Suppression of Heating in Quantum Spin Clusters under Periodic Driving as a Dynamic Localization Effect

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We investigate numerically and analytically the heating process in ergodic clusters of interacting spins 1/2 subjected to periodic pulses of an external magnetic field. Our findings indicate that there is a threshold for the pulse strength below which the heating is suppressed. This threshold decreases with the increase of the cluster size, approaching zero in the thermodynamic limit, yet it should be observable in clusters with fairly large Hilbert spaces. We obtain the above threshold quantitatively as a condition for the breakdown of the golden rule in the second-order perturbation theory. It is caused by the phenomenon of dynamic localization.

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The dynamics of many-particle quantum systems under periodic perturbations is a fascinating subject that has recently attracted renewed attention in various contexts. Examples include solid-state nuclear magnetic resonance (NMR) in the presence of a continuously applied radio frequency field [1,2], dynamics of ultracold atoms in the presence of oscillating laser potential [3], responses of electron-nuclear systems to optical pumping [4], Floquet topological insulators [5–7], and laser-driven multiferroics [8]. Periodic driving of qubit systems is also involved in proposals to engineer quantum simulators [9]. An important fundamental issue in this general context is to identify peculiarly quantum behavior under periodic driving [10]. A relevant quantum phenomenon here is dynamic localization (DL), which is the time-domain analog of Anderson localization [11–13]. DL is well understood for systems with one or a few degrees of freedom, such as a kicked quantum rotator [14–21]. The current effort is to understand the applicability of DL to many-particle systems.

DL in many-particle systems, if it occurs, would imply that the system stops absorbing energy, which, in turn, would be contrary to the continuous absorption picture based on the standard linear response theory [22]. On the other hand, the absence of the continuous energy absorption is often implied when the system is subjected to fast and strong periodic driving. In this case, the often-used framework is the average Hamiltonian theory, which can be justified by the Magnus expansion [23], which, in turn, has unclear applicability limits.

A lot of attention in recent years has been focused on the response of systems with strong spatial disorder to periodic driving [24–26]. Various studies [27–31] converged to the conclusion that systems that exhibit many-body localization without periodic driving can also exhibit many-body dynamical localization under periodic driving, when the driving strength is not too large. We, on the other hand, are primarily interested in the periodic driving of the systems, which are ergodic (i.e., thermalizable) without driving.

If one takes an ergodic isolated many-particle quantum system and starts kicking it, then one would reasonably expect (on the basis of the second law of thermodynamics) that the system absorbs energy after each kick, and therefore, the temperature of the system gradually increases without any limitation from above. If the time delay between the kicks is very long, one should further expect that it does not matter whether the kicks are strictly periodic in time or not. However, it has been shown in our previous numerical investigation that, surprisingly, the latter expectation does not hold for a system containing 16 spins 1/2 [32]. We found that the heating caused by the periodic kicks with very long delays was asymptotically much slower than that caused by slightly aperiodic kicks. We attributed the above difference to DL. The system of 16 spins 1/2 has 2^{16} quantum levels, leading one to suspect that the above quantum effects might survive in the thermodynamic limit. Later studies, however, arrived at the conclusion that the weak periodic driving of macroscopic ergodic systems leads to stationary states essentially indistinguishable from the infinite temperature state [27,33]. Such a conclusion is also supported in the present Letter. Yet, even in such a case, a practically important question remains concerning the size dependence of the DL effects. This question has also been discussed in the literature [34], but so far no quantitative criterion for the onset of dynamical localization as a function of the system size and the strength of the perturbation has been formulated. The present Letter aims at filling this gap. We develop a golden-rule-like theory of heating under the periodic driving and formulate the

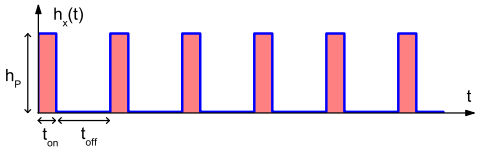

FIG. 1. Schematic plot of magnetic field pulses.

condition for the breakdown of that theory as a function of cluster size and perturbation strength. We verify this criterion by direct numerical simulations. The above breakdown is accompanied by the emergence of quantum corrections that can be detected through the suppression of heating under periodic driving when compared with aperiodic driving. We propose that the above difference can be used in practice to diagnose the sizes of quantum nanoclusters.

We consider a quantum spin-1/2 XXZ chain subjected to periodic pulses of external magnetic field. The system is governed by the Hamiltonian

$$\mathcal{H}(t) = \sum_{i=1}^{N_s} (J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) + \sum_{i=1}^{N_s} h_i^z S_i^z + h_x(t) \sum_{i=1}^{N_s} S_i^x, \quad (1)$$

where N_s is the total number of spins, $S_i^\alpha (\alpha = x, y, z)$ are the spin operators on the ith lattice site, and J_α are the nearest-neighbor coupling constants with values $J_x = J_y = -1$ and $J_z = 2$ chosen such as to mimic the NMR experiments in solids [1], h_i^z are the small static magnetic fields randomly chosen from the interval $(-0.2, 0.2)$, and finally, $h_x(t)$ is the external magnetic field along the x direction, which is switched on with the large amplitude $h_P = 10$ for a very short time $t_{on} \sim 0.01$ and then switched off for a very long time $t_{off} \sim 100$—see the sketch in Fig. 1. We set $\hbar = k_B = 1$.

The above setting is such that, during each pulse, the perturbation term dominates the dynamics; yet, due to the very small duration of the pulse, the overall effect of the perturbation is very small ($h_P t_{on} \ll 1$). We have used a similar setting in Ref. [32]. The only difference now is the addition of small disordered local fields h_i^z, which break the translational invariance of the Hamiltonian and hence make the entire Hilbert space of 2^{N_s} states connected by the perturbation. In Ref. [32] the size of the connected blocks in the Hilbert space was smaller than 2^{N_s} by a factor of roughly N_s, which created conditions more favorable to DL [35].

Following Ref. [32], let us illustrate the DL effect by comparing the heating process in our system under periodic and aperiodic pulses. We do this by exactly diagonalizing the Hamiltonian (1) up to 16 spins. Figure 2 presents the evolutions of average energy E_{av} per spin for spin chains of different length initially put either in the ground state of

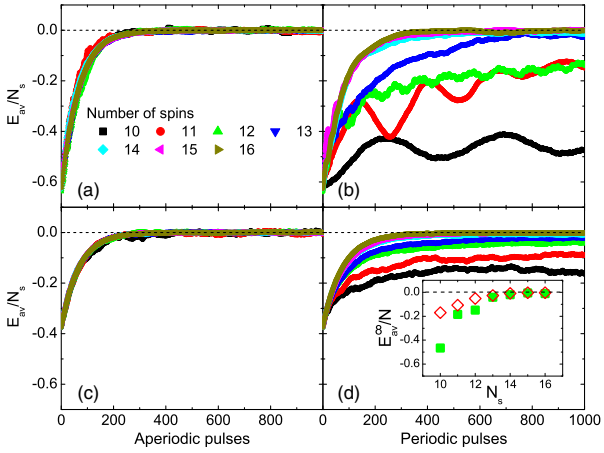

FIG. 2. Average energy per spin for (a),(c) aperiodic and (b),(d) periodic pulse sequences. The initial state in panels (a) and (b) is the ground state; in panels (c) and (d) it is the thermal state with $T = 1$. The inset in (d) shows the asymptotic long-time values of E_{av}/N_s under periodic driving from the ground state (green squares) and the thermal state (red diamonds).

Hamiltonian $\mathcal{H}_{off}$ [Figs. 2(a) and 2(b)], or in the thermal state [35] with temperature $T = 1$ [Figs. 2(c) and 2(d)]. Figures 2(a) and 2(c) present respective results for a series of slightly aperiodic pulses with t_{off} randomly chosen in the range 100 ± 10. In this case, the heating processes for different N_s all exhibit the same heating per spin towards the infinite temperature limit. In contrast, significant differences between different N_s arise in Figs. 2(b) and 2(d) representing the behavior under periodic driving. In particular, we see that the infinite temperature regime associated with $E_{av}/N_s = 0$ is not reached by clusters of size $N_s = 13$ and below.

In the rest of this Letter, we develop a theory of the above DL effect. We only consider periodically pulsed $h_x(t)$ with period $\mathcal{T} \equiv t_{on} + t_{off}$, where $t_{off} = 100$.

Let us denote the initial wave function as Ψ_0. After applying n periodic pulses, the system evolves to a state $\Psi_n = U(\mathcal{T})^n \Psi_0$, where $U(\mathcal{T})$ is the time evolution operator, which is related to a time-independent effective Floquet Hamiltonian $\mathcal{H}_{eff}$ as

$$U(\mathcal{T}) = e^{-i\mathcal{H}_{off} t_{off}} e^{-i\mathcal{H}_{on} t_{on}} \equiv e^{-i\mathcal{H}_{eff}\mathcal{T}}, \quad (2)$$

where $\mathcal{H}_{on}$ and $\mathcal{H}_{off}$ correspond to Hamiltonian (1) with $h_x = h_P$ and $h_x = 0$, respectively. We also introduce Floquet phase operator $\Phi \equiv \mathcal{H}_{eff}\mathcal{T}$, confining its eigenvalues ϕ_μ in the range of $[0, 2\pi)$, and then define the Floquet *quasienergies* (eigenvalues of $\mathcal{H}_{eff}$) as $\{\varepsilon_\mu \equiv \phi_\mu/\mathcal{T}\}$, which fall into the "first Floquet zone" $[0, E_F)$, where $E_F \equiv 2\pi/\mathcal{T}$.

Let us now describe qualitatively the situation of "normal" heating. In this case, an initial eigenstate φ_0 of the Hamiltonian $\mathcal{H}_{off}$ with eigenenergy E_0 becomes

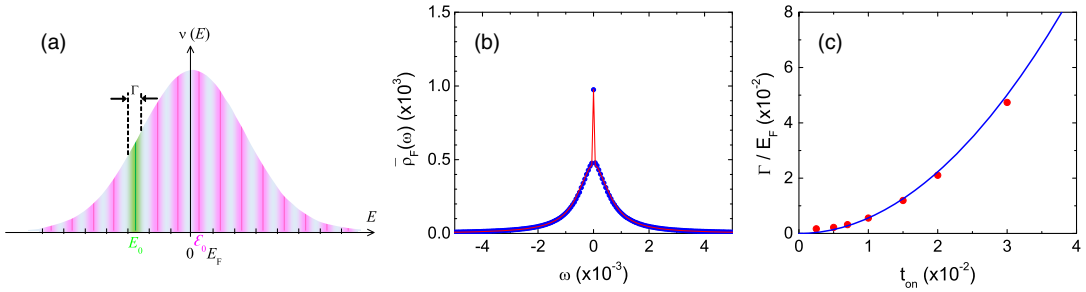

FIG. 3. (a) Schematic plot of the density of energy states $\nu(E)$ for $\mathcal{H}_{\rm off}$ with the indication of energy bands of width Γ coupled to the initial eigenstate of energy E_0 in the process of normal heating by periodic pulses. Adjacent bands are separated by energy E_F. (b) Average spectral density $\bar{\rho}_F(\omega)$ (blue dots) for a chain of 14 spins periodically driven by pulses with $t_{\rm on} = 0.02$ and $t_{\rm off} = 100$. The red line is the fit by the BW distribution and a δ-function peak at $\omega = 0$. (c) BW width Γ for a 14-spin chain with $t_{\rm off} = 100$ and different $t_{\rm on}$. The red circles are obtained numerically from $\bar{\rho}_{\rm F}(\omega)$; the blue line is from Eq. (3).

effectively coupled to other eigenstates φ_k of $\mathcal{H}_{\rm off}$, with eigenenergies E_k forming narrow bands around values $E_0 + nE_F$, where n is an integer number [see Fig. 3(a)]. The width of these bands Γ is simultaneously the inverse lifetime of the initial eigenstate φ_0 under the periodic perturbation, and it also controls the heating rate. In the Floquet theory, one can consider the spectral density $\rho_F(\omega) \equiv \sum_\mu |\langle\varphi_0|\psi_\mu\rangle|^2 \delta(\omega + \mathcal{E}_0 - \varepsilon_\mu)$ associated with the decomposition of the initial state φ_0 in terms of Floquet eigenstates ψ_μ [36,37]. Here $\mathcal{E}_0 \equiv E_0 \bmod E_F$. The shape of this spectral density can be well approximated by the Breit-Wigner (BW) formula, $\rho_F(\omega) = (1/2\pi)\Gamma/(\omega^2 + \Gamma^2/4)$. In Fig. 3(b), we show the above spectral density averaged over all eigenstates of $\mathcal{H}_{\rm off}$, $\bar{\rho}_F$, for a 14-spin chain. It can be perfectly fitted by a superposition of a δ-function peak at $\omega = 0$ (originating from uninteresting diagonal terms in the perturbation) and the BW distribution. At the same time, it can be shown analytically from a golden-rule-like calculation [35] that, in our setting, the value of Γ averaged over all initial eigenstates is

$$\Gamma = \frac{h_P^2 t_{\rm on}^2 N_s}{4\mathcal{T}}. \tag{3}$$

In Fig. 3(c), we compare the analytical result (3) with the value of Γ extracted from the numerically computed $\bar{\rho}_F$ for various $t_{\rm on}$ and find a very good agreement.

In the Floquet picture, the process of heating for the initial wave function φ_0 is simply the dephasing between different Floquet eigenstates participating in the expansion of φ_0. The participating Floquet eigenstates can, in turn, be decomposed into the eigenstates of the Hamiltonian $\mathcal{H}_{\rm off}$, forming the energy bands shown in Fig. 3(a), which sample the entire $\nu(E)$. As a result, the participating eigenstates of $\mathcal{H}_{\rm off}$ fairly represent the infinite-temperature state, even through they constitute only a small fraction Γ/E_F of all eigenstates of $\mathcal{H}_{\rm off}$.

In general, only a minority of the eigenstates of $\mathcal{H}_{\rm off}$ belonging to the above mentioned energy bands are directly coupled to φ_0 by the perturbation $\mathcal{H}_P \equiv h_x(t) \sum_{i=1}^{N_s} S_i^x$. At the same time, only the minority of the eigenstates of $\mathcal{H}_{\rm off}$ directly coupled to φ_0 would belong to the above energy bands. We formulate the criterion for the normal heating as a self-consistency condition on the validity of the golden-rule formula (3) for the BW width. Namely, in order for the normal heating to occur, it is necessary that, for a typical eigenstate φ_0 of Hamiltonian $\mathcal{H}_{\rm off}$, there be at least one other eigenstate φ_1 (with energy E_1) directly coupled to φ_0 by a typical perturbation matrix element, such that $\mathcal{E}_1 \equiv E_1 \mod E_F$ falls within the window $\mathcal{E}_0 \pm \Gamma/2$, where Γ is obtained from the golden-rule formula (3).

We then associate the onset of DL with the violation of the above criterion; i.e., DL sets in when the golden-rule-predicted Γ is too small, and as a result, none of the eigenstates of $\mathcal{H}_{\rm off}$ directly coupled to a typical φ_0 falls, after backfolding to the first Floquet zone, into the BW window $\mathcal{E}_0 \pm \Gamma/2$.

The above DL criterion addresses typical eigenstates of $\mathcal{H}_{\rm off}$. Therefore, it is applicable to the initial conditions close to the infinite-temperature limit, where the density of states of $\mathcal{H}_{\rm off}$ is the highest, and hence the tendency to DL is the weakest. From this perspective, the criterion is, certainly, a sufficient condition for the onset of DL at lower temperatures. It is also possibly the necessary condition [35]: In finite clusters with ergodic Hamiltonians, if the analog of our DL criterion is satisfied for low-temperature states φ_0, but high-temperature states are dynamically delocalized, then low-temperature states are still likely to "leak" to the high-temperature range due to the higher-order effects of the perturbations by $\mathcal{H}_{\rm on}$ not included in the second-order perturbation theory behind Eq. (3). In this scenario, the stronger tendency to DL at lower temperatures only delays the onset of normal heating during the *prethermalization* stage [34,38–44].

Let us now apply the above criterion to the spin system described by Hamiltonian (1). Since both $\mathcal{H}_{\rm off}$ and $\mathcal{H}_{\rm P}$ are local in the sense that they are sums of local terms, the perturbation $\mathcal{H}_{\rm P}$ does not have significant matrix elements

coupling the eigenstates of $\mathcal{H}_{\rm off}$ separated by an energy much larger than a typical one-particle energy of $\mathcal{H}_{\rm off}$, which can be estimated as the root-mean-squared value of the local field: $h_{\rm rms} = [N_{NN}(J_x^2\langle S_x^2\rangle + J_y^2\langle S_y^2\rangle + J_z^2\langle S_z^2\rangle)]^{1/2} = \sqrt{3}$, where $N_{NN} = 2$ is the number of nearest neighbors for each spin. If we represent $\mathcal{H}_{\rm P}$ in the eigenbasis of an ergodic Hamiltonian $\mathcal{H}_{\rm off}$, we expect to get a band random matrix which has its nonzero elements located within a diagonal band with a typical half-width of $h_{\rm rms}$. For our spin system, the total number of states per unit energy interval, $\mathcal{N}$, can be approximated as a Gaussian, $\mathcal{N}(E) \approx (2^{N_s}/\sqrt{2\pi}\sigma_E)\exp(-E^2/2\sigma_E^2)$, where $\sigma_E \approx [N_s N_{NN}(J_x^2\langle S_{ix}^2\rangle\langle S_{jx}^2\rangle + J_y^2\langle S_{iy}^2\rangle\langle S_{jy}^2\rangle + J_z^2\langle S_{iz}^2\rangle\langle S_{jz}^2\rangle)]^{1/2} = \sqrt{3N_s}/2$ is the root-mean-squared value of the total energy. Thus, the relative number of nonzero matrix elements of $\mathcal{H}_{\rm P}$ in the eigenbasis of $\mathcal{H}_{\rm off}$ can be estimated as $h_{\rm rms}/\sigma_E = 2/\sqrt{N_s}$.

Since the Hamiltonian $\mathcal{H}_{\rm off}$ is time independent, it can also be considered as being periodic with period $\mathcal{T}$. The perturbation problem can now be treated in the Floquet quasienergy representation. After the eigenenergies E_k of $\mathcal{H}_{\rm off}$ are folded into the first Floquet zone using relation $\mathcal{E}_k \equiv E_k \bmod E_F$, and then the respective eigenstates are ordered according to the value of $\mathcal{E}_k$, the perturbation $\mathcal{H}_{\rm P}$ becomes a sparse random matrix, where the nonzero elements are uniformly distributed over the entire matrix. This is because $h_{\rm rms} \gg E_F$. Thus, in each column (or line) of the matrix $\mathcal{H}_{\rm P}$, the total number of nonzero elements is $N_V \approx 2^{N_s} \times 2/\sqrt{N_s}$. Thus, in the first Floquet zone, the typical distance between the quasienergies of two unperturbed neighboring states coupled by nonzero elements of $\mathcal{H}_{\rm P}$ is

$$\Delta\mathcal{E} \approx \frac{E_F}{N_V} = \frac{E_F\sqrt{N_s}}{2^{N_s}\times 2}. \tag{4}$$

According to our criterion, normal heating takes place when, for a typical unperturbed state φ_0, the energy window $\mathcal{E}_0 \pm \Gamma/2$ contains at least one other state φ_1 directly coupled to φ_0. This implies the condition $\Gamma/\Delta\mathcal{E} \geq 2$, from which, using Eqs. (3) and (4), we find the threshold value

$$t_{\rm on} = \frac{2}{h_{\rm P}}\sqrt{\frac{2\pi}{2^{N_s}\sqrt{N_s}}}. \tag{5}$$

To test the crossover criterion (5), we numerically calculate the asymptotic average energy in the long-time limit [35] $E_{\rm av}^{\infty} \equiv \sum_\mu |\langle\varphi_0|\psi_\mu\rangle|^2\langle\psi_\mu|\mathcal{H}_{\rm off}|\psi_\mu\rangle$ for different $t_{\rm on}$ and N_s with different initial wave functions φ_0. Each φ_0 represents an eigenstate of $\mathcal{H}_{\rm off}$ with energy $E_{\rm av}^0 \equiv \langle\varphi_0|\mathcal{H}_{\rm off}|\varphi_0\rangle$. In Fig. 4(a), the ratio $E_{\rm av}^{\infty}/E_{\rm av}^0$ averaged over a representative ensemble is plotted as a function of $t_{\rm on}$. The ensemble consists of three statistical samples, each

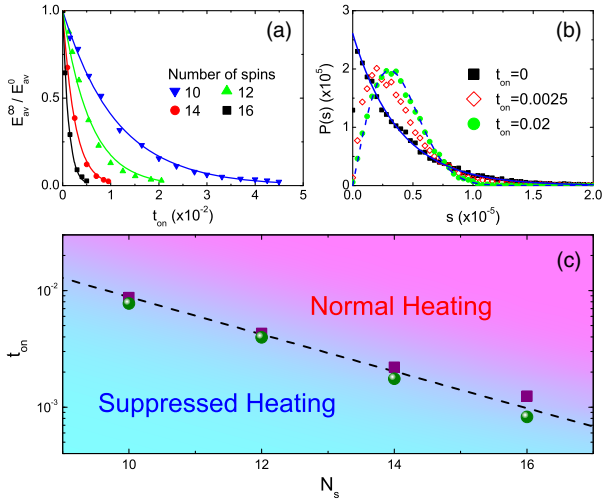

FIG. 4. (a) Ratio $E_{\rm av}^{\infty}/E_{\rm av}^0$ under periodic driving for different N_s as a function of $t_{\rm on}$ averaged over the ensemble of initial states, which are single eigenstates of $\mathcal{H}_{\rm off}$ [35]. Symbols show numerical results; lines denote exponential fits. (b) Probability distributions of spacings s between Floquet quasienergies for a 14-spin chain with different $t_{\rm on}$. Blue solid line: Poission distribution. Blue dashed line: Wigner-Dyson distribution. (c) Phase diagram of the crossover from normal to suppressed heating as a function of the pulse duration $t_{\rm on}$ and the number of spins N_s. Dashed line: Critical condition given by Eq. (5). Symbols are obtained numerically by the condition $E_{\rm av}^{\infty}/E_{\rm av}^0 = 0.5$. Green balls are obtained from panel (a); purple squares are obtained for the initial thermal state with $T = 1$.

including ~1% of 2^{N_s} eigenstates of $\mathcal{H}_{\rm off}$ with the initial $E_{\rm av}^0$ selected in the vicinity of three energies $\frac{1}{4}E_g$, $\frac{1}{2}E_g$, and E_g, where E_g is the (negative) energy of the ground state. With such a choice, we avoid large statistical noise near $E_{\rm av}^0 = 0$. We find that all three samples exhibit nearly the same dependence of $E_{\rm av}^{\infty}/E_{\rm av}^0$ on $t_{\rm on}$ [35], which implies that this dependence is representative of a larger ensemble of randomly chosen initial eigenstates of $\mathcal{H}_{\rm off}$. In turn, the ratio $E_{\rm av}^{\infty}/E_{\rm av}^0$ for the latter characterizes the heating process close to $T = \infty$.

For each N_s in Fig. 4(a), the ratio $E_{\rm av}^{\infty}/E_{\rm av}^0$ decreases nearly exponentially with increasing $t_{\rm on}$. Normal heating corresponds to $E_{\rm av}^{\infty}/E_{\rm av}^0 = 0$, while completely suppressed heating means $E_{\rm av}^{\infty}/E_{\rm av}^0 = 1$. We then define the value of $t_{\rm on}$ for the crossover between normal heating and DL as the one giving $E_{\rm av}^{\infty}/E_{\rm av}^0 = 0.5$, and we plot this value as a function of N_s in Fig. 4(c). The result exhibits a good agreement with the analytical criterion (5) plotted as a line in Fig. 4(c). Also plotted in Fig. 4(c) are the results for the ensemble of initial thermal states with $T = 1$ [35]. In accordance with our earlier discussion, we attribute the small difference between the results for $T = 1$ and $T = \infty$ to the longer pretherm-alization stage expected for finite temperatures [35].

An additional piece of evidence that the above suppression of heating is related to DL is the statistics of spacings s

between adjacent Floquet quasienergies. In Fig. 4(b), we plot the statistics for $N_s = 14$ and three values of t_{on} across the crossover from the normal heating to the suppressed heating, and we observe the simultaneous crossover from the Wigner-Dyson to the Poisson statistics.

The threshold (5) for the suppression of heating can be used to determine the number of spins in a nanocluster. For a finite cluster, by changing either t_{on} or the perturbation strength, one can observe the onset of significant differences of the heating response of the system to periodic and aperiodic perturbations of equal strengths, and then estimate N_s using Eq. (5). Given the exponential dependence on N_s in Eq. (5), such an estimate is supposed to be quite accurate.

In conclusion, we formulated the criterion for the onset of quantum suppression of heating in finite clusters, tested this criterion numerically, and illustrated that it is related to the phenomenon of DL. We further proposed that it can be used to diagnose the size of finite spin clusters. Our criterion should be generalizable to a broader class of systems and perturbations.

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