## Anomalous Behavior of Magnetic Susceptibility Obtained by Quench Experiments in Isolated Quantum Systems

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We examine how the magnetic susceptibility obtained by the quench experiment on isolated quantum systems is related to the isothermal and adiabatic susceptibilities defined in thermodynamics. Under the conditions similar to the eigenstate thermalization hypothesis, together with some additional natural ones, we prove that for translationally invariant systems the quench susceptibility as a function of wave vector  $\mathbf{k}$ is discontinuous at k=0. Moreover, its values at k=0 and the  $k\to 0$  limit coincide with the adiabatic and the isothermal susceptibilities, respectively. We give numerical predictions on how these particular behaviors can be observed in experiments on the XYZ spin chain with tunable parameters, and how they deviate when the conditions are not fully satisfied.

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Introduction.—Ultracold atoms [1,2] and molecules [3–5] in optical lattices offer nearly ideal playgrounds for studying quantum many-body systems experimentally. Various model systems [6-21] are realized on the optical lattices with various geometry [22–27] and with tunable physical parameters [2,28–31]. Furthermore, one can isolate the systems from the environments over a reasonably long period, which enables the direct observation of the dynamics of isolated quantum systems induced by suddenly changing a physical parameter [32–38]. After this socalled quench, the system often relaxes to a steady state, where the expectation values of local observables become almost time independent [21,39-44]. The nature of such a steady state has been discussed in terms of the eigenstate thermalization hypothesis (ETH) [45–56]. For example, if the "strong" ETH is satisfied, the steady state is an equilibrium state [45–51].

In this Letter, we study the susceptibility obtained by the quench experiment, and explore whether or not it coincides with a thermodynamic susceptibility. This problem is highly nontrivial since there are two kinds of thermodynamic susceptibilities, the isothermal and the adiabatic ones, which take different values. In other words, it is not even clear which thermodynamic susceptibilities should be compared with the quench one. Furthermore, the wave number dependences of these susceptibilities make the problem more nontrivial, as we will reveal in this paper.

To be concrete, we consider the magnetic susceptibility of a quantum spin system. Suppose that the initial equilibrium state is in a uniform "offset" magnetic field h, and a weak extra magnetic field of wave number k is suddenly applied. The quench susceptibility  $\gamma^{\text{qch}}(k)$  is defined as the rate of magnetization change induced by such a quench. We

explore its relation to the isothermal and the adiabatic thermodynamic susceptibilities,  $\chi^T(\mathbf{k})$  and  $\chi^S(\mathbf{k})$ , in the case where  $\chi^T(\mathbf{0}) > \chi^S(\mathbf{0})$ , which occurs when  $h \neq 0$ .

We reveal that  $\chi^{qch}(k)$  is discontinuous at k=0 as a function of k. Because of this discontinuity, both thermodynamic susceptibilities are obtained from the quench one, as  $\chi^{\text{qch}}(\mathbf{0}) = \chi^S(\mathbf{0})$  and  $\lim_{k\to \mathbf{0}} \chi^{\text{qch}}(k) = \chi^T(\mathbf{0})$ . The proof requires the conditions similar to the ETH, which hold when the dynamics of the system is complicated enough, as well as the natural conditions that are satisfied except at a phase transition point.

Furthermore, we numerically demonstrate how such anomalous behaviors should be observed in experiments on an isolated quantum spin system when it is nonintegrable. We also predict how the deviation from these behaviors is observed when the physical parameters of the system are tuned so that it becomes integrable.

Setup.—We deal with a quantum spin-1/2 system on a ddimensional cubic lattice  $\Omega_N$  with linear size L and  $N = L^d$ spins. The periodic boundary conditions and the invariance under the discrete spatial translations are assumed for the prequench Hamiltonian  $\hat{H}(h)$ , where h denotes the uniform offset magnetic field. The density matrix of the initial state is chosen as the canonical Gibbs one,  $\hat{\rho}_{\rm ini}=e^{-\beta\hat{H}(h)}/Z$  [57]. We are interested in the quantum quench process where

the additional magnetic field  $\Delta h(\mathbf{r})$ , with wave number  $\mathbf{k}$ and small magnitude  $\Delta h_k$ , is suddenly applied at t=0. At t > 0, the isolated system obeys the Schrödinger dynamics of the postquench Hamiltonian,  $\hat{H}(h) - \sum_{r \in \Omega_N} \hat{\sigma}^z_r \Delta h(r)$ , where  $\hat{\sigma}_r^{\alpha}$  ( $\alpha = x, y, z$ ) is the Pauli operator on site  $r \in \Omega_N$ . For simplicity, we assume that  $\Delta h(\mathbf{r})$  is parallel to the offset field h, pointing in the z direction. While the previous works regarding the quantum quench focused only on the final state, we here study the quench susceptibility,

$$\chi_N^{\rm qch}(\boldsymbol{k}) \coloneqq \lim_{T \to \infty} \lim_{\Delta h_k \to 0} \frac{\overline{{\rm Tr}[\hat{\rho}(t)\hat{m}_k]}^T - {\rm Tr}[\hat{\rho}_{\rm ini}\hat{m}_k]}{\Delta h_k}, \quad (1)$$

which quantifies the *difference* of the expectation values of the k component of magnetization,  $\hat{m}_k = (1/N) \sum_{r \in \Omega_N} e^{-ik \cdot r} \hat{\sigma}_r^z$ , between the final and the initial states. Here,  $\hat{\rho}(t)$  is the density matrix at time t, and  $\overline{f(t)}^T$  denotes the time average of f(t) over  $0 \le t \le T$ .

For comparison, we consider the isothermal and the adiabatic thermodynamic susceptibilities,  $\chi_N^T(k)$  and  $\chi_N^S(k)$ , which are defined via the quasistatic processes with constant temperature and entropy, respectively. At k=0, they satisfy

$$\chi_N^S(\mathbf{0}) = \chi_N^T(\mathbf{0}) - \frac{T}{c_h} \left[ \left( \frac{\partial m_\mathbf{0}}{\partial T} \right)_h \right]^2,$$
 (2)

where  $c_h$  is the specific heat at constant magnetic field and  $T=1/\beta$  is the temperature [61]. We assume  $0 < T < +\infty$ , and exclude phase transition points where  $c_h$  diverges as  $N \to \infty$  and the case where  $(\partial m_0/\partial T)_h$  vanishes, which is indeed unlikely for  $h \neq 0$ . This leads to the most interesting situation where the two susceptibilities take different values even in the thermodynamic limit,

$$\chi_{\infty}^{S}(\mathbf{0}) < \chi_{\infty}^{T}(\mathbf{0}), \tag{3}$$

where  $\chi_{\infty}^{\bullet}(\mathbf{k}) := \lim_{N \to \infty} \chi_{N}^{\bullet}(\mathbf{k})$ .

Main results.—Our main results are summarized as follows.

(i) The k = 0 value of the quench susceptibility agrees with that of the adiabatic one:

$$\chi_{\infty}^{\text{qch}}(\mathbf{0}) = \chi_{\infty}^{S}(\mathbf{0}), \tag{4}$$

if and only if condition (8), which is similar to but different from the ordinary ETH, is satisfied. Although the quench increases entropy, this equality implies it is irrelevant to  $\chi^{\rm qch}_{\infty}(\mathbf{0})$  [61]. By contrast, the quench induces relevant changes in energy and temperature [61], which results in  $\chi^{\rm qch}_{\infty}(\mathbf{0}) < \chi^T_{\infty}(\mathbf{0})$ .

(ii) The  $k \neq 0$  value of the quench susceptibility agrees with those of the adiabatic and the isothermal ones [65],

$$\chi^{\text{qch}}_{\infty}(\mathbf{k}) = \chi^{S}_{\infty}(\mathbf{k}) = \chi^{T}_{\infty}(\mathbf{k})$$
 for all  $\mathbf{k} \neq \mathbf{0}$ , (5)

if and only if condition (10), which is similar to but weaker than the ordinary "off-diagonal" ETH [44,49–51], is satisfied

(iii) The isothermal susceptibility,  $\chi_{\infty}^{T}(\mathbf{k})$ , is uniformly continuous as a function of  $\mathbf{k}$  [66] under two conditions

(12) and (13) regarding the spatial spin-spin correlation function, both of which are fulfilled in normal systems.

(iv) When the conditions for (ii) and (iii), [namely, Eqs. (10), (12) and (13)] are all satisfied,

$$\lim_{k \to \mathbf{0}} \chi_{\infty}^{\text{qch}}(k) = \lim_{k \to \mathbf{0}} \chi_{\infty}^{T}(k) = \chi_{\infty}^{T}(\mathbf{0}).$$
 (6)

This also shows that  $\chi^{\rm qch}_{\infty}(k)$  is discontinuous at k=0 because  $\chi^{\rm qch}_{\infty}(\mathbf{0}) < \chi^T_{\infty}(\mathbf{0})$  as seen from the thermodynamic inequality (3) [69] and the general relation [61],

$$\chi_N^{\text{qch}}(\mathbf{0}) \le \chi_N^S(\mathbf{0}). \tag{7}$$

(v) These results can be confirmed by a series of experiments in the isolated quantum systems, e.g., ultracold atoms, which simulate the XYZ spin chain. We predict the dependence of the above susceptibilities on k, N, and the exchange coupling parameters,  $J_x$ ,  $J_y$ ,  $J_z$ .

exchange coupling parameters,  $J_x$ ,  $J_y$ ,  $J_z$ . Condition for (i).—We introduce  $\hat{m}_k^0 := \lim_{T \to \infty} \overline{e^{i\hat{H}(h)t}} \hat{m}_k e^{-i\hat{H}(h)t}^T$ , which is the energy-diagonal part of  $\hat{m}_k$  [61]. Let  $|\nu\rangle$  be the simultaneous eigenstate of  $\hat{H}(h)$ , the translation operators, and  $\hat{m}_{k=0}^0$ , with eigenenergy  $E_{\nu}$  and crystal momentum  $K_{\nu}$ . We also introduce  $\delta\hat{\sigma}_r^z = \hat{\sigma}_r^z - \text{Tr}[\hat{\rho}_{\text{ini}}\hat{\sigma}_r^z]$  and  $\delta E_{\nu} = E_{\nu} - \text{Tr}[\hat{\rho}_{\text{ini}}\hat{H}(h)]$ . Then, we obtain the necessary and sufficient condition for (i) in the following form [61]: For almost all  $|\nu\rangle$  in a narrow energy region  $|\delta E_{\nu}| \lesssim T\sqrt{c_h N}$ , the diagonal elements  $\langle \nu | \delta\hat{\sigma}_0^z | \nu \rangle$  are related almost linearly with  $\delta E_{\nu}$  as

$$\langle \nu | \delta \hat{\sigma}_{\mathbf{0}}^{z} | \nu \rangle = C \delta E_{\nu} / N + o(1/\sqrt{N}),$$
 (8)

where  $C=\mathcal{O}(1)$  is some constant independent of  $\nu$  [70]. This is similar to but different from the ordinary two forms of ETH in the following points. The ordinary strong ETH [48–51] requires more stringently that  $all\ \langle\nu|\hat{\sigma}_0^z|\nu\rangle$  behave like a smooth function of  $E_{\nu}/N$ , which is often satisfied in nonintegrable systems [71]. Since a smooth function of  $E_{\nu}/N$  can be regarded as linear within the narrow region  $|\delta E_{\nu}|\lesssim T\sqrt{c_hN}$ , any system satisfying the strong ETH also satisfies condition (8). By contrast, the ordinary weak ETH [53–55] requires only that  $\langle\nu|\delta\hat{\sigma}_0^z|\nu\rangle=o(1)$  for almost all  $\nu$  in the same energy region. For this reason, some models that satisfy the ordinary weak ETH do not satisfy Eq. (8), as will be demonstrated shortly.

Demonstration of (i).—We now demonstrate how result (i) can be observed in experiments on the XYZ spin chain, which has the prequench Hamiltonian,

$$\hat{H}(h) = -\sum_{j=0}^{N-1} \sum_{\alpha = x, y, z} J_{\alpha} \hat{\sigma}_{j}^{\alpha} \hat{\sigma}_{j+1}^{\alpha} - \sum_{j=0}^{N-1} h \hat{\sigma}_{j}^{z}, \qquad (9)$$

with periodic boundary condition,  $\hat{\sigma}_N = \hat{\sigma}_0$ . Since spin systems [14–21] and a 1D ring [22,23] can be separately

realized in ultracold atoms and molecules, we expect this model can also be realized experimentally. This model alone covers three different classes of systems, (a) XYZ, (b) XXZ ( $J_x = J_y \neq J_z$ ), and (c) XY ( $J_z = 0$ ) models, by tuning the parameters  $J_\alpha$ . We here predict the behaviors of the susceptibilities by means of the numerical diagonalization for (a) and (b), and the analytic evaluation for (c), respectively.

Figure 1(a) shows the N dependence of the k=0 components  $\chi_N^{\rm qch}(0)$ ,  $\chi_N^T(0)$ , and  $\chi_N^S(0)$  in the XYZ model [72]. Since the model has no local conserved quantity for  $h \neq 0$  [73], it is expected that the condition (8) is fulfilled, so that Eq. (4) holds. In fact, Fig. 1(a) shows that  $\chi_N^{\rm qch}(0)$  approaches  $\chi_N^S(0)$  as N increases. Their difference decreases nearly exponentially, as shown in the inset, where the function  $0.083 \, e^{-0.193N}$  is also plotted as a guide to the eye. Both of them remain far off from  $\chi_N^T(0)$ .

Contrastingly, Eq. (4) does *not* hold for the *XXZ* or the *XY* models, as shown in Figs. 1(b) and 1(c), respectively. In these two cases, there exist some local conserved quantities that result in the violation of Eq. (8) and its equivalent (4). In other words, they do not satisfy Eq. (8) because of its integrability [74], while they do satisfy the ordinary "weak" ETH [53–56]. It should be noted that our results (a)–(c) are consistent with inequalities (3) and (7).

Conditions for (ii).—As is proved in Ref. [61], Eq. (5) holds if and only if almost all  $|\nu\rangle$  in a narrow energy region  $|\delta E_{\nu}| \lesssim T \sqrt{c_h N}$  satisfy

$$\sum_{\nu'} \delta_{E_{\nu}, E_{\nu'}} \delta_{K_{\nu}, K_{\nu'} + k} |\langle \nu' | \hat{\sigma}_{\mathbf{0}}^{z} | \nu \rangle|^{2} = o(1/N)$$
for all  $k \neq \mathbf{0}$ . (10)

This is similar to the "off-diagonal ETH" [44,49–52], except for the following points. First, the off-diagonal

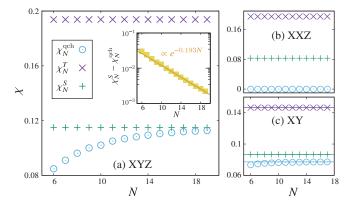


FIG. 1. Size-*N* dependence of  $\chi_N^{\rm qch}(0), \chi_N^T(0)$ , and  $\chi_N^S(0)$  of the (a) *XYZ*, (b) *XXZ*, and (c) *XY* models. We take (a)  $(J_x - J_y, J_z) = (1.2, 1.0)$ , (b) (0.0, 1.0) and (c) (1.2, 0.0), for fixed values of  $J_x + J_y = 0.6$ , h = 0.8,  $\beta = 0.15$ . Inset of (a):  $\chi_N^S(0) - \chi_N^{\rm qch}(0)$  in the logarithmic scale. Solid lines in (c):  $\chi_\infty^{\rm qch}(0), \chi_\infty^T(0)$ , and  $\chi_\infty^S(0)$ .

ETH requires that *all* off-diagonal elements of *all* local operators tend to vanish as  $N \to \infty$ . By contrast, Eq. (10) refers only to a *particular* spin operator  $\hat{\sigma}_0^z$  and to the off-diagonal elements between *specific* pairs of states such that

$$E_{\nu} = E_{\nu'}$$
 and  $\mathbf{K}_{\nu} = \mathbf{K}_{\nu'} + \mathbf{k}$ . (11)

Furthermore, it requires not all such off-diagonal elements but *most* of them tend to vanish. Second, the ordinary off-diagonal ETH [44,49–51] requires exponentially fast decay of all the off-diagonal elements, which is not necessarily satisfied in integrable models. By contrast, Eq. (10) is a weaker condition [61] that can be satisfied even in integrable models, as we will demonstrate shortly for the *XY* model.

It is noteworthy that if we impose Eqs. (8) and (10) not only on a particular spin operator  $\hat{\sigma}_0^z$  but also on all other local operators, we obtain a new necessary condition for thermalization, which is also a sufficient condition as long as the quench parameter  $\Delta h_k$  is small.

Conditions for (iii).—We introduce the canonical spinspin correlation function [61,75] as  $\phi_N^T(r) \coloneqq \beta \langle \delta \hat{\sigma}_0^z; \delta \hat{\sigma}_r^z \rangle_{\rm ini}$ . Then, we can show [61] that  $\chi_\infty^T(k)$  is uniformly continuous on the whole region (including k=0), if  $\phi_\infty^T(r)$  decays fast enough such that

$$\lim_{N \to \infty} \sum_{\mathbf{r} \in \Omega_N} |\phi_{\infty}^T(\mathbf{r})| < \infty \tag{12}$$

and if finite-size effects are small such that

$$\lim_{N \to \infty} \sum_{\mathbf{r} \in \Omega_N} |\phi_N^T(\mathbf{r}) - \phi_\infty^T(\mathbf{r})| = 0.$$
 (13)

Since we exclude phase transition points, condition (12) is expected to be satisfied in most systems. Moreover, it seems normal that the condition (13) holds, since the canonical ensemble well emulates a subsystem in an infinite system [76,77].

If conditions (10), (12), and (13) are all fulfilled, Eq. (6) follows from results (ii) and (iii). It also follows that  $\chi_{\infty}^{\text{qch}}(k)$  is discontinuous at k = 0, as discussed in (iv).

Demonstrations of (ii)–(iv).—The discontinuity of  $\chi_{\infty}^{\text{qch}}(k)$  may seem counterintuitive, but can be verified experimentally by adopting the isolated system representing Eq. (9). The observed susceptibility should follow the following results of the numerical simulation.

Figure 2 shows the k dependence of  $\chi_N^{\rm qch}(k)$ ,  $\chi_N^T(k)$ , and  $\chi_N^S(k)$  in the (a) XYZ, (b) XXZ, and (c) XY models. Recalling that the condition (10) is weaker than the ordinary off-diagonal ETH [44,49–51], we expect that it is fulfilled in all these models. In fact, our data show that Eq. (5),  $\chi_\infty^{\rm qch}(k) = \chi_\infty^S(k) = \chi_\infty^T(k)$  for all  $k \neq 0$ , holds in each model. We also find that  $\chi_N^T(k) - \chi_N^{\rm qch}(k)$  for  $k \neq 0$  scales as  $\Theta(1/N)$  in (c). This is because the off-diagonal

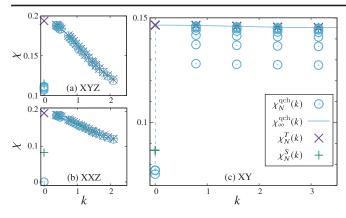


FIG. 2. k dependence of  $\chi_N^{\rm qch}(k)$ ,  $\chi_N^T(k)$ , and  $\chi_N^S(k)$  in (a) XYZ, (b) XXZ, and (c) XY models, with the same parameters as in Fig. 1. We take (a), (b) N=12–17 and  $k=2\pi n_k/N$ , and (c)  $N=2^n$  with n=3–9 and  $k=2\pi n_k/8$ , with  $n_k=0$ –4. Solid line in (c):  $\chi_\infty^{\rm qch}(k)$   $[=\chi_\infty^S(k)=\chi_\infty^T(k)]$  for  $k\neq 0$ , whereas the dashed line shows its discontinuous jump to  $\chi_\infty^{\rm qch}(0)$ .

elements  $|\langle \nu'|\hat{\sigma}_0^z|\nu\rangle|$  that satisfy Eq. (11) decay not exponentially but algebraically as  $\Theta(1/N)$  for the XY model.

The conditions (12) and (13) are the natural ones that will also be satisfied in all these models. In fact, Figs. 2(a)–2(c) indicate Eq. (6),  $\lim_{k\to 0}\chi_{\infty}^{\rm qch}(k) = \chi_{\infty}^T(0)$ , holds and hence  $\chi_{\infty}^{\rm qch}(k)$  is discontinuous at k=0 while  $\chi_{\infty}^T(k)$  is uniformly continuous.

For the parameters presented here, Eqs. (5) and (6) hold in all three cases, while Eq. (4) only in the XYZ one. By further varying  $J_x$  and  $J_y$ , we can also construct a model for which *none* of Eqs. (4)–(6) holds [61]. In such a case, the condition (10) is violated, while the conditions (12) and (13) are still fulfilled.

Discussion on discontinuity.—The discontinuity of  $\chi^{\rm qch}_{\infty}(k)$  at k=0 seems nontrivial. When results (i) and (ii) hold, this discontinuity is related to that of  $\chi^S_{\infty}(k)$ . To help understand the former, we here explain the latter discontinuity intuitively [66]. We also explain the continuity of  $\chi^T_{\infty}(k)$ .

Suppose that a huge system is enclosed by an adiabatic wall. We consider a thermodynamic process in which  $\Delta h(r)$  is applied quasistatically. If  $\Delta h(r)$  is localized and uniform in a subsystem with  $N=L^d$  sites, one obtains the adiabatic susceptibility of wave number  $|k|\sim 1/L$ . Since the total system size is huge, it is well approximated by  $\chi_{\infty}^S(k)$ . On the other hand, this thermodynamic process can also be regarded as an isothermal process for the subsystem because the rest of the system works as a heat reservoir. According to this picture, one obtains  $\chi_N^T(\mathbf{0})$ . Since the two pictures have to give the same results,  $\chi_{\infty}^S(k) = \chi_N^T(\mathbf{0})$  for  $|k| \sim 1/L$ . By increasing N, we obtain  $\lim_{k\to 0} \chi_{\infty}^S(k) = \chi_{\infty}^T(\mathbf{0})$ . Comparing this with inequality (3), we can see that  $\chi_{\infty}^S(k)$  is discontinuous at  $k=\mathbf{0}$ . By contrast, we can argue similarly the case where the adiabatic wall is replaced with a

heat reservoir. Then we have  $\lim_{k\to 0} \chi_{\infty}^T(k) = \chi_{\infty}^T(\mathbf{0})$ , which shows that  $\chi_{\infty}^T(k)$  is continuous at  $k=\mathbf{0}$ .

Relation to Kubo formula.—Since the Schrödinger dynamics is assumed, our results are applicable to experiments on isolated quantum systems. Moreover, since many formulas of physics were derived assuming the Schrödinger dynamics, our results contribute also to foundations of such formulas. As an example of the latter, we finally discuss the susceptibility obtained by the Kubo formula [78],  $\chi_N^{\text{Kubo}}(k, \omega + i\varepsilon)$ . Here,  $\omega$  is the frequency and  $\varepsilon$  is an infinitesimal positive number. While we have defined  $\chi_N^{\text{qch}}$  through a sudden quench of  $\Delta h(r)$ , Kubo derived  $\chi_N^{\text{Kubo}}$  assuming that  $\Delta h(r)$  is switched on gradually over a long timescale  $\sim 1/\varepsilon$ .

It is generally believed that the  $\varepsilon \to +0$  limit of  $\chi_N^{\text{Kubo}}$  should be taken after the  $N \to \infty$  limit [79–83]. However, some works took the  $\varepsilon \to +0$  limit keeping N finite [84–86]. For the latter limit, we can show [61]

$$\lim_{\epsilon \to +0} \chi_N^{\text{Kubo}}(\mathbf{k}, 0 + i\epsilon) = \chi_N^{\text{qch}}(\mathbf{k}) \quad \text{for all } N, \quad (14)$$

although the left-hand side and right-hand side correspond to the slow and fast processes, respectively, which would result in different final states. Therefore, all the statements (i)–(iv) for  $\chi_{\infty}^{\rm qch}(\mathbfit{k})$  hold also for  $\lim_{N\to\infty}\lim_{\varepsilon\to+0}\chi_N^{\rm Kubo}(\mathbfit{k},0+i\varepsilon)$  [87]. Moreover, the previous results on  $\lim_{\varepsilon\to+0}\chi_N^{\rm Kubo}(\mathbfit{0},0+i\varepsilon)$  [84–86] can be understood more precisely using (i) [61]. However, it is noteworthy that  $\chi_N^{\rm Kubo}$  is hard to measure in experiments in contrast to  $\chi_N^{\rm qch}$ , since the system cannot be isolated for the infinitely long timescale.

In conclusion, we have revealed the anomalous natures of the quench susceptibility, demonstrating together that experimental verifications are feasible enough.

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