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Replica resummation of the Baker-Campbell-Hausdorff series

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We developed a novel perturbative expansion based on the replica trick for the Floquet Hamiltonian governing the dynamics of periodically kicked systems where the kick strength is the small parameter. The expansion is formally equivalent to an infinite resummation of the Baker-Campbell-Hausdorff series in the un-driven (non-perturbed) Hamiltonian, while considering terms up to a finite order in the kick strength. As an application of the replica expansion, we analyze an Ising spin 1/2 chain periodically kicked with magnetic field of strength h, which has both longitudinal and transverse components. We demonstrate that even away from the regime of high frequency driving, if there is heating, its rate is nonperturbative in the kick strength, bounded from above by a stretched exponential: $e^{-\mathrm{const}\, h^{-1/2}}$. This guarantees the existence of a very long pre-thermal regime, where the dynamics is governed by the Floquet Hamiltonian obtained from the replica expansion.

Introduction.— Time-periodic modulation of interactions is a powerful tool to engineer properties of materials in both artificial and condensed matter systems [1]. In particular, high frequency driving is the cornerstone of various experiments and proposals inducing interactions such as spin-orbit coupling [2], artificial gauge fields for uncharged particles [3, 4]; it has been applied to dynamically tune or suppress hopping amplitude in optical lattices [5], and also to change topological properties of materials [6–8].

Given a periodic driving protocol, however, determining the Floquet Hamiltonian that governs the stroboscopic evolution is usually a highly non-trivial task. Except for some special integrable cases [9–12], one is compelled to apply approximate methods, e.g. variants of high frequency expansion (Magnus [13], van Vleck [14] or Brillouin-Wigner [15] expansions). These provide a local effective Hamiltonian in each order of the expansion, however, until recently, not much had been known about the convergence properties of these series. A conjecture based on the generalization of the eigenstate thermalization hypothesis suggests that generic closed periodically driven systems heat up in the thermodynamic limit, i.e. they approach a completely structureless, infinite temperature steady state [16–18]. The convergence of the expansions of the effective Hamiltonian is intimately related to heating. Recently upper bounds on heating had been reported in the linear response regime [19] and for the Magnus expansion [20, 21], with the central result that the heating is *at least* exponentially suppressed in the driving frequency for periodically driven models characterized by local Hamiltonians with bounded energy spectrum. This theoretical finding implies that one can engineer nontrivial phases of matter, which remain stable for the experimentally relevant timescales. In some situations heating seems to be either absent completely or remain well below exponential bounds [22–25]. Another recent theoretical work showed that nontrivial non-equilibrium Floquet phases can be stabilized by large driving amplitude [26] or by weak coupling to environment [27].

One of the most studied driving protocols is a time-periodic sequence of sudden quenches between different Hamiltonians [24, 29, 30], which is interpreted as kicked dynamics if one of the time intervals on which the Hamiltonians act is much shorter than the other. Such protocols naturally appear e.g. in the context of digital quantum simulation in trapped

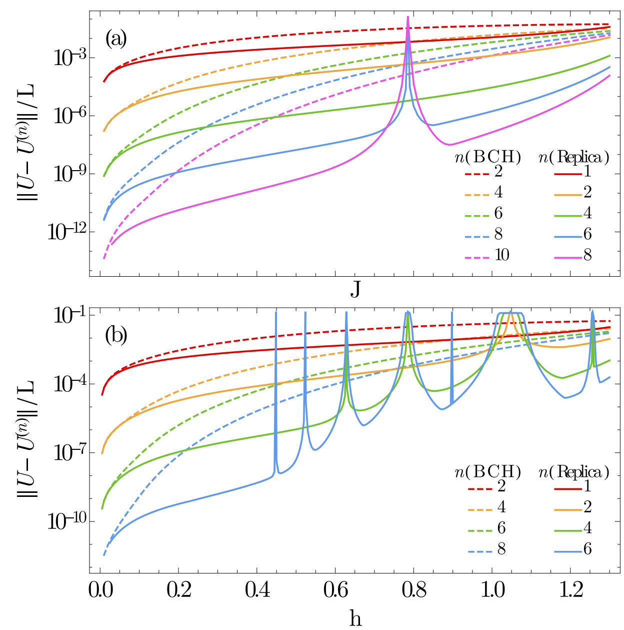

FIG. 1. The replica expansion (solid lines) beats the traditional Magnus (BCH) expansion (dashed lines) by several orders of magnitude away from the narrow resonances at rational fractions of π. The performance of the expansions is measured by the l_2 distance of the exact (U) and the approximate time evolution operator ($U^{(n)} = \exp(-iH_F^{(n)})$) within a single time-period, in the kicked tilted field Ising model defined in Eq. (7). In the top (bottom) panel the magnetic field (Ising interaction) is considered as the periodic kick. The orders are chosen such that for the matching colors the replica expansion contains all the nested commutators appearing in the corresponding order of the BCH expansion. The curves were obtained by exact diagonalization using the QuSpin package [28] on a system of $L = 16$ sites and kick strength (a) $h = 0.1$ (b) $J = 0.1$. The direction of the magnetic field is defined by $c_\theta = 0.8$, $s_\theta = 0.6$.

ions [31–33] and are frequently realized in other experimental platforms (see e.g. Refs. [34, 35]).

In the present work a novel expansion for the effective Floquet Hamiltonian is introduced for periodically kicked systems, which clearly outperforms the traditional high frequency expansions in a wide parameter range, as illustrated using two examples shown in Figure 1. Our approach uses the replica trick to calculate the logarithm of the time evolution operator describing a single period. The small parameter is the kick strength and we do not assume high frequency driving. The Magnus expansion is equivalent to the Baker-Campbell-Hausdorff (BCH) series in periodically kicked systems, and the replica expansion can be thought of as an infinite resummation of the BCH formula. As such, the possible applications of the replica expansion can reach far beyond periodically driven systems, including the theory of differential equations [13], Lie group theory [36], analysis of NMR experiments [37] or estimation of Trotterization errors in various numerical integration schemes. As an application of the replica expansion, we establish a conjecture for a non-perturbative – stretched exponential $\exp(-\mathrm{const}\, h^{-1/2})$ in the kick strength h – upper bound for the heating rate in the kicked tilted field Ising model. Our conjecture supplements the bounds introduced in Refs. [19–21], which address only the regime of high frequency driving.

Kicked dynamics.— The effective Floquet Hamiltonian evolving the kicked system is given by the logarithm of the stroboscopic time evolution operator over one period $U = U_0 U_1 = e^{-iJH_0} e^{-ihH_1}$ as

$$H_F = i\log(e^{-iJH_0} e^{-ihH_1}), \tag{1}$$

where we incorporated the time intervals of the Hamiltonians $H_{0,1}$ to the coupling constants J, h. The BCH formula provides a series expansion for H_F assuming both J and h are small as

$$\begin{aligned} H_F =& JH_0 + hH_1 - iJh\frac{1}{2}[H_0,H_1] - \\ & Jh\frac{1}{12}(J[H_0,[H_0,H_1]] + h[H_1,[H_1,H_0]]) + \dots \end{aligned} \tag{2}$$

In the usual setup of kicked systems, where $J \gg h$, that is, at intermediate frequencies and weak kick strengths, the terms with low order in H_1 but high order in H_0 are not negligible. A series expansion in the small parameter of h could be obtained formally by a resummation of the BCH series in H_0. The first order resummation is well known [24, 38],

$$H_F = JH_0 + \frac{-iJ\mathrm{ad}_{H_0} e^{-iJ\mathrm{ad}_{H_0}}}{e^{-iJ\mathrm{ad}_{H_0}} - 1} hH_1 + \mathscr{O}(h^2) \tag{3}$$

where $\mathrm{ad}_X(Y) = [X,Y]$ is the Lie derivative. However, to the best knowledge of the authors, closed form expressions for the infinite resummation in higher orders of H_1 have not yet been reported in the literature.

Replica expansion.— We tackle this problem by constructing a series expansion in h in Eq. (1). Because of the noncommutativity of H_0 and H_1, the higher order derivatives of the logarithm of the time evolution operator cannot be obtained easily. To circumvent this obstacle, we apply the replica trick to express the logarithm,

$$\log U = \lim_{\rho\to 0} \frac{1}{\rho}(U^\rho - 1). \tag{4}$$

This idea has been proven to be uniquely useful in various fields of science, such as in the statistical physics of spin glasses [39], machine learning [40], and also in calculation of the entanglement entropy [41]. Assuming that the replica limit $\mathscr{L}(\bullet) \equiv \lim_{\rho\to 0}\frac{1}{\rho}(\bullet)$ commutes with the differentiation, the series expansion of the Floquet Hamiltonian in Eq. (1) reads

$$H_F^{(n)} = \sum_{r=0}^{n} h^r \Gamma_r, \tag{5}$$

with $\Gamma_0 = JH_0$ and $\Gamma_r = \mathscr{L}\frac{1}{r!}\partial_h^r U^\rho$. The derivatives of the powers of the time evolution are easy to calculate at integer values of the replica index ρ, and the replica limit is taken following an analytical continuation to arbitrary real values. Algebraic and combinatorical manipulations lead to the Floquet Hamiltonian expressed in terms of nested commutators [42]:

$$\Gamma_0 = JH_0 \tag{6a}$$

$$\Gamma_1 = \mathscr{L}\sum_{0\le m<\rho} \tilde{H}_m \tag{6b}$$

$$\Gamma_r = \frac{(-i)^{r-1}}{r!}\mathscr{L}\sum_{0\le m_1\le \dots m_r<\rho} [\tilde{H}_{m_r}, \dots [\tilde{H}_{m_2}, \tilde{H}_{m_1}]]] c_{m_2\dots m_r} \tag{6c}$$

where $\tilde{H}_m = U_0^{-m} H_1 U_0^m$ and $c_{m_2\dots m_r} = \frac{(r-1)!}{n_0! n_1! \dots}$. The expansion can be constructed similarly for different initial phases of the driving, $U' = e^{-iJH_0(1-\varphi)} e^{-ihH_1} e^{-iJH_0\varphi} = e^{-iH_F'}$, which results in the same equations as Eq. (6) except for a simple substitution $\tilde{H}_{m_i} \to \tilde{H}_{m_i+\varphi}$. Our method provides a remarkably simple derivation of the known first order term in Eq. (3) giving a certain degree of confidence in the replica expansion (see [42]). Having established the first main result of this Letter, we now demonstrate its performance in the example of the kicked Ising model in a tilted field [23].

Kicked Ising model.— The time evolution is characterized by time-periodic quenches between the Hamiltonians $H_{0,1}$,

$$H_0 = \sum_i \sigma_i^z \sigma_{i+1}^z \tag{7a}$$

$$H_1 = \sum_i c_\theta \sigma_i^x + s_\theta \sigma_i^z, \tag{7b}$$

where c_θ and s_θ are shorthand notations for $\cos\theta$ and $\sin\theta$. The purpose of introducing the tilt angle is to break the integrability of the model at $\theta = 0$ and $\pi/2$ [43]. Figure 1 shows the performance of the replica expansion for the kicked Ising model in two different limits: when the kick parameter is the magnetic field h, or the Ising interaction J. The spectral norm of the difference between the approximate and exact time evolution operators, $\Delta_n = \|U - U^{(n)}\|$ shown in Figure 1, bounds the accuracy of the expansion for the dynamics of *any observable* A, as $|\langle A\rangle(t)-\langle A\rangle_n(t)|\le 2t\|A\|\Delta_n+\mathscr{O}(\Delta_n^2)$, where $\langle A\rangle(t)$ ($\langle A\rangle_n(t)$) is the expectation value of the observable following t periods with respect to the exact (approximate) time evolution, starting from an arbitrary initial state [44]. As the two cases, kicking with H_0 or H_1, show qualitatively similar behavior, we discuss here only the replica expansion for kicking magnetic field.

The time evolution of kicking Hamiltonian H_1 with respect to unperturbed dynamics H_0 for m periods reads explicitly

$$\tilde{H}_m=\sum_i s_\theta\sigma_i^z-c_\theta\Big(\frac{1}{2}\sin(4mJ)(\sigma_{i-1}^z\sigma_i^y+\sigma_i^y\sigma_{i+1}^z)+\sin^2(2mJ)\sigma_{i-1}^z\sigma_i^x\sigma_{i+1}^z-\cos^2(2mJ)\sigma_i^x\Big), \tag{8}$$

and is the main building block of the replica expansion. The computation of the nested commutators of these objects is trivial, following which one has to deal with the multiple sums and the replica limit. It is convenient to separate the operator part of the expansion from the replica coefficients by expressing $\tilde{H}_m$ in Fourier harmonics as $\tilde{H}_m=\mathscr{O}_0+e^{i4Jm}\mathscr{O}_1+e^{-i4Jm}\mathscr{O}_{-1}$, where

$$\mathscr{O}_0=\sum_i s_\theta\sigma_i^z+\frac{c_\theta}{2}(\sigma_i^x-\sigma_i^z\sigma_{i+1}^x\sigma_{i+2}^z) \tag{9a}$$

$$\mathscr{O}_{\pm1}=\sum_i\frac{c_\theta}{4}[\sigma_i^x+\sigma_i^z\sigma_{i+1}^x\sigma_{i+2}^z\pm i(\sigma_i^z\sigma_{i+1}^y+\sigma_i^y\sigma_{i+1}^z)], \tag{9b}$$

which brings us to the simplest formulation of the replica expansion,

$$\Gamma_1=\sum_{x_1}\mathscr{R}_{x_1}\mathscr{O}_{x_1} \tag{10}$$

$$\Gamma_r=\frac{(-i)^{r-1}}{r!}\sum_{x_1,x_2,\dots,x_r}\mathscr{R}_{x_1x_2\dots x_r}[\mathscr{O}_{x_r},\dots[\mathscr{O}_{x_2},\mathscr{O}_{x_1}]] \tag{11}$$

where $x_i\in\{0,\pm1\}$ and we introduced the replica sum

$$\mathscr{R}_{x_1x_2\dots x_r}=\mathscr{L}\sum_{0\le m_1\le\dots m_r<\rho}e^{i4Jm_1x_1}e^{i4Jm_2x_2}\dots e^{i4Jm_rx_r}c_{m_2\dots m_r}. \tag{12}$$

These sums are evaluated gradually (with attention to the combinatorial factors) as

$$\sum_{m_j=0}^{m_{j+1}-1}m_j^y e^{i\tilde{J}m_j}=\Big(\frac{\partial}{i\partial_{\tilde{J}}}\Big)^y\frac{e^{i\tilde{J}m_{j+1}}-1}{e^{i\tilde{J}}-1}, \tag{13}$$

with $m_{r+1}=\rho$, and $\tilde{J}$ is an integer multiple of $4J$. The prefactor m^y, $0\le y\in\mathbb{N}$ may arise from the previous sum with respect to m_{j-1}, e.g. from the sum of constant terms. This way of evaluating the sums already defines the analytical continuation to arbitrary real values of ρ, allowing one to take the replica limit $\mathscr{L}$. This analytical continuation leads to $\mathscr{L}e^{i\tilde{J}\rho}-1=\log e^{i\tilde{J}}=i\tilde{J}$, which tries to enforce a Floquet Hamiltonian continuous in J at a price of breaking the periodicity $H_F(J)=H_F(J+2\pi)$. Alternatively, one can choose a different branch of the logarithm, e.g. which folds J into the interval $(-\pi,\pi]$ by applying a different analytical continuation [42]. This ambiguity in choosing the branch of the logarithm can be potentially used to further improve the expansion, restore the periodicity in J and eliminate divergences which are discussed below.

The sum is especially simple in the first order correction: $\mathscr{R}_0=0$, $\mathscr{R}_{\pm1}=2J(\cot 2J\mp i)$, yielding

$$\Gamma_1=\sum_i a_+\sigma_i^x+a_-\sigma_{i-1}^z\sigma_i^x\sigma_{i+1}^z+s_\theta\sigma_i^z+c_\theta J(\sigma_{i-1}^z\sigma_i^y+\sigma_i^y\sigma_{i+1}^z) \tag{14}$$

with $a_\pm=c_\theta(J\cot 2J\pm1/2)$.

The second order correction is written in a compact form by noticing that $\mathscr{O}_{\pm1}^\dagger=\mathscr{O}_{\mp1}$ and $\mathscr{R}_{x_1,x_2}^*=\mathscr{R}_{-x_1,-x_2}$,

$$\Gamma_2=\frac{-i}{2}\{(\mathscr{R}_{10}-\mathscr{R}_{01})[\mathscr{O}_0,\mathscr{O}_1]+\mathscr{R}_{1-1}[\mathscr{O}_{-1},\mathscr{O}_1]\}+\text{h.c.} \tag{15}$$

The replica coefficients are evaluated as

$$\mathscr{R}_{10}-\mathscr{R}_{01}=(1-2J\cot 2J)(1+i\cot 2J) \tag{16}$$

$$\mathscr{R}_{1-1}=\frac{1}{2}-i\frac{\sin 4J-4J}{4\sin^2 2J}, \tag{17}$$

which finally yields

$$\Gamma_2=\sum_i c_\theta a_-(\sigma_i^y\sigma_{i+1}^x\sigma_{i+2}^z+\sigma_i^z\sigma_{i+1}^x\sigma_{i+2}^y)-s_\theta a_-[\sigma_i^y+\sigma_i^z\sigma_{i+1}^y\sigma_{i+2}^z+\cot 2J(\sigma_i^x\sigma_{i+1}^z+\sigma_i^z\sigma_{i+1}^x)]+(b+c)\sigma_i^z\sigma_{i+1}^x\sigma_{i+2}^x\sigma_{i+1}^z-b\sigma_i^y\sigma_{i+1}^y-c\sigma_i^z\sigma_{i+1}^z. \tag{18}$$

The coefficients are $b=\frac{c_\theta^2}{8}\frac{4J\cos 4J-\sin 4J}{\sin^2 4J}$ and $c=\frac{c_\theta^2}{4}\frac{4J-\sin 4J}{\sin^2 4J}$. The higher order corrections can be calculated similarly [42].

Resonances.— Notice that the first order correction diverges near $J_{k,1}=k\pi/2$, which was identified as a signal of a heating (or nonergodicity–ergodicity) transition in a different spin model [24], similar to the divergence of high-temperature expansion signaling phase transition in statistical physics. The source of this divergence is easily identified as the zero of the denominator in Eq. (13). Similar to the high frequency expansion, the higher order corrections become less and less local due to the increasing number of commutators. The degree of divergence at $J_{k,1}$ also increases with the order, as the denominators from the consecutive sums become multiplied, and it can also increase because of the derivative in Eq. (13), leading to a divergence $\sim|J-k\pi/2|^{-r}$ at the r^{th} order of expansion. Additional lower order divergences may appear at $J_{k,m}=k\pi/2m$, $m=1\dots r$. Consider e.g. the replica sum $\mathscr{R}_{11}=2J(\cot 4J-i)$ appearing in the second order expansion, which diverges at $J_{k,2}=k\pi/4$. Many of these possible divergences do not enter the expansion because of the vanishing commutators in the operator part or due to cancellations, e.g. $[\mathscr{O}_1,\mathscr{O}_1]=0$, $[\mathscr{O}_1,[\mathscr{O}_1,\mathscr{O}_0]]=0$, etc. For instance, the divergence at $k\pi/4$ only appears at the 5^{th} order of the expansion, see Figure 1. In spite of the cancellations we conjecture that *in the thermodynamic limit* new divergences keep appearing in increasing orders similar to the dual case with interaction kicks (Figure 1(b)), and the expansion blows up near every rational fraction of $\pi/2$ (similar to KAM series). In contrast, we find that *finite-size* systems are characterized by a finite set of resonances $\{J_{k,m_1},\dots J_{k,m_{\max}}\}$, where $m_{\max}\sim L$. For instance, the replica expansion of a two-level system (e.g. a single kicked spin) has a single divergence at $J_{k,m_1}=k\pi$, and no singularities appear at rational fractions.

The stationary expectation value of few-body operators do not show any signature of transition at these resonances in finite-size systems, and it is not clear if these resonances are just an artifact of the expansion, or they herald some hidden physical effect. The divergences restrict the applicability of the replica method to non-resonant frequencies. As shown in Figure 1, at low orders, it can provide an accurate estimate of the Floquet Hamiltonian for an extended range of frequencies, while increasing orders lead to more accurate results inside a narrower domain. That is, given a fixed J, similar to the method introduced in Ref. [20], one can introduce an optimal order of expansion n^*, up to which the corrections increase the accuracy of the approximation of the Floquet Hamiltonian.

Bound on heating.— It is natural to assume that the width of the resonances is proportional to the small parameter h, which is further supported by the analysis of the magnitude of the corrections Γ_r [45]. As an illustration, we give the scaling of the Hilbert-Schmidt norm $\|\Gamma_r\|_{\mathrm{HS}}=\sqrt{\mathrm{Tr}\,\Gamma_r^\dagger\Gamma_r}\sim f_J^r(J-\pi/4)$ near the resonance $\pi/4$,

$$f^r_{\pi/4}(\delta J)=\frac{c_{\pi/4}(r)}{\delta J^{r-4}}+\mathscr{O}(\delta J^{-(r-5)})\,. \tag{19}$$

The r dependence of the prefactor is illustrated in [42]. Up to the highest order we had access to, we found $c_J(r)$ to decrease with r. For our purposes it is enough to assume that it grows at most exponentially $\lesssim\alpha^r$, and we expect that at high orders this exponential growth indeed appears as the asymptote of $c_J(r)$. Then the series $\sum_r\|\Gamma_r\|h^r$ diverges for $\delta J<\alpha h$, which gives the width of the resonances. The optimal order of the expansion is hence estimated by the maximal order at which the closest resonance is located further than $\sim\alpha h$. As the resonances appear at the rational fractions of $\pi/2$, $J=\frac{k\pi}{2m}$, where $m=1,\dots,n$ at the n^{th} order of the expansion, the question is how far one can get in the expansion without having a resonance approaching a fixed J.

Rational approximation of irrational numbers has been thoroughly studied in the mathematical literature [46], and is the cornerstone of the KAM theorem in classical dynamical systems, where the stability of the (quasi)periodic motion to integrability-breaking perturbations depends on the irrationality of the corresponding frequencies. The irrationality of a number is defined by how difficult it is to approximate by rational numbers. The number x is of type (K,ν) if it satisfies $|x-p/q|>Kq^{-\nu}$ for all integer pairs (p,q) [47]. For example, the most irrational number in this sense is the golden ratio, which is of type $(1/\sqrt{5},2)$. Such badly approximable numbers are generic in the sense that for any $\nu>2$, almost all irrational numbers x are of type (K,ν) for some K [46, 47]. In the following we choose a J for which $\frac{2J}{\pi}$ is of type (K,ν), such that

$$\left|J-\frac{k\pi}{2m}\right|=\frac{\pi}{2}\left|\frac{2J}{\pi}-\frac{k}{m}\right|>\frac{\pi}{2}\frac{K}{m^\nu}\,. \tag{20}$$

Hence J is not affected by any resonances as long as $n<n^*$

$$n^*=\left(\frac{\pi K}{2\alpha h}\right)^{\frac{1}{\nu}}, \tag{21}$$

which we set as the optimal order of expansion. By the construction of the expansion,

$$\|U-e^{-iH_F^{(n)}}\|\sim h^{n+1}\,, \tag{22}$$

which gives

$$\|U-e^{-iH_F^{(n^*)}}\|\sim h^{n^*+1}\sim h^{\frac{C}{h^{1/\nu}}}\lesssim e^{-\frac{C'}{h^{1/2-\varepsilon}}} \tag{23}$$

at the optimal order with some constants C, C' and arbitrary $\varepsilon>0$, by choosing ν close enough to 2. Consequently, the Floquet Hamiltonian in the optimal order is conserved for stretched exponentially long time in the inverse kick strength, and, if the steady state is the infinite temperature ensemble, it is approached at least stretched exponentially slowly. We remark that this bound is not sharp, and our analysis does not rule out the possibility of absence of heating in the model. We also stress that the resonances in the replica expansion do not imply heating, but the breakdown of the expansion, which leads to an upper bound on heating. This bound could possibly be improved by a resummation with better convergence properties. We have given an estimate for the accuracy of the replica expansion. We leave a more rigorous mathematical analysis, similar to the ones in Refs. [20, 21], to future work.

Further applications.— It is straightforward to apply the replica expansion not only to spin models but to fermionic or bosonic models as well. An example of a kicked harmonic oscillator is given in the supplemental material [42]. Although we constructed the replica expansion for quantum mechanical systems, similar to the BCH expansion, it can be readily applied to classical systems [38] either by using Hamiltonian vector fields, or by taking the classical limit of the quantum effective Hamiltonian. We compare our expansion to the Birkhoff normal form [48], which, similar to the replica expansion, produces an approximate constant of motion perturbatively in the kick strength [49]. We find that the classical limit of the replica expansion reproduces the Birkhoff normal form Hamiltonian. The higher order resonances hence are not just an arifact of the replica expansion, but they appear in a classical calculation without any reference to the replica trick.

Conclusion.— We have developed a novel expansion applicable to periodically driven systems where the driving consists of sudden quenches between different Hamiltonians. The expansion takes into account all orders in one of the Hamiltonians and is perturbative in the other. As such, it is an infinite resummation of the BCH formula, whose coefficients can be reproduced by taking the derivatives of the terms in the replica expansion [42]. We demonstrated that, similar to the high frequency expansions, the replica expansion is asymptotic for systems with unbounded Hamilton operators, that is, it may not converge, but performs very well when evaluated at an optimal order. In infinite systems the expansion suffers from resonances near rational frequencies, whose avoidance determines the optimal order of expansion, whereas in finite systems the resonances remain sparse, leading to better convergence properties. It is an interesting question whether these resonances have a physical meaning, and whether one could remove the resonances by a proper choice of analytical continuation in the replica trick. Similar structure of resonances appear in classical chaotic systems, which demonstrate the potential of our approach towards buildiing a quantum KAM theory.

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