Fidelity of the diagonal ensemble signals the many-body localization transition

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In this work, we use exact matrix diagonalization to explore the many-body localization (MBL) transition in a random-field Heisenberg chain. We demonstrate that the fidelity and fidelity susceptibility can be utilized to characterize the interaction-driven many-body localization transition in this closed spin system which is in agreement with previous analytical and numerical results [S. Garnerone, N. T. Jacobson, S. Haas, and P. Zanardi, Phys. Rev. Lett. **102**, 057205 (2009); P. Zanardi and N. Paunkovic, Phys. Rev. E **74**, 031123 (2006)]. In particular, instead of ground-state fidelity, we test the fidelity between two diagonal ensembles related by a small parameter perturbation δh , it is special that here the parameter perturbation δh_i for each site are random variables like h_i . It shows that fidelity of the diagonal ensemble develop a pronounced drop at the transition. We utilize fidelity to estimate the critical disorder strength h_c for different system size, we get $h_c \in [2.5, 3.9]$ and get a power-law decay with an exponent of roughly -1.49(2) for system size N, and can extrapolate h_c^{in} of the infinite system is about 2.07 which all agree with a recent work by Huse and Pal, in which the MBL transition in the same model was predicted to be hc [2,4]. We also estimate the scaling of maximum of averaged fidelity susceptibility as a function of system size N, it shows a power law increase with an exponent of about 5.05(1).

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I. INTRODUCTION

The concept of Anderson localization is established and well known since Anderson proposed it in his seminal paper [1] more than half a century ago [2]. It shows that a static disordered potential can lead to a complete absence of diffusion in an closed quantum system which has received extensive attention since then and has formed a complete conclusions that non-interacting systems in one and two dimensions will be localized for arbitrary disorder, even for very small disorder [3,4]. In Ref. [1], Anderson also conjectured that a closed interacting quantum system with sufficiently strong disorder would fail to approach thermal equilibrium. Until much more recently, Basko et al. [5] gave new arguments to revive this idea of many-body localization (MBL). Note that this is a quantum glass transition that occurs at nonzero (even infinite) temperature, where equilibrium quantum statistical-mechanics breaks down. In the localized phase the system fails to thermally equilibrate. Like the more familiar ground-state quantum-phase transitions, this transition is a sharp change in the properties of the many-body eigenstates of the Hamiltonian, unlike ground-state phase transitions, the many-body localization transition at nonzero temperature appears to be only a dynamical-phase transition that is invisible in the equilibrium thermodynamics [6].

Many studies [6–18] have studied and confirmed the phenomenon of MBL recently, showing that a novel dynamical phase transition can happen in the interacting disordered systems. Many features of the MBL phase have been explored. It has been displayed that bipartite entanglement entropy between two sectors of the system shows a characteristic logarithmic growth in the many-body localized phase [19–24].

Recently, generous efforts [25-39] have been devoted to the role of fidelity, a popular concept in quantum information theory [40], in quantum critical phenomena [41], demonstrating that fidelity is useful in characterizing distinct phases of quantum many-body systems [42]. In particular, the minimum of fidelity near a critical point has been studied in several models [27-29]. It has also been shown that fidelity plays a crucial role in quantum phase transitions (QPTs) in quantum fields [30]. Particularly, fidelity as well as the Berry phase have also been recently used to analyze quantum phase transitions from a geometrical perspective. In [35], Venuti et al. unified these two approaches showing that the underlying mechanism is the critical singular behavior of a complex tensor over the Hamiltonian parameter space. The advantage of the fidelity is that it is a space geometrical quantity, no a priori knowledge of the order parameter and symmetry breaking is required in studies of QPTs.

Considering the special and crucial role of fidelity in quantum critical phenomena, in this work, we apply the fidelity approach to MBL transitions. In Ref. [26], the authors applied the fidelity approach to estimate random transitions of the disordered quantum model. They showed that the fidelity susceptibility and its scaling properties provide useful information about the phase diagram. So the point here is phenomenological, we think it should work based on previous analysis [26,27], we do the numerics and we see that it indeed works. Since MBL is concerned with all energies, and recently it was widely studied with high excited state [6–11], the states in the middle of the spectrum are important in MBL [6,7], and one can see that such states and their corresponding weights

It has also been found that the total correlations scales extensively in the localized phase developing a pronounced peak at the transition [17]. Even though, still many features of MBL are unexplored and their broader connections are unknown.

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are nicely and naturally included in the dephased state from the definition of the dephased state in the following Eq. (1), so here instead of the ground state which represents low temperature, our focus is on the time-averaged, dephased state which is the unique state that maximizes the von Neumann entropy [43] and has also been used to study MBL recently [17]. So fingerprints of the MBL transition are expected in the fidelity of this dephased state. It is worth noting that to test the dephased-state fidelity, the parameter perturbation δh_i for each site used in this paper are not determinate, but random variables like h_i .

Next we first review the definition of the dephased state. For a fixed initial state ρ and non-degenerate Hamiltonian H, the dephased state or time-averaged state ω has the following form [17]:

$$\omega := \sum_{n} |E_{n}\rangle \langle E_{n}|\rho|E_{n}\rangle \langle E_{n}| = \lim_{\tau \to \infty} \frac{1}{\tau} \int_{0}^{\tau} dt e^{-itH} \rho e^{itH},$$
(1)

where $|E_n\rangle$ are the eigenvectors of H. This is long-time equilibrium state, and is often referred to as the diagonal ensemble, since for the non-degenerate Hamiltonian H, the off-diagonal elements each time average to zero. It is known that the dephased or time-averaged state is the unique state that maximizes the von Neumann entropy, holding all constants of motion fixed [43]. If the expectation value of an observable equilibrates on average during the time evolution of a system, then the equilibrium expectation value can be computed from it [44,45].

To test the fidelity of the dephased state ω , we use the mixed-state fidelity, which is given by [46]

$$F(\rho_0, \rho_1) := \operatorname{tr} \sqrt{\rho_1^{\frac{1}{2}} \rho_0 \rho_1^{\frac{1}{2}}}.$$
 (2)

This quantity measures the degree of distinguishability between the two quantum states ρ_0 and ρ_1 . The fidelity is related to the statistical Bures distance: $D(\rho_0, \rho_1) = \sqrt{2(1 - F)}$ [32]. We will use Eq. (2) to compare two diagonal ensembles ω_0 and ω_1 related by a small parameter perturbation δh , then we get $F(\omega_0, \omega_1)$ corresponding to $F(h, h + \delta h)$. In the limit, the fidelity is close to unity and it can be approximated by the lowest-order nontrivial Taylor expansion

$$F(h,h+\delta h) \simeq 1 - \chi(h) \frac{\delta h^2}{2}.$$
 (3)

The prefactor in the quadratic term, $\chi(h)$, is called the fidelity susceptibility [37]. It has been recently intensively studied as a probe of quantum criticality [27,29,42].

II. MODEL USED FOR NUMERICS

It has been shown that many-body localization appears to occur for a wide variety of particle, spin, or qubit models. Here we study a spin model, the Heisenberg spin chain with random fields in the z direction [7]. The Hamiltonian of this model is given by

$$H = \sum_{i=1}^{N} \left[J \left(s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + s_i^z s_{i+1}^z \right) + h_i s_i^z \right], \quad (4)$$

where the h_i represent identically distributed static fields on each site i, each with a probability distribution that is uniform in [-h,h]. We consider the chains are of size N with periodic boundary conditions. The system is completely characterized by the disorder strength h and the coupling constant J. This is one of the simpler models that shows a many-body localization transition. Through dephased-state fidelity and fidelity susceptibility we will present evidence that the MBL transition at $h = h_c \cong 3.5 \pm 1.0$ also dose occur in this model, in correspondence with the prediction in [7]. For all values of the parameters, this model has two global conservation laws: total energy and total magnetization S^z along the z direction, so in the numerics we only pay attention to states with zero total S^z . Here the initial states we take are all eigenstates of the Hamiltonian $\sum_{i=1}^{N} s_i^z$ from the subspace with total $S^z = 0$. These initial states are product states, for each initial state, according to Eq. (1), we can compute the corresponding diagonal ensemble ω_0 . To test the fidelity of the diagonal ensemble, for the small parameter perturbation δh_i for each site, we have three options: (a) $\delta h_i = \epsilon$, (b) $\delta h_i = \epsilon h$, (c) $\delta h_i = \epsilon h_i$ (ϵ is a small constant). The parameter perturbation δh_i for each site is the same constant as in cases (a) and (b), but different random variables in case (c). We have tried these three cases, only in the case (c) $\delta h_i = \epsilon h_i$, we can see the phenomenon of MBL transition through fidelity to denote. So in this paper we do all computation in the case (c) $\delta h_i = \epsilon h_i$, and let $\epsilon = 10^{-3}$, we then compute for each initial state the diagonal ensemble ω_1 , fidelity $F(\omega_0, \omega_1)$ and fidelity susceptibility χ . Averaging over all selected initial states and disorder realizations yields the mean values E[F] and $E[\chi]$. The numerics were performed using standard libraries for matrix exact diagonalization. Total S^z symmetry and parallel programming techniques were employed to make

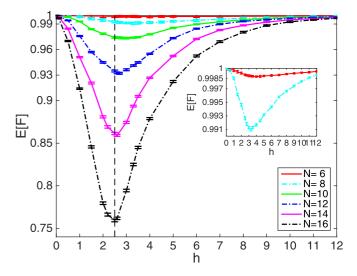


FIG. 1. Averaged fidelity of the depased state as a function of h for system size from 6 to 16. The system size N is indicated in the legend. Statistical error bars for every data points are given. In the ergodic phase [7] (small h) E[F] decays substantially under the dynamics until h approaches to the critical point h_c , then in the localized phase (large h) E[F] turns to increase approximately approaching to 1. The drop gets sharper as system size N increases. The inset corresponds to enlarged pictures for system size N = 6 and 8 with the same data.

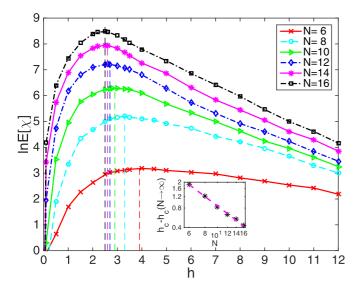


FIG. 2. Averaged fidelity susceptibility of the depased state as a function of *h* for system sizes from 6 to 16. The system size *N* is indicated in the legend. For every system size, the critical line is plotted. In the inset, subtracting the values of h_c^{inf} (the critical disorder strength in the infinite system) from h_c one can see that the decrease versus system size *N* (the asterisks) is well captured by a power-law with exponent of approximately -1.49(2) (dashed line guide to the eye $\propto N^{-1.49(2)}$).

computations feasible. The number of disorder realization for each disorder amplitude |h| and system size N we used in the data shown in this paper is 10^4 for N = 6 and N = 8, 2000 for N = 10 and N = 12, 200 for N = 14, and 50 for N = 16.

III. RESULTS AND DISCUSSION

Here we take J = 1, for this case the MBL transition in the model (4) was predicted to be $h_c \in [2, 4]$ in [7]. According

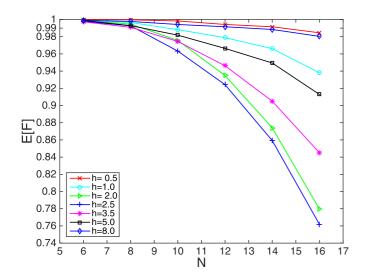
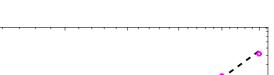
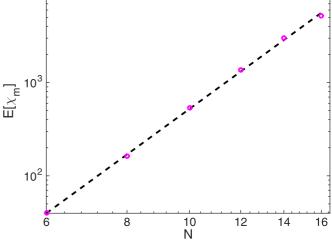


FIG. 3. Averaged fidelity E[F] as a function of system size N for different values of disorder strength h from small to large. The value of h is indicated in the legend. E[F] decays as the system size increases, it decays the fastest when h = 2.5.



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FIG. 4. Maximum of averaged fidelity susceptibility as a function of system size *N* and the fitting curve to the data points, one can see that the increase of $E[\chi_m]$ for system size *N* (the circles) is well captured by a power-law exponent of approximately 5.05(1) (dashed line guide to the eye $\propto N^{5.05(1)}$).

to the pronounced data change shown in Figs. 1 and 2, one can obtain the approximate critical disorder strength h_c for different system size N. For $N = 6, h_c \rightarrow 3.9, N = 8, h_c \rightarrow$ 3.3, N = 10, $h_c \rightarrow 2.9$, N = 12, $h_c \rightarrow 2.7$, N = 14, $h_c \rightarrow$ 2.6, $N = 16, h_c \rightarrow 2.5$. So we obtain $h_c \in [2.5, 3.9]$ for the breakdown of ergodic phase, which agrees with the prediction in [7,13]. In Fig. 1, we show one standard-deviation error bars, and from this figure, one can see the E[F] versus h show an initial decrease at low h towards a minimum and then increase at higher disorder approximately approaching to 1. The critical disorder strength h_c is size dependent, we do the fitting h_c with expression as $h_c \sim A + B/N^C$, where A, B, C are the fitting parameters, and get A = 2.07, B = 26.7, C = 1.49(2). So one can extrapolate the critical disorder strength h_c^{inf} of the infinite system is about 2.07 which also agrees with the prediction in [7]. In the inset of Fig. 2, subtracting the values of h_c^{inf} from h_c one can see that the decrease of $(h_c - h_c^{inf})$ for system size N is well captured by a power-law with exponent of approximately -1.49(2). As the data change of Figs. 1 and 2, it shows that here MBL transition is not a sharp transition which can also be seen in recent studies [7,14]. In Fig. 3, $\mathsf{E}[F]$ decays as the system size increases, it decays the fastest when h = 2.5, and one can see that when the value of h is small, h = 0.1, and when it is large, h = 8, E[F] decays very little with system size N. It can be predicted that the fidelity E[F] will be independent of system size N at very large h, namely fidelity E[F] approximately is not to be changed in the localized phase. In Fig. 4, scaling of maximum of averaged fidelity susceptibility $E[\chi_m]$ is estimated. It shows a power-law increase of $E[\chi_m]$ for system size with an exponent of roughly 5.05(1), i.e., $\mathsf{E}[\chi_m] \propto N^{5.05(1)}$.

IV. SUMMARY

In this paper, the numerical simulations performed show that the fidelity and fidelity susceptibility of the diagonal ensemble denote the MBL transition in a special way which is in agreement with previous analytical and numerical results [26,27]. We test the fidelity between two diagonal ensembles related by a small parameter perturbation δh , it is special that here the parameter perturbations δh_i for different site are random variables like h_i . Undoubtedly the transition from an ergodic to a MBL phase is a highly non-equilibrium phenomenon which is poorly understood at present. Our study of the exact matrix diagonalization of the model in Eq. (4) can demonstrate some of the properties of the ergodic and localized phases. It shows that in the ergodic phase (small h) E[F] decays substantially under the dynamics until h approaches the critical disorder strength h_c , then in the localized phase (large h) $\mathsf{E}[F]$ turns to increase approximately approaching 1. If the disorder strength is large enough, the fidelity E[F] will not be changed in the localized phase for arbitrary system size. We also get the critical disorder strength $h_c \in [2.5,3.9]$ for the breakdown of the ergodic phase, the fitting h_c with expression as $h_c \sim A + B/N^C$, A = 2.07, B = 26.7, C = 1.49(2). Then one can extrapolate the critical

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strength of the disorder in the infinite system h_c^{inf} to be about 2.07. The decrease of $(h_c - h_c^{\text{inf}})$ for system size N is well captured by a power-law with exponent of approximately -1.49(2), i.e., $(h_c - h_c^{\text{inf}}) \propto N^{-1.49(2)}$. We also estimate the scaling of maximum of fidelity susceptibility as a function of system size N, it shows a power-law increase of $\mathsf{E}[\chi_m]$ for system size N with an exponent of roughly 5.05(1), i.e., $\mathsf{E}[\chi_m] \propto N^{5.05(1)}$. We hope that the present work provides a novel window into the remarkable phenomenon of many-body localization.

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