos as the underlying universal (across models) and global (throughout Hilbert space) cause of the Trotterisation performance breakdown threshold first noticed in the context of Ising DQS in Refs [36, 37]. To consider this in context, it is worth discussing how RMT is also arising in other areas of quantum information. In recent years, the classical computational complexity of the random matrices underpinning quantum chaos [101] has motivated a range of pioneering experiments designed to implement random unitary circuits, like quantum supremacy and information scrambling [102–107]. For example, in contrast to our main results, where target models are explicitly integrable and quantum chaotic dynamics arise from simulation errors, quantum supremacy experiments target the accurate simulation of quantum chaotic target dynamics specifically because it pushes the classical complexity. This provides further motivation for many open questions around how to optimise DQS of a target model which is itself quantum chaotic, a situation which is likely to arise often in real DQS applications. In Appendix D 4b, we note already that sharp Trotterisation thresholds may still be observable for quantum chaotic target models, but quantum supremacy experiments illustrate that this context merits much more detailed investigation. For example, does the remarkable universality of Trotterisation performance across system types observed here extend to Trotterisations of quantum chaotic target models? Do similar sharp thresholds appear in other contexts where hardware-error-induced quantum chaos appears [95–100], and (how) are these situations connected? We anticipate that the new analytical tools we have introduced, like the goodness-of-fit test statistic X_{RMT}^2 , will provide invaluable insight into such questions.

In a different direction, while we can connect pre-threshold Trotter errors to perturbative corrections in the Floquet-Magnus expansion [36, 37] and identify the threshold as an emergent radius of convergence, it remains a fascinating open question to find some mechanistic origin for the threshold and the onset of quantum chaotic dynamics beyond it. Given the key role of RMT in establishing the classical computational complexity of quantum supremacy experiments [101, 102], we suggest that RMT could perhaps be used to build an information theoretic understanding of the breakdown of DQS performance in terms of computational complexity.

Finally, in this work, we show that digitisation-induced quantum chaotic dynamics can be realised in quite modestly sized systems. While this heralds a breakdown in performance in DQS, it is intriguing to speculate whether

this can be used as a resource in other contexts, such as open-system simulations (using the deep connection between quantum chaos and thermalisation in closed quantum systems [45, 81, 82]), or quantum metrology [108].

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Appendix A: Random Matrix Theory and Quantum Chaos

Dynamical signatures of quantum chaos are manifestations of certain random matrix properties in the eigenvectors of quantum chaotic systems. Here, we provide an overview of quantum chaos and its relation with random matrix theory (RMT). We also discuss the technical subtleties and nuances involved in the calculation of the quantum chaos signatures used in this paper, and we use quantum kicked-top models of different symmetries to explain these for both statistical and dynamical signatures.

1. Random Matrix

A random matrix has all or most of its entries as independent random numbers satisfying certain probability laws, and random matrix theory is concerned with the statistical properties of (all or a few of) the eigenvalues and eigenvectors of such matrices [49]. Wigner used RMT analyses to explain certain spectral properties of heavy nuclei [110], motivating much subsequent theoretical work [49, and references therein], and Dyson showed that physically relevant random matrices fall (mainly) into one of three universality classes according to their symmetries [88]. These classes are categorised into circular or Gaussian ensembles for unitary and Hermitian random matrices, respectively. Ensembles are categorised according to the Dyson parameter β into orthogonal (COE/GOE, $\beta = 1$), unitary (CUE/GUE, $\beta = 2$) and symplectic (CSE/GSE, $\beta = 4$), related to degrees of freedom in random entries and degeneracies of the matrices [49, 51].

2. Quantum Spectra of Classically Chaotic Systems

Over the years, many studies connected RMT with quantum chaos [45, 46, 50, 51, 85, 86], by showing that the distribution of energy levels in the Hamiltonians of classically chaotic systems, commonly referred to as the eigenvalue or level (spacing) statistics, adhere to the Wigner-Dyson statistics [45, 46, 85], given by

$$P(s) = A_\beta s^\beta e^{-B_\beta s^2} \quad (\text{A1})$$

where s is the spacing between neighbouring levels, and the coefficients

$$A_\beta = \begin{cases} \pi/2 & \beta = 1 \\ 32/\pi^2 & \beta = 2 \\ 2^{18}/3^6\pi^3 & \beta = 4 \end{cases} \quad (\text{A2})$$

and

$$B_\beta = \begin{cases} \pi/4 & \beta = 1 \\ 4/\pi & \beta = 2 \\ 64/9\pi & \beta = 4 \end{cases} \quad (\text{A3})$$

are calculated by normalising $P(s)$ with the mean level spacing fixed to 1 [46]. These distributions do not have closed forms for a given Hilbert space dimension \mathcal{D} . They are generalisations of the results obtained for ensembles of small dimensional matrices, and are exact for $\mathcal{D} = 2$ (see Ref. [45] for further details). In appendix A 4 a, we discuss the nuances involved in the calculation of level spacing statistics and illustrate them with the quantum kicked top.

It is conjectured by Bohigas-Giannoni-Schmit (BGS conjecture) [85] that, even for single particle quantum systems that are chaotic in the classical limit, level spacings exhibit Wigner-Dyson statistics. For quantum systems

with an integrable classical limit, Berry-Tabor conjectured that the level spacings exhibit Poisson statistics [86]. There are a few counterexamples to both of these conjectures, including: (i) a classically chaotic system without Wigner-Dyson statistics in its quantised spectrum [111], (ii) a 1D integrable system with Wigner-Dyson statistics [112], and (iii) an integrable system without Poisson statistics [113]. Additionally, these statistics can be tricky to interpret in a context where the natural classical limit of a quantum system is not clear. Therefore, the existence of Wigner-Dyson statistics in level spacings is neither a necessary nor a sufficient condition of quantum chaotic dynamics, but it still is a strong signature of quantum chaos.

3. Eigenvector Statistics

Despite the popularity of using level statistics as a signature for quantum chaos, the conclusive and defining RMT property of quantum chaotic dynamics is found in the statistics of the dynamics' eigenvectors, which are rigorously defined in a closed form for any arbitrary dimension \mathcal{D} [50, 51, 87].

Eigenvectors $\{|\psi_i\rangle_U\}$ of a random unitary matrix U are also random (column) matrices, and once they are expanded in a generic-basis $\{|k\rangle\}$, as $|\psi_i\rangle_U = \sum_{k=1}^{\mathcal{D}} c_{ik} |k\rangle$ with the constraint $\sum_{k=1}^{\mathcal{D}} |c_{ik}|^2 = 1$, the squared moduli (component populations/probabilities) $\eta = |c_{ik}|^2$ obey a certain distribution depending on the universality class [50, 51, 87]. As stated in the main text, the reduced probability densities corresponding to these classes are given as

$$\tilde{P}_{\text{COE/GOE}}(\eta) = \frac{\Gamma(\frac{\mathcal{D}}{2})}{\Gamma(\frac{\mathcal{D}-1}{2})} \frac{(1-\eta)^{(\mathcal{D}-3)/2}}{\sqrt{\pi\eta}} \quad (\text{A4})$$

$$\tilde{P}_{\text{CUE/GOE}}(\eta) = (\mathcal{D}-1)(1-\eta)^{\mathcal{D}-2} \quad (\text{A5})$$

$$\tilde{P}_{\text{CSE/GSE}}(\eta) = (\mathcal{D}-1)(\mathcal{D}-2)\eta(1-\eta)^{\mathcal{D}-1}, \quad (\text{A6})$$

where \mathcal{D} is the dimension of the Hilbert space, and $\Gamma(x)$ (the Gamma function) is the generalized factorial. In the figures of this paper, we denote these (and Wigner-Dyson) distributions by the appropriate three letter acronym, depending on whether the unitary or the Hamiltonian is used to calculate the eigenvectors (and eigen-phases/values). The distributions in Eqs (A4–A6), contrary to Wigner-Dyson distributions in Eq. (A1), have a closed form for a given dimension of the Hilbert space \mathcal{D} .

The eigenvector statistics analysis in this work is carried out on the eigenvectors of each Trotter step unitary using the following recipe:

1. Choose an appropriate reference basis $\{|k\rangle\}$ to calculate $|\psi_i\rangle_U = \sum_{k=1}^{\mathcal{D}} c_{ik} |k\rangle$ (discussed below).
2. Create a histogram from the component populations $\eta = |c_{ik}|^2$. Some care is required here to ensure that the histogram is sufficiently well behaved (e.g., does

not contain too many low-count bins) to ensure it can be compared meaningfully to a target distribution.

3. Convert the histogram to a probability density by normalising the area under the histogram to 1.
4. Compare with the appropriate target probability density for unitaries \tilde{P}_a ($a \in \{\text{COE, CUE, CSE}\}$) for the appropriate dimension in Eqs (A4–A6).

a. Choosing the reference basis

The question of how to choose the reference basis is important and a little subtle. It turns out that the above construction will almost always lead to eigenvector statistics satisfying the probability distribution of one of the randomness universality classes for an arbitrary basis: A non-random basis will give random eigenvector statistics when expanded in a random basis, and an arbitrary basis will almost always be random. So the reference basis needs to be chosen in such a way that the eigenvector statistics satisfy one of the universality classes *if and only if* the underlying unitary matrix derives from non-integrable/quantum chaotic dynamics (i.e., is a random matrix), and this means that the reference basis must itself not be random. The easiest way to ensure this is to use the eigenbasis of an integrable system unitary as the reference basis: the eigenvector statistics of an integrable system will not satisfy RMT distributions when expanded in the eigenbasis of another integrable system, whereas the eigenvector statistics of a non-integrable system, using the same reference basis, will. It must be acknowledged that there is some risk of falling into a circular argument here, but with care, it can be avoided. One way to ensure that the reference basis derives from an integrable system is to test the robustness/sensitivity of eigenvectors to small perturbations [45, 87, 114]. Under small perturbations, the eigenvectors of a regular quantum system only negligibly differ from the unperturbed basis, while the eigenvectors of perturbed quantum chaotic systems become random matrices in the unperturbed basis [45, 114]. However, more straightforwardly, the free, uncoupled evolution of a quantum system (without any non-interacting terms) is integrable by construction. The eigenvectors of the uncoupled system can therefore reliably be used to define a non-random reference basis, and this is the approach taken in this work.

As a final note, the dynamical distinctions between regular and quantum chaotic systems derive from this robustness (sensitivity) of the eigenvectors of integrable (quantum chaotic) systems to small perturbations [46]. Therefore, eigenvector statistics are used in this paper as the defining property of quantum chaotic dynamics.

b. *Chi-squared goodness-of-fit test for agreement with RMT*

As illustrated in Fig. 4, comparing eigenvector histograms with the expected statistical distributions visually can be very misleading. To make this comparison both quantitative and objective, we therefore characterise the agreement of a given histogram with RMT predictions using a reduced chi-squared χ^2_V goodness-of-fit test. Specifically, we define a reduced RMT goodness-of-fit test statistic according to:

$$X_{\text{RMT}}^2 = \min_{a \in \{\text{COE}, \text{CUE}, \text{CSE}\}} X_a^2, \quad (\text{A7})$$

where

$$X_a^2 = \frac{1}{N_{\text{bin}} - 1} \sum_{i=1}^{N_{\text{bin}}} \frac{(n_i - \tilde{P}_a(x_i))^2}{\tilde{P}_a(x_i)}. \quad (\text{A8})$$

follows the usual definition for a reduced-chi-squared goodness-of-fit test [115, 116]. Here, N_{bin} is the number of bins, n_i is the number of elements in the i th bin (ranging from $[x_i - \frac{\delta}{2}, x_i + \frac{\delta}{2})$), and δ is the width of the bins. Defined in this way, if the eigenvector statistics agree with one of the universal RMT probability distributions, the residuals in the X_{RMT}^2 test statistic will reduce to independent random variables, and the value for X_{RMT}^2 should be distributed according to a chi-squared probability distribution. If needed, this comparison can be formulated as a hypothesis test to determine whether to reject the *null hypothesis* that the eigenvector statistics do agree with RMT predictions.

It is not necessary to be too strict in how we apply the *minimum* in the above definition. For example, to create plots like those in Fig. 5, to observe the onset of quantum chaos at the threshold, it is generally useful to define the X_{RMT}^2 test statistic relative to a particular choice of distribution, such as whichever is the closest RMT distribution in the post-threshold region. Obviously, that may not be known in advance for an arbitrary system, so that is where the minimum in the definition can be used. However, there may also be situations where the universality class may transition from one to another [117], such as could in principle occur at a Trotterisation threshold for a non-integrable target system, in which case it may be useful to look specifically at the X^2 test statistic for more than one distribution. Generally, we will simply leave this choice implicit and write X_{RMT}^2 , but occasionally, we may write explicitly, e.g., X_{COE}^2 .

4. Quantum Kicked Top

The kicked top is one of the best-studied models, both in classical and quantum chaos, and is extensively used to demonstrate the connection between the two [118]. Here, we use quantum kicked tops of different symmetries to provide concrete examples of both the dynamical signatures of quantum chaos and the RMT properties discussed

above. Quantum kicked-kicked toptops of COE and CSE symmetries are given by the Floquet operator:

$$F = e^{-iV} e^{-iH_0}, \quad (\text{A9})$$

with

$$H_0 = pJ_y \quad (\text{A10})$$

$$V = \lambda J_z^2 / 2j, \quad (\text{A11})$$

for COE, and

$$H_0 = pJ_z^2 / j \quad (\text{A12})$$

$$V = k [J_z^2 + k' (J_x J_z + J_z J_x) + k'' (J_x J_y + J_y J_x)] / j, \quad (\text{A13})$$

for CSE. The kicked top with CUE symmetry is obtained by the following Floquet operator:

$$F = \exp(-ik' J_x^2 / 2j) \exp(-ik J_z^2 / 2j) \exp(-ip J_y) \quad (\text{A14})$$

For further details on these different quantum kicked-top symmetries, see the Refs [51, 118]. The parameters used for the numerical simulation below are: (COE) $p = 1$, $\lambda = 0.01$ (regular) & 10 (chaotic), and $j = 400$, (CUE) $p = 1.7$, $k = 6$, $k' = 0.5$, and $j = 400$, and (CSE) $p = 4.5$, $k = 1.5$, $k' = 2$, $k'' = 3$, and $j = 399.5$. In the dynamical simulations, we use the COE symmetry with the initial state $|j, m = j - 1\rangle$, and the perturbation fidelity decay signature is obtained by comparing the quantum kicked tops with kick strengths of λ and 1.001λ .

a. *Static Signatures*

Here, we discuss the procedures and nuances involved in calculating the level-spacing and the eigenvector statistics, illustrating them with quantum kicked-top examples.

a. Level-spacing statistics In this paper, for the quantum kicked-top models here and the DQS models in the main text, we mostly calculate the level spacing statistics using the eigenphases $\{\phi_U\}$ of a unitary evolution operator $U(t)$, which are unique up to a $\{\phi_U \pm 2n\pi\}$ difference for any integer n . This means that, for a given unitary operator, there are infinitely many corresponding Hermitian operators with the same eigenvectors but different $\{\phi_U \pm 2n\pi\}$ eigenvalue spectrums. This is an important limitation for level-spacing statistics. Moreover, regardless of the non-uniqueness, an unfolding procedure is required to remove system-dependent secular variations and make the level spacings of any eigen-phase/value spectrum comparable with Wigner-Dyson distributions. Full details on level spacing statistics and unfolding are already found in many references [45, 46, 119, 120], but the main calculation steps are:

- Sort the eigen-values/phases and group them into symmetry-reduced sub-spaces.

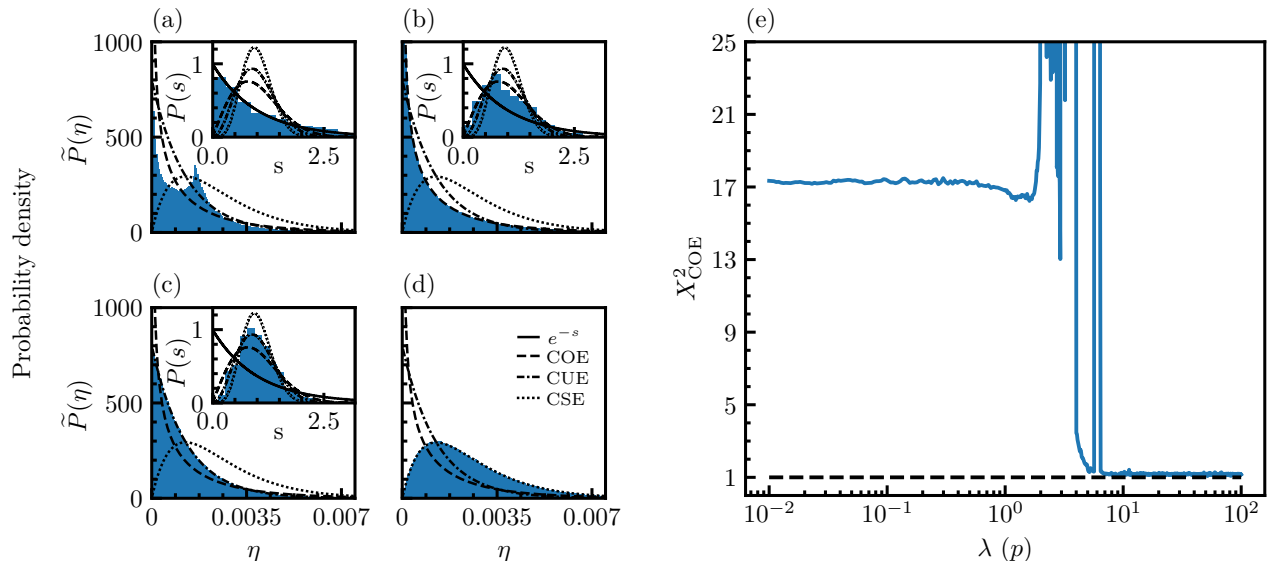


Figure 7. Eigenvector and eigenvalue (insets) statistics for quantum kicked top with (a) regular parameters (i.e. weak kick) and COE, (b) chaotic (i.e. strong kick) and COE, (c) chaotic and CUE, and (d) chaotic and CSE, and (e) the X_{RMT}^2 test statistic for COE eigenvector statistics as a function of kick strength λ . X_{RMT}^2 shows three main regions: (i) regular dynamics $\lambda \lesssim 1$, (ii) $1 \lesssim \lambda \lesssim 7$ transition region with mixed-phase space and stable islands, and (iii) $\lambda \gtrsim 7$ quantum chaotic system. $j = 400$ for COE and CUE, and $j = 399.5$ for CSE, and the other parameters are given in appendix A 4.

- Unfolding: renormalise the local density of states by a smooth function to have both global and local unit-average level spacings.
- Calculate the level spacings for each symmetry-reduced sub-spaces and create histograms with these spacings.
- Normalise the area under the histogram to 1 and compare it with Wigner-Dyson distributions.

We can also superimpose the statistics of all these sub-spaces to have better resolution in the histogram plots [118].

Insets in Fig. 7 show the level spacing statistics for (a) COE with regular, (b) COE with quantum chaotic, and (c) CUE with quantum chaotic parameters. For regular parameters, it closely follows the Poisson statistics, and chaotic cases follow the corresponding Wigner-Dyson distribution of each class. They are super-imposed histograms of two sub-spaces. CUE and COE unitaries given above are symmetric under a π rotation around the y-axis, and two symmetry reduced sub-spaces are determined by even and odd eigenstates of $e^{-i\pi J_y}$ [118].

Obviously, it is also possible to define a goodness-of-fit X^2 test statistic to quantify agreement with Wigner-Dyson level-spacing statistics, but since the eigenvector statistics already provide a necessary and sufficient condition for quantum chaotic dynamics (and are generally easier to calculate), we have not included any such calculations here.

b. Eigenvector statistics Once an appropriate basis $\{|k\rangle\}$ is chosen, calculation of eigenvectors is almost trivial using the prescription in appendix A 3. The only subtlety in this procedure arises when the system has degeneracies. For example, when comparing eigenvector statistics against the CSE distribution, which exhibits Kramers degeneracies, you need to take the degeneracies into account by summing the amplitudes for the degenerate levels, and this procedure decreases the degrees of freedom by half. The derivation of the CSE distribution in Eq. (A6) already takes these into account [51]. Note that it can be any two levels, so you do not have to identify the exact degeneracies [51]. For the other symmetries, the same procedure also applies for degenerate cases, and the distributions in Eqs (A4–A5) need to be used with the decreased degree of freedom, e.g., $\mathcal{D}/2$, see Heisenberg model DQS with σ_z . In degenerate cases, however, the diagonalization routine may give random results even in non-random cases, due to the linear freedom in choosing the degenerate eigenvectors [99], and one needs to ensure that results are not affected by the diagonalization routine.

Figures 7 (a–d) show the eigenvector statistics, respectively, for (a) COE with regular, and (b) COE, (c) CUE and (d) CSE with quantum chaotic parameters. We observe close agreements (disagreement) between the eigenvector statistics of quantum chaotic (regular) systems and the corresponding RMT distributions. We also quantify the agreement/disagreement by calculating the X_{RMT}^2 goodness-of-fit test statistic between the eigenvector statis-

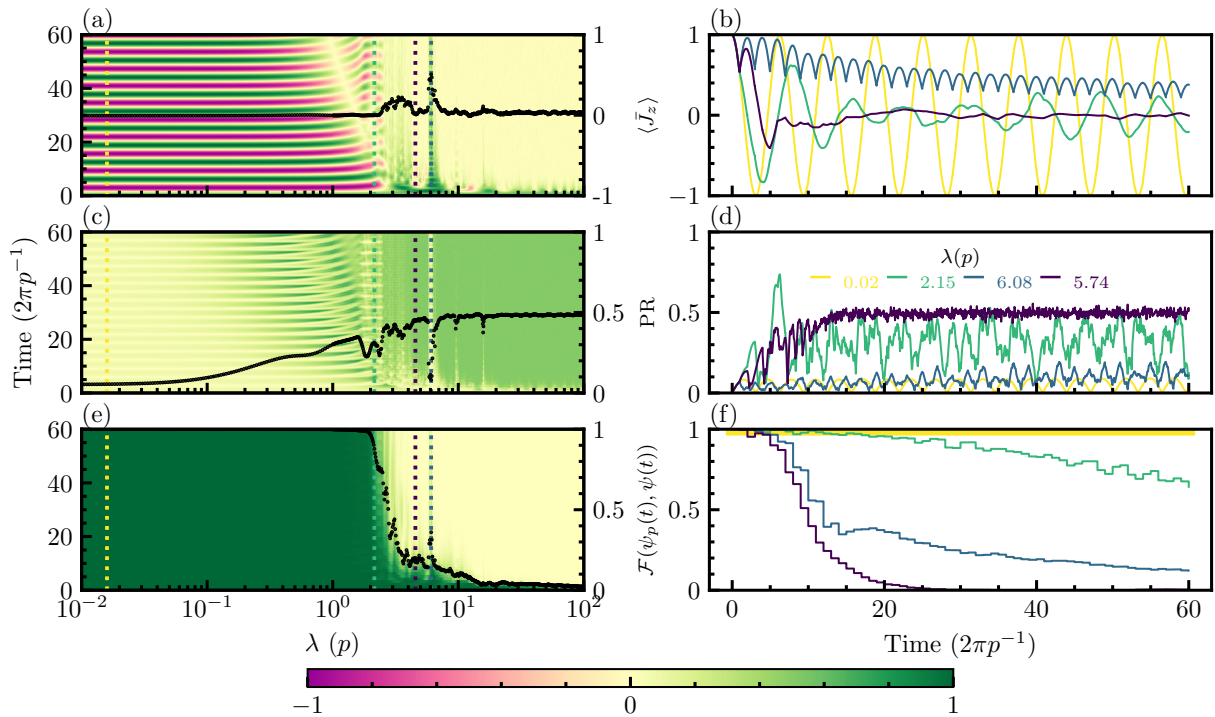


Figure 8. Dynamical signatures of quantum chaos in quantum kicked top with COE and $j = 400$ (The other parameters are given in appendix A 4). Dynamical evolutions of (a) (normalised) expectation value $\langle \bar{J}_z \rangle = \frac{1}{j} \langle J_z \rangle$, (c) participation ratio PR, and (e) fidelity under perturbation $\mathcal{F}(\psi_p(t), \psi(t))$ show quantum chaotic signatures for sufficiently large kicking strength λ . Black dots are temporal averages with y-axes on the right. (b), (d), and (f) show time traces, respectively, from (a), (c), and (d) for the kick-strengths values given in the legend of (d) and also marked by the line colours on colour plots. expectation values lose (quasi)periodicity (a)&(b), system gets delocalised (c)&(d), and fidelity decays exponentially (e)&(f) in the chaotic regime, while they all recover in the stable island ($\lambda = 6.08(p^{-1})$).

tics of quantum kicked top of COE symmetry and the corresponding RMT distribution as a function of kick strength. In Fig. 7 (e), X_{RMT}^2 shows three main regions: (i) regular dynamics for $\lambda \lesssim 1$, (ii) a transition region for $1 \lesssim \lambda \lesssim 7$ with mixed-phase space and stable islands, and (iii) the quantum chaotic region for $\lambda \gtrsim 7$. Next, we demonstrate the same transition and regions in dynamical signatures of quantum chaos.

b. Dynamical Signatures

Here, we demonstrate onset of quantum chaos in the dynamics of a quantum kicked top with COE symmetry as a function of kick strength. Figure 8 shows the time evolutions of (a) (normalised) expectation value $\langle \bar{J}_z \rangle = \frac{1}{j} \langle J_z \rangle$, (b) participation ratio (PR), and (c) fidelity under perturbation. Beyond the critical kicking strength $\sim 2p$, the system starts to show quantum chaotic characteristics: (i) destruction of (quasi)periodicity in expectation values, (ii) high delocalisation, (iii) rapid perturbation fidelity decay. Figures 8 (d–f) show time traces for various kick-strengths, and we clearly see the quantum chaotic (and regular) dynamics as well as the revival of regular dynamics on the stable island marked (and plotted) by blue, which is also

identified in the X_{RMT}^2 analysis of eigenvector statistics.

Appendix B: Ising Model

1. Dynamics in Small Systems

Here, we show dynamics for the magnetisation $\langle \bar{J}_z \rangle = \langle J_z \rangle / j$ for small j values in A2A-Ising Trotterisation. Figure 9 shows that the threshold gets sharper as the dynamics start to show quantum chaotic characteristics, namely the destruction of (quasi)periodicity, beyond the threshold. Even though the approximate threshold position is still clear for any system size in Fig. 9, it is a smooth transition when the system is still (quasi)periodic beyond the threshold, and it gets sharper only when the (quasi)periodicity is destroyed for sufficiently large j values. In Fig. 9, we observe that the sharp threshold and signatures of quantum chaotic dynamics start to appear for $j \geq 4$, and this observation is consistent with our X_{RMT}^2 analysis in the main text, which shows $X_{\text{RMT}}^2 \leq 1$ for $j \geq 4$.

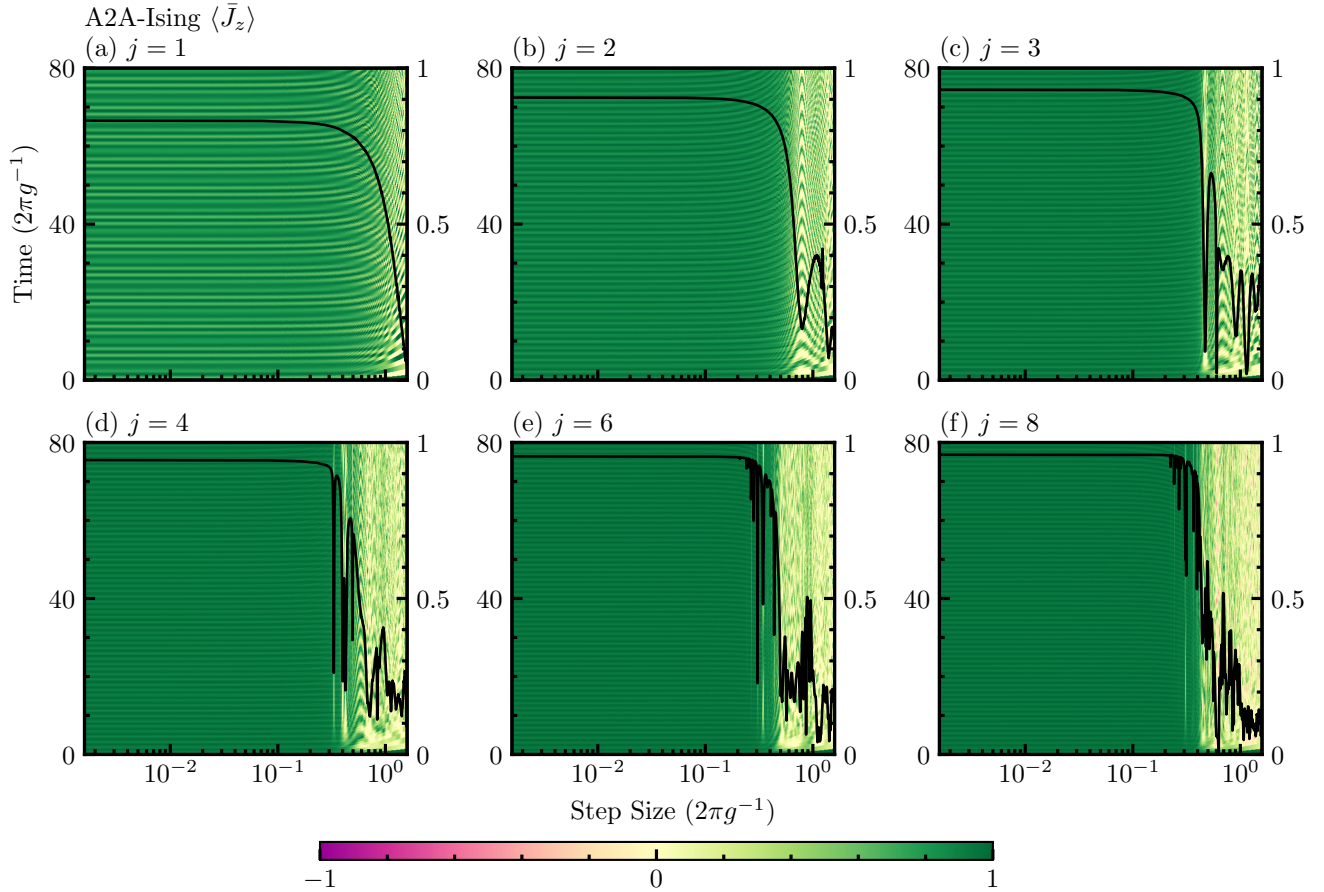


Figure 9. The onset of quantum chaos and Trotterisation threshold as the system size increases in A2A-Ising. The *lack* of sharp threshold in small sizes is understood from the dynamical evolutions. (a), (b) and (c) show that the dynamics beyond the threshold is still (quasi)periodic, respectively, for the small spin sizes $j = 1$, $j = 2$ and $j = 3$, which consistently do not produce a good agreement with RMT statistics analyses. The smallest system size with $X_{\text{RMT}}^2 \approx 1$ is $j = 4$ and (d-f) shows that the dynamics beyond the threshold start losing (quasi)periodicity for $j > 4$. The system parameters and the initial state are the same as in the main text of the paper.

2. Eigenvector Statistics

In the main text of the paper, we show eigenvector statistics histograms for $j = 64$ and calculate X_{RMT}^2 for the other system sizes. Here, to illustrate how system size affects the histograms themselves, we provide example histograms for several j values and three step sizes, which are chosen from regular (before the threshold), quantum chaotic (after the threshold), and stable island regions. Figure 10 shows the eigenvector statistics for different j values on each column and different step sizes on each row: (top to bottom) before the threshold ($\tau = 0.02$ ($2\pi g^{-1}$)), quantum chaotic ($\tau = 0.5$ ($2\pi g^{-1}$)), and stable island (seen only in large system sizes) ($\tau = 0.7$ ($2\pi g^{-1}$)) regions, respectively. The smallest system size, in Fig. 10 (a), does not have enough components to produce meaningful statistics, and the visual comparisons in Figs 10 (b–c) do not provide very clear conclusions. The X_{RMT}^2 goodness-of-fit test statistic, on the other hand, provides consistent conclusions in terms of successfully identifying the dis-

agreement/agreement of eigenvector statistics with RMT distributions. For the large system sizes, the regular and chaotic regions are clearly distinguishable in the eigenvector statistics, shown respectively for (d) $j = 64$ and (e) $j = 256$ in Figs 10 (d–e). However, the stable islands ($\tau = 4.5$ ($2\pi g^{-1}$)) are visually indistinguishable from the quantum chaotic $\tau = 3.5$ ($2\pi g^{-1}$) case, and, once again, X_{RMT}^2 proves useful and identifies these weak islands (see main text).

Appendix C: Heisenberg Model

1. Eigenvector Statistics

In the main text, we present only the X_{RMT}^2 analysis for the Heisenberg Trotterisations. Therefore here, Fig. 11 explicitly shows the eigenvector statistics histogram plots for 3, 6, and 9 qubits Heisenberg Trotterisations on each column and different step sizes on each row. The step sizes

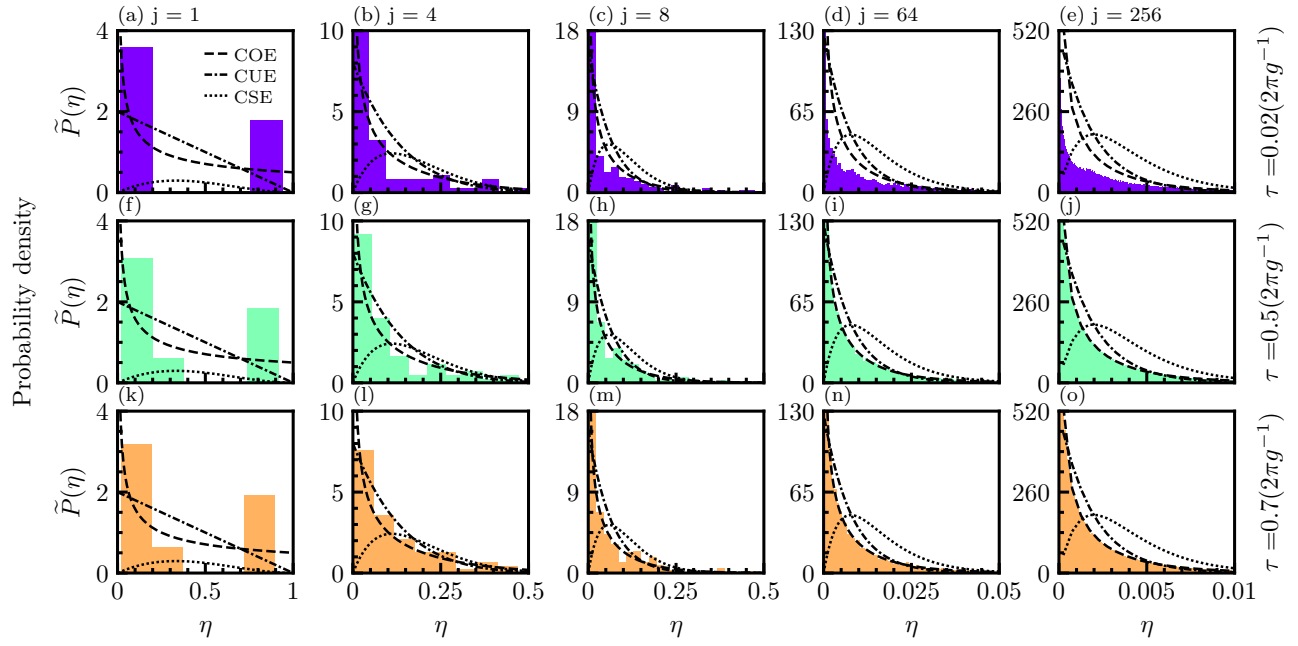


Figure 10. Eigenvector statistics for Trotterised A2A-Ising unitary. Columns show increasing j values from left-to-right, and the rows, from top-to-bottom, are for step sizes before the threshold ($\tau = 0.02 (2\pi g^{-1})$), chaotic ($\tau = 0.5 (2\pi g^{-1})$), and stable island (seen only in large system sizes) ($\tau = 0.7 (2\pi g^{-1})$) regions. The coloured lines are RMT distributions as shown by the legend.

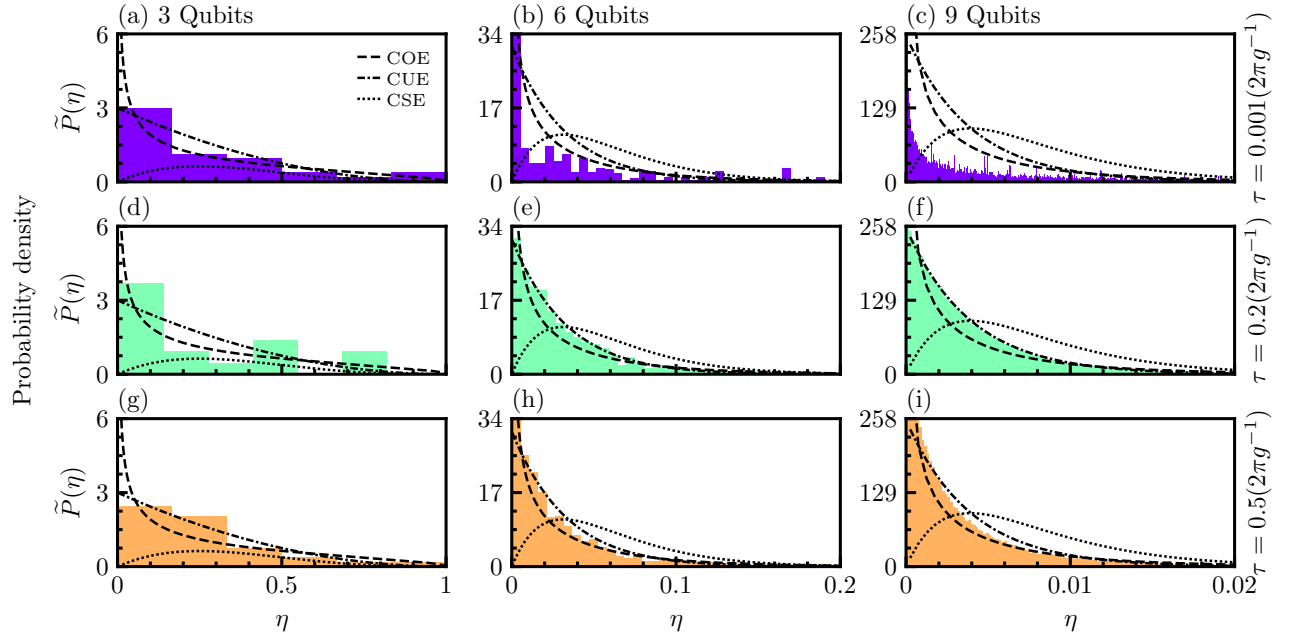


Figure 11. Eigenvector statistics for Trotterised Heisenberg unitary. Columns, left to right, show 3, 6, and 9 qubit chains, and rows, top-to-bottom, are for step sizes before the threshold ($\tau = 0.001 (2\pi g^{-1})$), quantum chaotic ($\tau = 0.2 (2\pi g^{-1})$), and stable island ($\tau = 0.5 (2\pi g^{-1})$) regions. 9 qubits show clear deviations from the RMT distributions (c) before the threshold and (i) in the stable island, and it closely follows the CUE distribution in (f) quantum chaotic region. 6 qubits show clear deviation from RMT (c) before the threshold, while it is quite close to CUE distribution both in (e) stable island and (h) quantum chaotic regions, while X_{RMT}^2 clearly distinguishes the two in the main text of the paper. 3 qubits cases in (a,d,g) do not have enough components to give good statistics. The coloured lines are RMT distributions as shown by the legend.

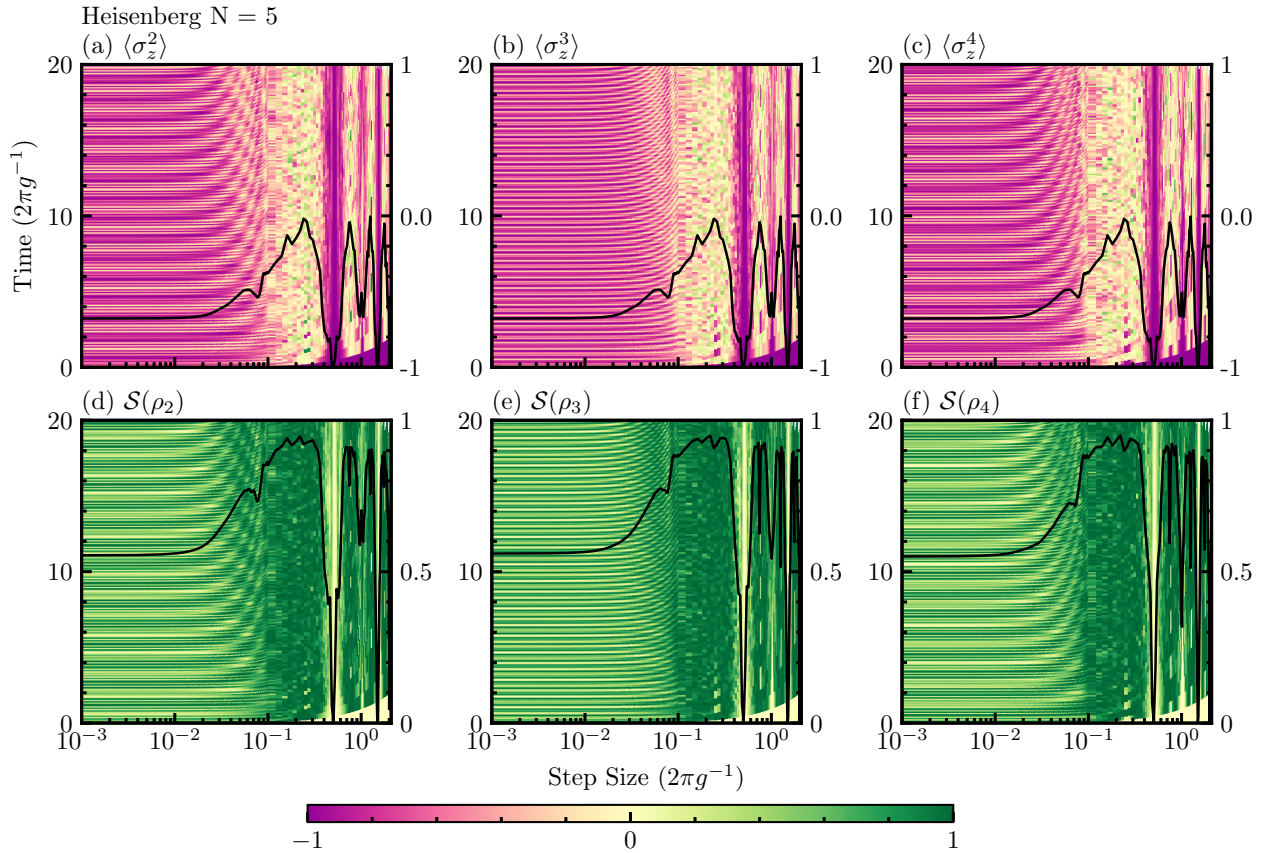


Figure 12. Dynamical evolutions of qubit polarization $\langle \sigma_z^k \rangle$ and sub-system entropy $\mathcal{S}(\rho_k)$ for qubit $k = 2, 3, 4$ in the $N = 5$ Heisenberg chain. The black lines, with y-axes on the right, are the time averages of the colour plots. System parameters are the same as in the main text of the paper.

shown in the columns of Fig. 11 are, respectively from top-to-bottom, from before the threshold ($\tau = 0.001$ ($2\pi g^{-1}$)), quantum chaotic ($\tau = 0.2$ ($2\pi g^{-1}$)), and stable island ($\tau = 0.5$ ($2\pi g^{-1}$)) regions. For the case of 9 qubits, the histogram plots clearly agree/disagree with the RMT distributions in all three cases as seen in Figs 11 (c,f,i). The eigenvector statistics of the 6 qubits case show visually convincing agreement (and disagreement) in the quantum chaotic (and regular) regime as shown in Fig. 11 (b) (and (e)). However, for the 6 qubits case, the distinction between the stable island and quantum chaotic regimes is not as clear as it is for 9 qubits. Finally, for the smallest system size in Fig. 11, none of the histogram plots provides any clear conclusion. By contrast, in each case, the X_{RMT}^2 analysis used in the main text of the paper provides quantitative measures of these visual comparisons, and successfully identifies all these regimes providing conclusive and consistent results.

As a final note, this Trotterisation has degeneracies. Therefore, the eigenvector statistics in Fig. 11 are calculated using the procedure discussed in appendix A 4 a b. Consequently, the number of independent components is reduced by half, so the theoretical lines in Fig. 11 are for $\mathcal{D} = 2^{N-1}$ for the case of N qubits. These degenera-

cies are removed when the longitudinal field σ_z term is replaced with the transverse field $\sigma_{y/x}$ term. Then, the regular procedure can be followed, and we observed a good agreement with RMT distributions of the full dimension $\mathcal{D} = 2^N$. In both cases, the results regarding the threshold and the onset of quantum chaos beyond it are qualitatively the same both in the eigenvector statistics and the dynamical signatures (not shown, data available).

2. Dynamics of the Other Qubits in the Chain

In the main text of the paper, we use the first qubit of the chain to demonstrate the dynamics of the expectation values and subsystem entropies in the Trotterisation of the Heisenberg model, and we argue that the onset of quantum chaos and the threshold position is independent of this particular choice by using eigenvector statistics of the Trotter step unitary as well as sub-system independent dynamical quantities such as PR and simulation fidelity. Here, we provide the dynamics of the expectation values and the subsystem entropies for the second, third and fourth qubits of the chain of 5 qubits. Figs 12 (a-c) (and (d-f)) show the dynamics of expectation values (and sub-

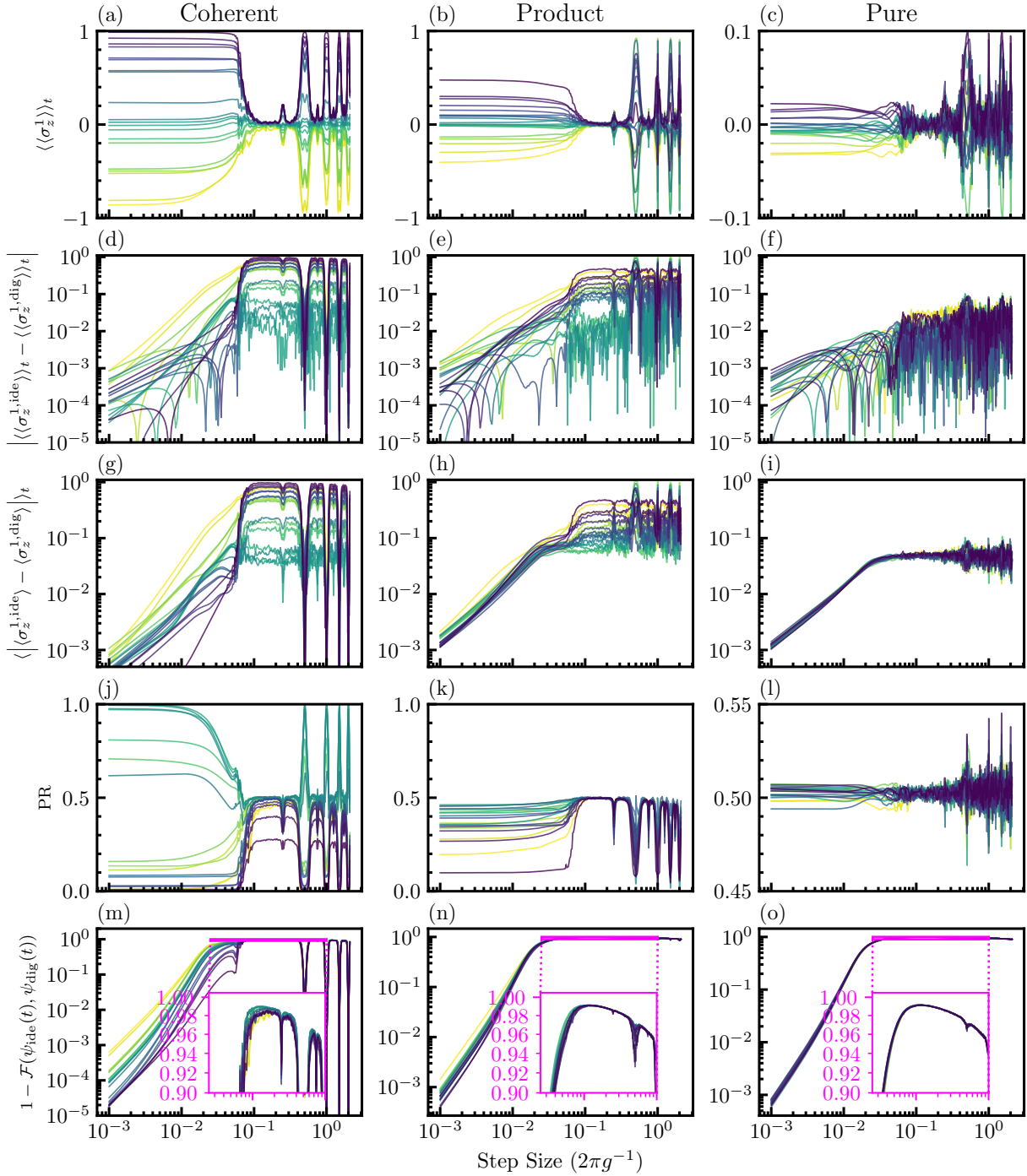


Figure 13. Threshold position for 9 qubits Heisenberg chain with various initial states. The columns, left-to-right, show the results for 20 spin-coherent, 20 product, and 20 pure initial states sampled uniformly at random. In each column, the same line colours correspond to the same initial state. Here, the second layer of brackets $\langle \cdot \rangle_t$ represents time averaging. The rows, top-to-bottom, show time averaging of (a–c) the qubit polarization of the first qubit in the chain $\langle\langle\sigma_z^1\rangle\rangle_t$ for Trotterised evolution, (d–f) the absolute difference $|\langle\langle\sigma_z^{1,\text{ide}}\rangle\rangle_t - \langle\langle\sigma_z^{1,\text{dig}}\rangle\rangle_t|$ between the time averaged expectation values obtained from the Trotterised ($\langle\langle\sigma_z^{1,\text{dig}}\rangle\rangle_t$) and ideal dynamics ($\langle\langle\sigma_z^{1,\text{ide}}\rangle\rangle_t$) sampled at every step size τ , (g–i) time average of the point-to-point absolute difference $|\langle\langle\sigma_z^{1,\text{ide}} - \sigma_z^{1,\text{dig}}\rangle\rangle_t|$ at each step of the evolution, (j–l) participation ratio $\langle PR \rangle_t$ for the Trotterised dynamics, and (m–o) simulation infidelity $1 - \mathcal{F}(\psi_{\text{dig}}(t), \psi_{\text{ide}}(t))_t$. We find the threshold at the same position. The smooth deviations from the ideal value (i.e. the value at $\tau \rightarrow 0$) in the time averages of $\langle\langle\sigma_z^1\rangle\rangle_t$ start before the threshold for the states with larger Trotter errors, which is also explained as the result of the change in (quasi)periodicity in the main text.

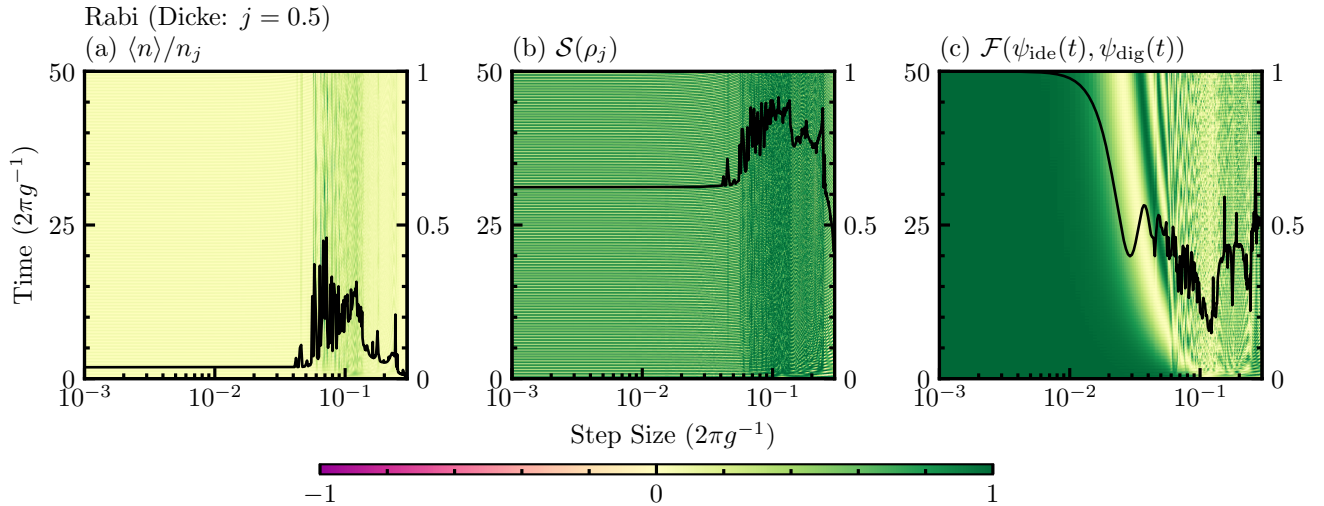


Figure 14. The sharp threshold in the Trotterised quantum Rabi evolution. Dynamical evolutions of the smallest case of the Dicke model ($j = 0.5$ i.e. the quantum Rabi model) show the dynamical signatures of quantum chaos beyond the threshold.

system entropies), respectively, for (a) (and (d)) second, (b) (and (e)) third, and (c) (and (f)) fourth qubit. We clearly observe the same threshold and same behaviours observed for the first qubit.

3. Effect of Initial State on the Threshold

Trotterisation of the Heisenberg model show certain initial-state-dependent effects in the main text of the paper. Here, we analyse the dynamics of the 9-qubit Trotterised Heisenberg model for various initial states (of 3 types) and provide results for expectation values, PR values, and the Trotter errors. The results show that the initial state does affect the size of the Trotterisation errors before the threshold and we note that the threshold might not seem sharp for the states with larger errors. Still, the breakdown of digitisation occurs at a sharp threshold largely independent of the initial state.

We sample 20 initial states uniformly at random from each spin-coherent, product, and pure state types, where the spin-coherent state

$$|\theta, \phi\rangle_N = \otimes_N (\cos(\theta/2) |1\rangle + e^{-i\phi} \sin(\theta/2) |0\rangle), \quad (\text{C1})$$

is just a subset of product states $|N\rangle = \otimes_{i=1}^N |i\rangle$, which is a subset of pure states. Figure 13 shows various averaged quantities calculated from the digital simulations for $t = 20$ ($2\pi g^{-1}$). Even for initially highly delocalised states (and the pure state samples), there is a noticeable difference at the same threshold position, and we observe the same threshold in each quantity and initial state.

Appendix D: Dicke Model

1. Threshold in Rabi model

Here, we include the full dynamics of photon number, subsystem entropy, and simulation fidelity in the Rabi model (i.e., Dicke model with $j = 0.5$). Figure 14 shows that the Rabi model already shows a strong threshold in all these quantities, and we observe signatures of quantum chaotic dynamics beyond the threshold. We see that the (quasi)periodic dynamics of the (normalised) photon number is destroyed beyond the threshold (Figure 14 (a)), and that the subsystem entropy of the spin component is considerably larger than the pre-threshold value (Fig. 14 (b)), which is maximised for sufficiently large spin components in the Dicke model (Fig. 3 (i)). Finally, the threshold in simulation fidelity, shown in Fig. 14 (c), again appears as the secondary transition from (quasiperiodic) oscillatory-in-time to decaying behaviour. Despite the threshold and signatures of quantum chaotic dynamics beyond it, we do not find an agreement with RMT in the eigenvector statistics of the Rabi model. Instead, the Dicke model, similar to the other models, shows agreement with RMT predictions only for sufficiently large system sizes (in this case, a sufficiently large spin component), but it also shows certain cavity dimension truncation dependencies discussed in appendix D3. We leave further analyses of the threshold in the Rabi model, and why it appears at the smallest sizes, as an open question for future research.

2. Normalisation of the Photon Number and the Participation Ratio

In this section, we present numerical data supporting our choice of normalisation coefficients n_j and \mathcal{D} for, re-

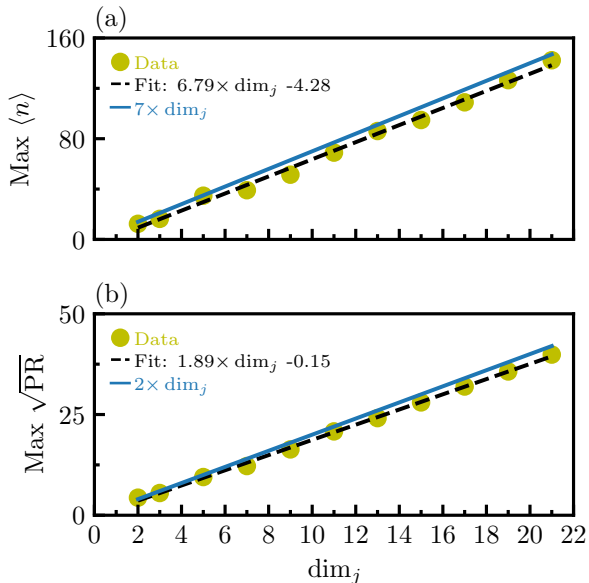


Figure 15. The maximum of (a) the photon numbers $\langle n \rangle$ and (b) the PR (shown as its square root) values of the quantum chaotic dynamics are, respectively, linear and quadratic (linear for $\sqrt{\text{PR}}$) in dim_j . In each sub-figure, the circles are the data points obtained numerically from the dynamical simulations, and the black lines are the numerical fits. The blue lines are the normalisation coefficients used in this paper.

spectively, the photon numbers $\langle n \rangle$ and PRs in the Dicke model. Figures 15 (a–b) show that the maximum of (a) the photon numbers $\langle n \rangle$ and (b) the $\sqrt{\text{PR}}$ values of the quantum chaotic regions are linear in dim_j . We use $n_j = 7 \times \text{dim}_j$ and $\mathcal{D} = (2 \times \text{dim}_j)^2$ for the normalisations of the photon number and participation ratio, respectively, and the blue lines in Figs 15 (a–b) show these values. The constant coefficients 7 and 2 are determined numerically. The dynamical signatures are independent of the cavity truncation dimension dim_c , provided that dim_c is large enough for the simulation to support all the components of the time evolving state. Therefore, these observations (together with the maximised subsystem entropy of the spin component) suggest that the quantum chaos in this model is driven by the spin- j component. The eigenvector statistics analyses, in the next section, support this intuition as they show agreement with the RMT distributions only when the cavity truncation is $\text{dim}_c \sim \text{dim}_j$.

3. Eigenvector Statistics and the Effect of Truncated Cavity Dimension

In the numerical analyses of the Dicke DQS, the finite truncation of the cavity dimension poses a non-trivial problem. Here, we provide detailed numerical analysis of the truncation dependency in the eigenvector (and also eigenvalue) statistics of the Trotter step unitary of the

Dicke model. We first present the histogram plots for the case $j = 6$ for different step sizes and cavity dimensions. Then, we carry out the X_{RMT}^2 analysis for the eigenvector statistics for various j values and as a function of various parameters. Our numerical analysis gives us some intuitive physical insight and suggests that the spin component of the system drives the quantum chaotic dynamics beyond the threshold. We report our numerical findings to support and explain our choice for cavity truncation in the main text of the paper, and to provide initial motivation for further research. This is a subtle problem which merits further investigation of how to apply these statistics for truncated dimensions in unbounded systems, as well as a more rigorous understanding and explanation of these numerical results.

a. Level-spacing and Eigenvector Statistics

In this section, we provide the eigenvector statistics histograms for the Dicke DQS to show the cavity dimension truncation dependency, and we also employ an additional static signature of quantum chaos as a supporting tool, namely the level-spacing (or eigen-phase/value) statistics (discussed in appendix A 2). Here, the level-spacing statistics are calculated for each parity subspace of the Dicke system ($\Pi = e^{i\pi(a^\dagger a + J_z + j)}$, see appendix A 4 a), and the figures in this section show the super-imposed statistics of these subspaces. Additionally, the eigenvector statistics of the Dicke DQS are obtained using the degenerate system procedure (discussed in appendix A 4 a b). Therefore we use the RMT distributions with half the total size of the truncated space $\mathcal{D} = \frac{1}{2} \text{dim}_j \times \text{dim}_c$.

Figure 16, for the $j = 6$ Dicke DQS, shows the level-spacing statistics in the upper-right insets, and the eigenvector statistics in the main figures with its *tail* in the lower-right insets. In Figs 16 (a–b), we use the step size $\tau = 0.01$ ($2\pi g^{-1}$) (i.e. before the threshold), and we show that neither the eigenvector nor the eigenphase statistics have an agreement with RMT distributions, as expected. The eigenphase statistics are actually Poisson distributed for this step size, which is a signature of regular dynamics according to the Berry-Tabor conjecture [86]. For the step size $\tau = 0.12$ ($2\pi g^{-1}$) (beyond the threshold) and the cavity dimension $\text{dim}_c = 25$, both the eigenvector and eigenphase statistics show agreement with RMT distributions, shown in Fig. 16 (c). However, once dim_c exceeds a certain value (that increases with j , as shown in the next section), agreement with RMT is lost in both of these cases, shown for $\text{dim}_c = 200$ in Fig. 16 (d) where the level-spacing statistics are actually closest to a Poisson distribution.

Aside from the dim_c dependency, both eigenvector and level-spacing statistics simultaneously agree/disagree with RMT beyond/before the threshold, and they show the same behaviour in various other system parameter regimes (not shown). Indeed, this even holds for examples the

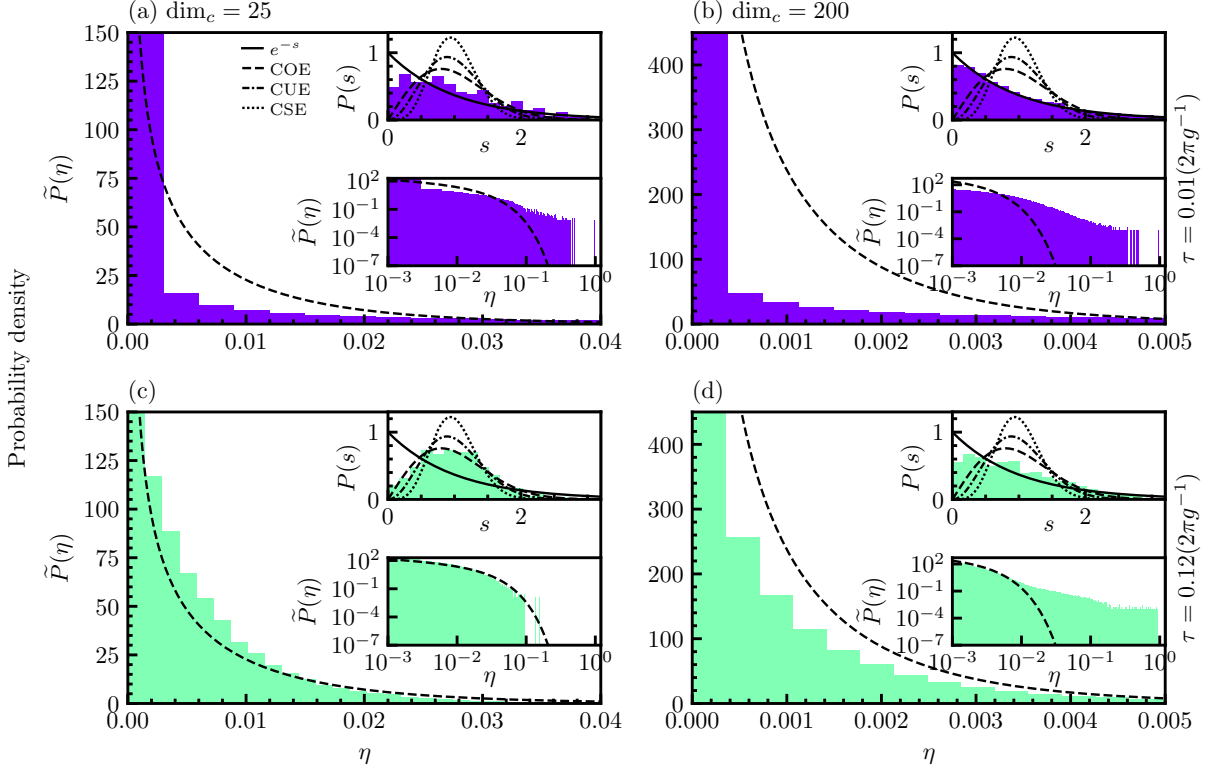


Figure 16. Eigenvector and eigenvalue statistics of Trotterised Dicke unitary with $j = 6$, and the system parameters are the same as the main text of the paper. In each panel (a–d), the main histogram plots show the eigenvector statistics, upper insets show the corresponding eigenvalue statistics, and the lower insets show the *tail* of the main histogram plots. Before the threshold $\tau = 0.01$ ($2\pi g^{-1}$) neither the eigenvector nor the eigenvalue statistics show an agreement with RMT distributions for cavity dimension truncations (a) $\text{dim}_c = 25$ and (b) $\text{dim}_c = 200$. Beyond the threshold $\tau = 0.12$ ($2\pi g^{-1}$), both the eigenvalue and the eigenvector statistics are observed to be *close* to RMT distributions for (c) $\text{dim}_c = 25$, and such agreements are lost both in the eigenvalue and the eigenvectors statistics for (d) $\text{dim}_c = 200$.

regime where the ideal Dicke model itself is known to be quantum chaotic [79, 80], where we still observe a sharp threshold, beyond which the PR values and sub-system entropies are larger for the digitised system than the ideal system. Since our focus in this paper is the digitisation-induced onset of quantum chaos, detailed analysis of this case is beyond the scope of this paper, but we provide some illustrative data in appendix D 4.

b. Goodness-of-fit Analyses

In this section, we analyse the dependency of eigenvector statistics on the truncation value of cavity dimension via the X_{RMT}^2 goodness-of-fit test statistic. In the previous section, we presented the eigenvector (and eigenphase) statistics histograms of the Trotter step unitary of the Dicke model with $j = 6$ for two different step sizes and two cavity truncation values. We compared these statistics with RMT distributions of dimension $\mathcal{D} = \frac{1}{2} \text{dim}_j \times \text{dim}_c$ (i.e. half the total size of the truncated space). Here, we calculate X_{RMT}^2 as a function of various parameters:

namely cavity truncation dim_c , Trotter step size τ , spin size j , and fit dimension dim_f . Here, we use the fit dimension dim_f to explore the effective system dimension. That is, with the other parameters fixed (including the cavity dimension), we instead sweep the dimension variable of the RMT distributions: we calculate X_{RMT}^2 by comparing the numerical eigenvector histograms to RMT distributions with dimension $\text{dim}_f/2$ instead of $\mathcal{D} = \frac{1}{2} \text{dim}_j \times \text{dim}_c$.

The main observation from the results below is that the maximum cavity truncation dimension to obtain $X_{\text{RMT}}^2 \sim 1$ is $\text{dim}_c = \text{dim}_j$. Together with the behaviours of the dynamical quantities (discussed in the main text and appendix D 2), these X_{RMT}^2 results suggest that quantum chaotic dynamics in the Dicke DQS is mainly driven by the spin component. This is consistent with a simple intuition that the non-commutations in the Dicke DQS result from single qubit rotations that affect only the collective spin component. We nevertheless note the importance of developing a more theoretically rigorous understanding of these numerical results as an open question for further studies.

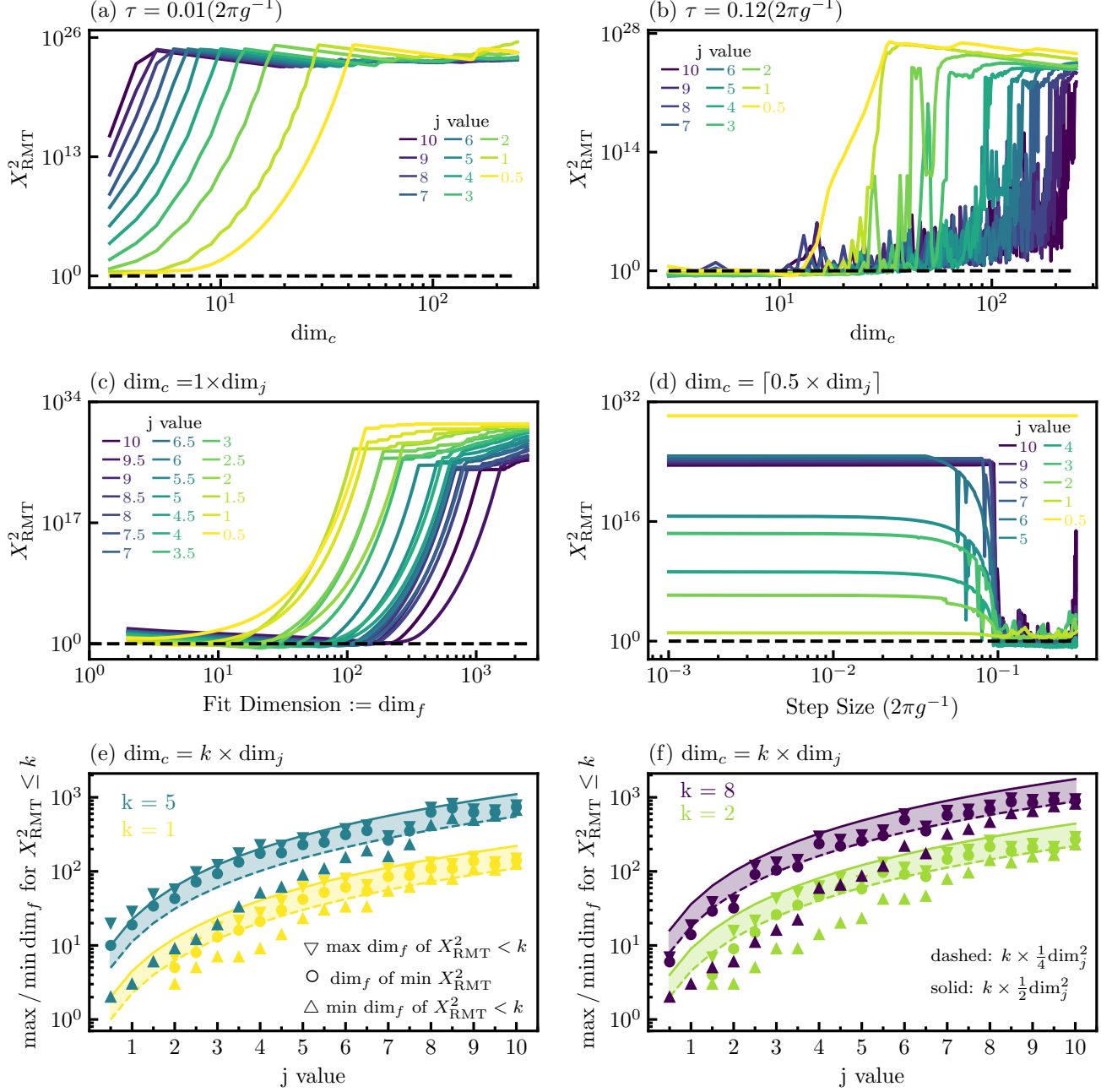


Figure 17. X^2_{RMT} analysis of the cavity truncation dependency in eigenvector statistics of the Trotterised Dicke unitary. The system parameters are the same as in the main text of the paper. Calculating X^2_{RMT} by sweeping the cavity truncation dimension \dim_c , (a) X^2_{RMT} values are always (much) larger than 1 before the threshold $\tau = 0.01(2\pi g^{-1})$, and (b) in the chaotic region beyond the threshold $\tau = 0.12(2\pi g^{-1})$. X^2_{RMT} reaches below 1 up to a maximum \dim_c that is observed to increase as the spin dimension \dim_j (i.e. the j value) increases. Fixing cavity truncation to $k \times \dim_j$ and fitting it against COE distribution of different *fitting* dimensions \dim_f , (c) shows $X^2_{\text{RMT}} < k$ is observed for $\dim_f \sim \frac{k}{2} \times \dim_j^2$ for $k = 1$. This relation is also shown in (e) and (f) where the maximum (downward triangles) and minimum (upward triangles) dimensions of $X^2_{\text{RMT}} < k$ and the dimension of the minimum X^2_{RMT} (circles) are plotted against j values for different k values. The minimum of X^2_{RMT} in (e) (and (f), which is separated for visual clarity) stays between $k \times \frac{1}{2} \dim_j^2$ (solid lines) and $k \times \frac{1}{4} \dim_j^2$ (dashed lines). X^2_{RMT} as a function of step size corresponding to solid line is presented in the main text of the paper, and (d) shows X^2_{RMT} as function of step size for various j values and $\dim_c = \lceil 0.5 \times \dim_j \rceil$ corresponding to dashed line.

a. Cavity truncation First, we analyse X_{RMT}^2 as a function of dim_c for two step sizes before ($\tau = 0.01$ ($2\pi g^{-1}$)) and after ($\tau = 0.12$ ($2\pi g^{-1}$)) the threshold and various j values. In this case, the fit dimension is equal to the total dimension of the truncated system, i.e. $\text{dim}_f = \text{dim}_j \times \text{dim}_c$. Figure 17 (a) shows that the eigenvector statistics before the threshold do not show agreement with RMT for any value of j or dim_c . For the quantum chaotic region beyond the threshold, however, we observe that $X_{\text{RMT}}^2 \sim 1$ up to a maximum dim_c (that increases with increasing j) as shown in Fig. 17 (b), and X_{RMT}^2 quickly diverges to larger values beyond these truncations.

b. Fit dimension Having observed agreement with RMT for $\text{dim}_c \sim \text{dim}_j$ in Fig. 17 (b), we now fix the cavity dimension to $\text{dim}_c = \text{dim}_j$ and calculate X_{RMT}^2 while varying the fit dimension dim_f for various j values. The data in Figure 17 (c) confirm that $X_{\text{RMT}}^2 \sim 1$ is observed only for $\text{dim}_f \sim \text{dim}_j \times \text{dim}_c$: specifically, we observe that X_{RMT}^2 stays below 1 when dim_f is between a minimum ($\min \text{dim}_f$) and a maximum $\max \text{dim}_f$. In Fig. 17 (e), we plot the minimum and maximum dim_f values with upper and lower (yellow) triangles, respectively. The dim_f at which X_{RMT}^2 achieves its minimum is shown in yellow circles. These values appear to converge towards each other as the j value increases, and stay mainly between $\frac{1}{2} \text{dim}_j^2$ and $\frac{1}{4} \text{dim}_j^2$. Accounting for the additional $1/2$ factor in dim_f due to the degeneracies in the system (as discussed in appendix A 4 a b), this means that the maximum dim_f after which X_{RMT}^2 starts to quickly increase is equal to the $\text{dim}_c = \text{dim}_j$, which is the cavity dimension we set.

c. max and min dim_f Next, we analyse these max and min dim_f values for larger cavity truncations. We already know from Fig. 17 (b) that X_{RMT}^2 does not reach below 1 for cavity truncations that are much larger than dim_c , but they are fit against the full system dimension D while we here use the fit dimension as a free parameter. In this case, we observed that the qualitative shape of curves similar to Fig. 17 (c) (not shown) stays the same provided that dim_c is an integer multiple of $k \times \text{dim}_j$ and that the curves shift upwards in X_{RMT}^2 as the cavity truncation increases. Therefore, X_{RMT}^2 again does not go below 1 for these large cavity truncations, but it does become smaller than the integer multiplicative factor k . Figs 17 (e–f) show that max and min dim_f at which the X_{RMT}^2 reaches below k are k multiples of the above dimension, respectively $k \times \frac{1}{2} \text{dim}_j^2$ and $k \times \frac{1}{4} \text{dim}_j^2$, and they again converge towards each other for larger j values and stay approximately between these two values.

d. Step size These results, though we leave it as an open question to find a rigorous explanation, show that the maximum truncation dimension that gives close agreement (i.e., $X_{\text{RMT}}^2 \sim 1$) with RMT is $\text{dim}_c \sim \text{dim}_j$, which is also the value we used in the main text to analyse RMT correspondence as a function of step size. In the above results, the minimum cavity truncation that gives close agreement is observed to be $\text{dim}_c \sim \frac{1}{2} \text{dim}_j$. For comparison, here we plot X_{RMT}^2 for $\text{dim}_c = \frac{1}{2} \text{dim}_j$, as function

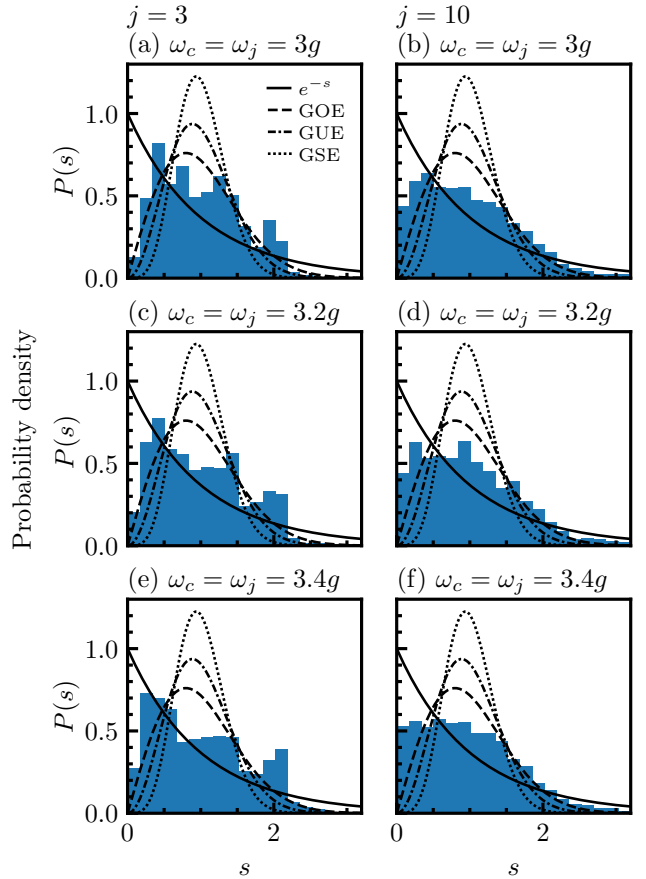


Figure 18. Finding *non-chaotic* parameters of the Dicke Hamiltonian by calculating the level spacing statistics for $j = 3$ and $j = 10$ on each column. It is qualitatively insensitive to dim_c , which is set to 100 in these calculations. The red, green, and blue lines are RMT statistics respectively for COE, CUE, and CSE classes, and the black line is Poisson distribution.

of step size and for various system sizes (Fig. 17 (d)). It is qualitatively the same as the main text and shows the same threshold, showing that within this small range for dim_c , the X_{RMT}^2 results for the Dicke model do not depend sensitively on dim_c .

4. Quantum Chaos in Dicke model

In order to focus on digitisation-induced quantum chaos, we focus exclusively on *regular* parameters of the Dicke Hamiltonian in the main text of the paper. Here, we discuss how we choose these parameters, and also provide example results for the Trotterisation of the Dicke Hamiltonian with quantum chaotic parameters.

In two papers [79, 80], the Dicke model is shown to be quantum chaotic for the coupling strengths g around the critical coupling $g_c = \sqrt{\omega_c \omega_j}$ of the super-radiant phase transition (it becomes regular, if g is either too much smaller or larger than g_c). For these regimes, Refs [79, 80]

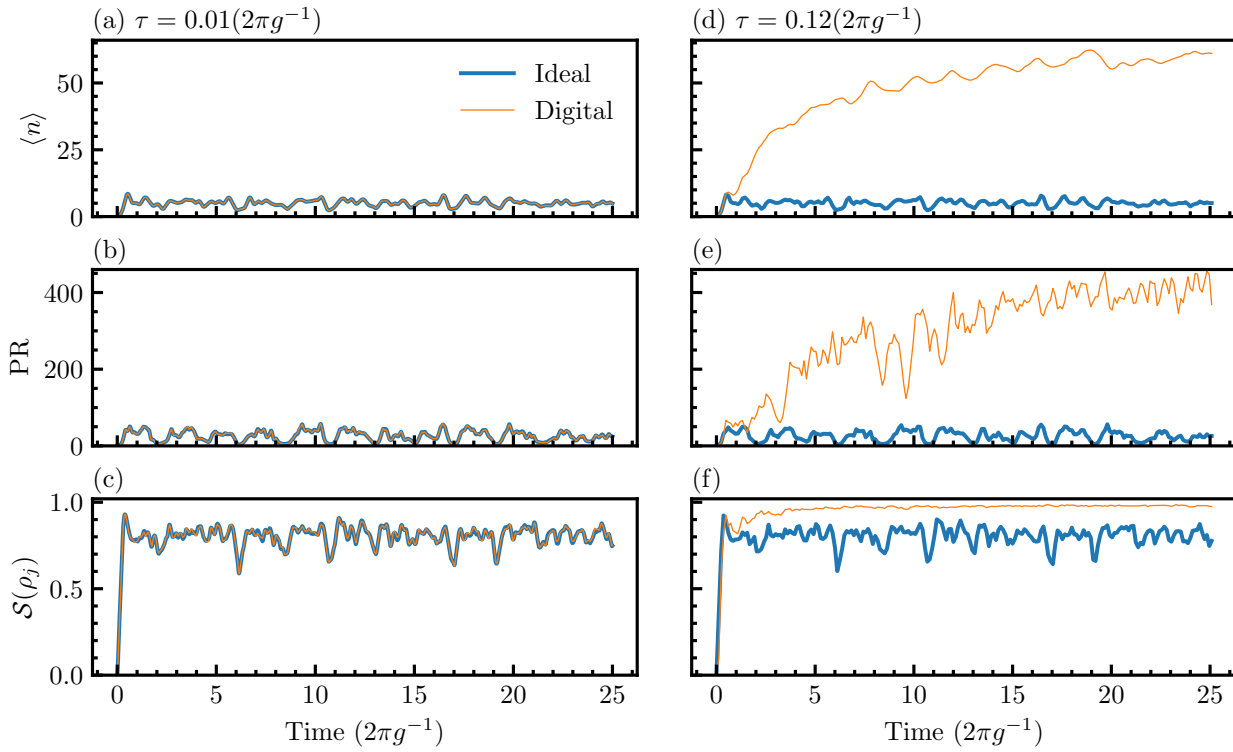


Figure 19. Trotterisation of the Dicke model in its quantum chaotic regime ($0.5\omega_c = \omega_j = g = 1$ and $j = 6$). The dynamical evolutions of (a) and (d) $\langle a^\dagger a \rangle$ expectations, (b) and (e) PR, and (c) and (f) entropy of the reduced state of spin component $S(\rho_j)$ show more dominant quantum chaotic characteristic for digital simulation (orange) beyond the threshold (a–c). The digital simulation before the threshold (d–f) accurately simulate the quantum *chaotic* Dicke.

show that the level spacing statistics of the Dicke Hamiltonian follow Wigner-Dyson statistics. They support these observations by obtaining a classical correspondence using Holstein-Primakoff transformations, together with certain approximations, and showing that the classical limit is chaotic for the parameters that give Wigner-Dyson statistics in the quantum case.

a. Choice of the Parameters for the Main Text of the Paper

Here, we choose the Dicke model parameters used in the main text of the paper, by calculating the nearest-neighbour level-spacing statistics of the Dicke Hamiltonian for two j values, and we find a parameter regime where it does not follow the Wigner-Dyson distribution. To do this, we need to find a combination of spin and cavity frequencies that are *far enough* from the superradiant phase transition point of the Dicke Hamiltonian. We can move far into either the superradiant or normal phase regime, and here we use the latter. Specifically, we gradually increase the product of the frequencies $\omega_c \times \omega_j$ (which increases the critical coupling g_c of the superradiant phase transition) until we stop observing Wigner-Dyson statistics. Using resonant spin and cavity frequencies, Fig. 18 shows this analysis for $j = 3$ and $j = 10$, and we find that the level statistics fairly obviously do not agree with

Wigner-Dyson statistics at both $j = 3$ and $j = 10$ by the time we have $\omega_c = \omega_j = 3.4g$. Thus, any combination of spin and cavity frequencies that satisfy $\omega_c \times \omega_j \geq (3.4g)^2$ should be far enough from the quantum chaotic regime (which appears only for coupling frequencies near the super-radiant phase transition critical coupling).

b. Trotterisation of the Dicke Model with Quantum Chaotic Parameters

Our goal in this paper is to analyse digitisation-induced quantum chaos, therefore we use regular parameters of the Dicke model in the main text. We also, however, observed (not shown in detail) that the threshold behaviour is qualitatively the same for both regular and quantum chaotic parameters. It is not in the scope of this paper to provide detailed results for the threshold in the quantum chaotic regime of the Dicke model, but, here, we provide some example results (two different step sizes) for the Dicke model with *quantum chaotic* parameters ($0.5\omega_c = \omega_j = g$ and $j = 6$). We show that the digitised dynamics closely follow the target dynamics for the small step size, and, for the large step size, it produces noticeably larger photon numbers, PR values, and sub-system entropies than the ideal Dicke evolution.

In Fig. 19, we compare the ideal and Trotterised dynam-

ics for two step sizes, before and after the threshold, and observe that the Trotterised dynamics beyond the threshold show *stronger* signatures of quantum chaos than ideal dynamics. Figures 19 (a–c) show that ideal (blue) and Trotterised (orange) dynamics produce the same results before the threshold for (a) $a^\dagger a$ expectation, (b) PR, and (c) sub-system entropy of the spin component $S(\rho_j)$. We

then compare the ideal dynamics with the Trotterised evolution beyond the threshold in Figs 19 (d–f), and we observe that the Trotterised dynamics produce stronger dynamical signatures of chaos, namely: (i) the destruction of (quasi)periodicity in expectation values is much more prominent, (ii) PR for DQS is an order of magnitude greater than ideal, and (iii) entropy is maximised in DQS and larger than the ideal.

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