I. INTRODUCTION

The nonequilibrium dynamics of generic quantum systems denies a fully understanding up to now, even if the thermalization in the long-time asymptotic state has been explained by the eigenstate thermalization hypothesis which proposes a universal form of the observable matrix elements in the eigenbasis of the Hamiltonian. In this paper, we study the form of the quantum state, i.e., of the density matrix elements. We propose that the density matrix has also a universal form in chaotic systems, which is used to understand the nonequilibrium dynamics in the whole time scale, from the transient regime to the long-time steady limit, and then extends the applicability of eigenstate thermalization hypothesis to true nonequilibrium phenomena such as nonequilibrium steady states. Our assumption is numerically tested in various models, and its intimate relation to the eigenstate thermalization hypothesis is discussed.

Nonequilibrium dynamics of the density matrix in chaotic quantum systems

Xinxin Yang and Pei Wang

1Department of Physics, Zhejiang Normal University, Jinhua 321004, People’s Republic of China
(Dated: August 22, 2018)

The nonequilibrium dynamics of quantum many-body systems keeps on attracting attention of both experimentalists and theorists. For integrable systems, the case-by-case study of exact solutions revealed exotic properties of the quantum states driven out of equilibrium. The long-time asymptotic state is far from thermal equilibrium, but should be described by the generalized Gibbs ensemble. On the other hand, for systems whose classical counterparts are chaotic, it is widely believed that they will finally thermalize in the long time limit. But the dynamics in the transient and intermediate time scale is still hard to explore, due to the lack of a reliable analytical or numerical method.

The study of the dynamics in quantum chaotic systems dated back to the early days of quantum mechanics, when the question has been raised as to how the statistical properties of equilibrium ensembles arise from the linear dynamics of Schrödinger equation in a complex system. A breakthrough was made in 1950s by Wigner, who stated that the statistics of the eigenenergies of a chaotic system should be as same as that of a random matrix, that is the level spacing follows the Wigner-Dyson distribution. This statement was verified by both experiments and numerical simulations. But for an integrable system, the level spacing satisfies a Poisson distribution according to Berry and Tabor.

In the random matrix theory (RMT), the eigenstates of the Hamiltonian are considered to be random vectors in the Hilbert space. This oversimplified picture ignores the dependence of the structure of the eigenstate on the eigenenergy, and then fails to explain why the observables are in fact a function of the energy or temperature of the system. A further step was made in the eigenstate thermalization hypothesis (ETH), which proposed a generic form of the matrix elements of observable operators in the eigenbasis of the Hamiltonian:

\[ O_{\alpha \beta} = O(\bar{E}) \delta_{\alpha \beta} + D^{-\frac{1}{2}}(\bar{E}) f_O(\omega, E) R_{\alpha \beta}^O, \]

where \( \alpha \) and \( \beta \) are the eigenstates of the Hamiltonian with \( E_\alpha \) and \( E_\beta \) being their eigenenergies, respectively. \( \bar{E} = (E_\alpha + E_\beta)/2 \) and \( \omega = E_\alpha - E_\beta \) denote the average energy and the energy difference of \( \alpha \) and \( \beta \), respectively. \( D(\bar{E}) \) is the density of many-body states, which increases exponentially with the system size (or the total number of particles). \( O(\bar{E}) \) and \( f_O(\omega, E) \) are both smooth functions, with the former describing how the expectation value of the observable changes with energy. The randomness of the eigenstates is reflected in Eq. (1) by the random number \( R_{\alpha \beta}^O \), which has zero mean and unit variance according to definition.

When a chaotic system is driven out of equilibrium, its density matrix evolves according to the quantum Liouville equation. In the asymptotic long-time state, the off-diagonal elements of the density matrix obtain completely randomized phases, therefore, only the diagonal elements, which construct the so-called diagonal ensemble, have a contribution to the expectation value of observables. ETH builds the equivalence between the microcanonical ensemble and the diagonal ensemble, and then explains thermalization successfully. Its correctness has been verified in plenty of numerical simulations, while its limitation was also noticed. ETH has to be modified for the order parameter in the presence of spontaneous symmetry breaking, and it fails in a many-body localized system which cannot thermalize.

In spite of the success of ETH, it cannot explain how an observable relaxes towards steady value, because it says nothing about the off-diagonal elements of density matrix which are important in the transient and intermediate time scale. The off-diagonal elements of density matrix are even the key of describing an asymptotic long-time state, in the case that the thermodynamic limit and the long-time limit are noncommutative. This noncommutativity defines an important class of nonequilibrium states - the nonequilibrium steady states, which is the basis of understanding mesoscopic transport phenomena. A stationary current flows through a central region which is coupled to multiple thermal reservoirs at different temperatures and chemical potentials. The description of such a quantum state goes beyond the ability of diagonal ensemble, Gibbs ensemble or generalized Gibbs ensem-
ble, but requires the knowledge of the off-diagonal elements. This motivated one of the authors to propose the nonequilibrium steady state hypothesis (NESSH)\textsuperscript{25}.

In this paper, we make NESSH complete by proposing the form of both the diagonal and off-diagonal elements in the density matrix, which is

\[
\rho_{\alpha\beta} = D^{-1}(E) \left( \frac{-\alpha^2}{2\pi \sigma_\alpha^2} \right) \delta_{\alpha\beta} + D^{-1}(E) f(\omega, E) R_{\alpha\beta}^s, \tag{2}
\]

where \(\mu_\alpha\) and \(\sigma_\alpha^2\) denote the mean and variance of the system’s energy, respectively. Note that the first term in Eq. (2) is absent in the previous paper\textsuperscript{24}, \(f(\omega, E)\) is the dynamical characteristic function, which is determined by the initial state and contains all the information for understanding the real-time dynamics of a chaotic system from the transient regime to the long-time steady limit. It is worth emphasizing that Eq. (2) stands for the density matrix of arbitrary chaotic system whether it thermalizes or evolves into a nonequilibrium steady state. In this paper, we will carry out numerical simulations in different models of spins in different dimensions to support our assumption \textsuperscript{24}, supplement to the numerical simulations of fermionic models in the previous study. Furthermore, we will show how to derive ETH by using Eq. (2), and then build an intimate connection between NESSH and ETH, which both stand in quantum chaotic systems.

The rest of the paper is organized as follows. The physical meaning of Eq. (2) will be discussed in Sec. \textsection \textsection III in which we also derive a generic expression for the real-time dynamics of an observable based on our assumption and ETH. The numerical evidence of our assumption is presented in Sec. \textsection III and \textsection IV The connection between NESSH and ETH is the content of Sec. \textsection IV Sec. \textsection V summarizess our results.

\section{II. Nonequilibrium Dynamics of the Density Matrix}

Let us consider an isolated system with the Hamiltonian \(\hat{H}\). Without loss of generality, we suppose \(t = 0\) as the initial time, at which the quantum state of the system is denoted by \(|s\rangle\). According to quantum mechanics, the expectation value of an arbitrary observable evolves as

\[
O(t) = \sum_{\alpha, \beta} e^{-i\omega t} \rho_{\alpha\beta} O_{\beta\alpha}, \tag{3}
\]

where \(\alpha\) and \(\beta\) denote the eigenstates of \(\hat{H}\), and \(\omega = E_\alpha - E_\beta\) is the difference between their eigenenergies. \(\rho_{\alpha\beta} = \langle \alpha | \hat{\rho} | \beta \rangle\) with \(\hat{\rho} = |s\rangle \langle s|\) denotes the element of the initial density matrix in the eigenbasis of \(\hat{H}\), and \(O_{\beta\alpha} = \langle \beta | \hat{O} | \alpha \rangle\) denotes the matrix element of the observable operator.

In the case that the initial state is not an eigenstate of \(\hat{H}\), the system is out of equilibrium at \(t > 0\). To study the nonequilibrium dynamics of a system is equivalent to calculate \(O(t)\). For this purpose, we need to know the eigenenergies, the initial density matrix and the observable matrix. For integrable systems, \(E_\alpha\), \(\rho_{\alpha\beta}\) and \(O_{\alpha\beta}\) differ from model to model. There is no common way of understanding nonequilibrium dynamics of integrable systems. But it is not the case for chaotic systems, which are "similar" to each other. RMT tells us that the eigenenergies of chaotic systems all follow the Wigner-Dyson distribution\textsuperscript{26}.

\[
P(E_1, E_2, \cdots) = \frac{1}{N} e^{-\frac{E_1^2 + E_2^2 + \cdots}{2 \sigma^2}} \prod_{\alpha > \beta} (E_\alpha - E_\beta), \tag{4}
\]

where \(\sigma\) is connected to the energy bandwidth and \(N\) is a normalization constant. And according to ETH, \(O_{\alpha\beta}\) has the universal form \textsuperscript{1}, independent of the model being of fermions, bosons or spins, or in which dimensions. Once if we know the form of \(\rho_{\alpha\beta}\), \(O(t)\) can be calculated, even if the exact solution of any specific chaotic model is inaccessible. Different from integrable models, our knowledge of \(E_\alpha\), \(O_{\alpha\beta}\) and \(\rho_{\alpha\beta}\) in chaotic models is not precise, but only statistical. Eq. (3) only gives the statistics of the eigenenergies, and Eq. (4) contains a random number \(R_{\alpha\beta}\). This is what we have to pay for not really solving the model. But it does not prevent us from obtaining the information that we are interested in, i.e. \(O(t)\).

Before discussing the form of \(\rho_{\alpha\beta}\), we need to make clear which kind of initial states are interesting to us. The initial state \(|s\rangle\) should be some quantum state that we can prepare in a laboratory. Preparing a quantum state is usually equivalent to measuring the state which inevitably causes the wave function collapsing into an eigenstate of the observable operator. Therefore, it is natural to choose \(|s\rangle\) as an eigenstate of a complete set of observable operators. For example, in a spin lattice model, we can choose \(|s\rangle\) to be a configuration of spin eigenstates in the \(z\)-direction on each lattice site, or we choose \(|s\rangle\) to the spin eigenstates in the \(x\)- or \(y\)-directions. Such kind of initial states will be called natural states in next. Of course, \(|s\rangle\) cannot be an eigenstate of \(\hat{H}\), otherwise, the system is already thermalized at the initial time according to ETH. \(|s\rangle\) is also not a fine-tuned state, such as the superposition of a few eigenstates of \(\hat{H}\). Such kind of fine-tuned states are difficult to creat in experiments for a many-body chaotic system. On the other hand, \(|s\rangle\) can be an eigenstate of a Hamiltonian \(\hat{H}_0\) which includes no interaction between particles and is then integrable, e.g., a spin model without interaction between spins at different sites. Usually, this kind of \(\hat{H}_0\) is commutative with some observable operators so that they have common eigenstates. \(|s\rangle\) can also be the eigenstate of a chaotic Hamiltonian \(\hat{H}'\) which is noncommutative with \(\hat{H}\). For example, \(\hat{H}'\) and \(\hat{H}\) describe interacting spins with different interaction strength. In this case, the eigenstate...
of $\hat{H}'$ looks like a random vector in the eigenbasis of $\hat{H}$, which is the foundation of our assumption (2).

Starting from a natural state, the dynamics of the density matrix follows the quantum Liouville equation. We propose that $\rho_{\alpha\beta} = \langle \alpha | s \rangle \langle s | \beta \rangle$ has a universal form which can be expressed as

$$\rho_{\alpha\beta} = D^{-1} \left( \langle \rho \hat{E} \rangle \delta_{\alpha\beta} + D^{-\frac{1}{2}} \hat{E} \right) \left( \hat{f} (\omega, \hat{E}) R_{\alpha\beta}^{s} \right),$$

(5)

where the first term in the bracket denotes the diagonal element, while the second term denotes the off-diagonal element. $\hat{E} = (E_{\alpha} + E_{\beta}) / 2$ and $\omega = E_{\alpha} - E_{\beta}$ are the energy average and the energy difference, respectively.

The density of states $D(\hat{E})$ appears in Eq. (5) to indicate how $\rho_{\alpha\beta}$ scales with increasing system’s size $N$. Note that both ETH and NESSH should be treated as assumptions in the thermodynamic limit $N \to \infty$. But $\rho_{\alpha\beta}$ vanishes as $N \to \infty$, therefore, we have to start from a finite $N$ and separate the diverging factor in $\rho_{\alpha\beta}$, which is $D$. $D$ increases exponentially with $N$ and diverges in thermodynamic limit. The exponents of $D$ in the diagonal and off-diagonal terms can be deduced from the fact that a local observable $O(t)$ must be convergent in thermodynamic limit.

Let us consider the diagonal term in Eq. (5). $\rho_{\alpha\alpha} = \langle \alpha | s \rangle \langle s | \alpha \rangle$ is in fact the probability of measuring the energy of state $| s \rangle$ and finding it is $E_{\alpha}$. This probability distribution should be centered around the mean energy of $| s \rangle$. It is natural to think that this distribution is a Gaussian distribution, which is also supported by our numerics. $\rho(\hat{E})$ can then be expressed as

$$\rho(\hat{E}) = \frac{1}{\sqrt{2\pi\sigma_{s}^{2}}} e^{-\frac{(\hat{E} - \mu_{s})^{2}}{2\sigma_{s}^{2}}} + C_{s}R_{ss},$$

(6)

where $\mu_{s}$ and $\sigma_{s}^{2}$ denote the mean energy and the energy fluctuation of the state $| s \rangle$. An additional term $C_{s}R_{ss}^{s}$ is added to fit the numerics into Eq. (5). $C_{s}R_{ss}^{s}$ describes the deviation from the Gaussian distribution with $C_{s}$ being a constant and $R_{ss}^{s}$ being an independent random number with zero mean and unit variance. The properties of $C_{s}$ and $R_{ss}^{s}$ will be further discussed in Sec. 11. They indeed vanish in thermodynamic limit. Anyway, $C_{s}R_{ss}^{s}$ has no effect on the value of $O(t)$.

The parameters $\mu_{s}$ and $\sigma_{s}^{2}$ in Eq. (6) can be determined. We have

$$\mu_{s} = \int \hat{E} \rho(\hat{E}) \, d\hat{E}$$

$$= \sum_{\alpha} E_{\alpha} \langle \alpha | s \rangle \langle s | \alpha \rangle$$

$$= \langle s | \hat{H} | s \rangle,$$

(7)

where we have used $\int dE_{\alpha} D(E_{\alpha}) = \sum_{\alpha}$ and $E_{\alpha} = \hat{E}$ for the diagonal elements. Note $\int C_{s}R_{ss}^{s} \hat{E} d\hat{E} = 0$, because $R_{ss}^{s}$ at different $\alpha$ are independent random numbers with zero mean. Similarly, we obtain the variance of energy

$$\sigma_{s}^{2} = \int \hat{E}^{2} \rho(\hat{E}) \, d\hat{E} - \left( \int \hat{E} \rho(\hat{E}) \, d\hat{E} \right)^{2}$$

$$= \langle s | \hat{H}^{2} | s \rangle - \langle s | \hat{H} | s \rangle^{2}$$

$$= \sum_{s' \neq s} H_{ss'}^{2}.$$  

(8)

Here the sum with respect to $s'$ is over the natural states, i.e., the common eigenstates of the complete set of observable operators, which form a natural basis of the Hilbert space. Different from $\mu_{s}$, the variance is determined by the off-diagonal elements of the Hamiltonian in the natural basis.

Next we consider the off-diagonal elements in Eq. (9). The factor $D^{-1/2}$ indicates that the off-diagonal elements are exponentially smaller than the diagonal elements. RMT says that the eigenstates are random vectors in the Hilbert space, therefore, $| s \rangle \langle \alpha |$ and $| s \rangle \langle s | \beta \rangle$ are both random numbers, so is $\rho_{\alpha\beta}$. The randomness of $\rho_{\alpha\beta}$ in Eq. (6) is reflected by the random number $R_{\alpha\beta}^{s}$, which by definition has zero mean and unit variance. And $R_{\alpha\beta}^{s}$ at different $(\alpha, \beta)$ are independent to each other. But the variance of $\rho_{\alpha\beta}$ is not a constant, but depends on the energies $E_{\alpha}$ and $E_{\beta}$. In order to describe the structure of $\rho_{\alpha\beta}$ which is ignored by RMT, we introduce the dynamical characteristic function $f(\omega, \hat{E})$ with $\hat{E} = (E_{\alpha} + E_{\beta}) / 2$ and $\omega = E_{\alpha} - E_{\beta}$. One can understand the off-diagonal term of Eq. (5) as follows. $\rho_{\alpha\beta}$ fluctuates heavily as $E_{\alpha}$ or $E_{\beta}$ changes. But if we integrate out the fluctuation, the average of $| \rho_{\alpha\beta} |^{2}$ changes smoothly with $E_{\alpha}$ and $E_{\beta}$, or with $\hat{E}$ and $\omega$. This is the central idea of NESSH and is highly nontrivial, being true only for chaotic systems. Our numerics in the previous study already showed its breakdown in integrable models.

By substituting Eqs. (1) and (6) into Eq. (5), we obtain

$$O(t) = \int \int_{-\infty}^{\infty} d\hat{E} \rho(\hat{E}) \hat{O}(\hat{E})$$

$$+ \int_{-\infty}^{\infty} d\hat{E} \int_{-\infty}^{\infty} dw e^{-i\omega t} f(\omega, \hat{E}) f_{O}(\omega, \hat{E}),$$

where we have used $\int dE_{\alpha} D(E_{\alpha})$ and $D(\hat{E} \pm \omega / 2) \approx D(\hat{E})$. The latter approximation comes from the fact that the integration function $f_{O}$ decays to zero quickly with increasing $\omega$. $C_{sO} = \int R_{\alpha\beta}^{s} R_{\alpha\beta}^{O}$ denotes the correlation between the random numbers $R_{\alpha\beta}^{s}$ and $R_{\alpha\beta}^{O}$, which can be estimated numerically by averaging $R_{\alpha\beta}^{s} R_{\alpha\beta}^{O}$ over a small energy box centered at a specific value of $(\hat{E}, \omega)$. $C_{sO}$ changes slowly with $\hat{E}$ or $\omega$, and can be treated as a constant and taken out of the integral. Note that the density of states disappears in Eq. (9), therefore, $O(t)$ converges in thermodynamic limit, as we expect.

The first term of Eq. (9) is independent of time, being exactly the expectation value of the observable with respect to the diagonal ensemble. Since $\rho(\hat{E})$ is a Gaussian
distribution (the second term of Eq.\,(13) cancels out in the integral), the first term of Eq.\,(13) evaluates \( O(\mu_s) \), once if \( O(E) \) changes slowly in the range \((\mu_s - \sigma_x, \mu_s + \sigma_x) \). \( O(\mu_s) \) is indeed the value of the observable after thermalization. Imagine the evolution processes starting from two different microscopic states \( |s_1\rangle \) and \( |s_2\rangle \) that have the same mean energy \( \mu_s \). In the long-time steady limit, one cannot distinguish \( |s_1\rangle \) from \( |s_2\rangle \) by any measurement. This is exactly what thermalization means - the memory of initial state is lost and the properties of the system is only determined by few parameters such as the mean energy.

The second term of Eq.\,(13) is more interesting. It is time-dependent and displays how \( O(t) \) relaxes to its stationary limit. Note that the second term is a Fourier transformation of \( f f \) with respect to the variable \( \omega \). The transient dynamics of \( O(t) \) is determined by the asymptotic behavior of \( f f \) in the large-\( \omega \) limit, while the long-time asymptotic behavior of \( O(t) \) is determined by the asymptote of \( f f \) at small \( \omega \). In this way, \( f \) influences the dynamics of an arbitrary observable in the whole time scale, which is the reason why \( f \) is called the dynamical characteristic function.

In thermodynamic limit, two different situations can be distinguished in the long-time asymptotic behavior of \( O(t) \). First, since numerics already shows that \( f f \) always develops a plateau at small \( \omega \), if \( f \) converges in the limit \( \omega \to 0 \), according to Riemann-Lebesgue lemma, the Fourier transformation of \( f f \) must decay to zero in the limit \( t \to \infty \). The second term of Eq.\,(13) then vanishes in the long-time limit, and \( \lim_{t \to \infty} O(t) \) coincides with the value of \( O \) in the diagonal ensemble. In this case, the system thermalizes. Second, if \( f \) asymptotes to \( 1/\omega \) in the small-\( \omega \) limit, the second term goes to a nonzero value in the limit \( t \to \infty \). In this case, the system does not thermalize but evolves into a nonequilibrium steady state, in which the values of observables are different from their equilibrium counterparts. The failure of thermalization is attributed to the infinite imbalance in the initial state \( \rho \), which cannot be removed for thermalization to happen. Moreover, the first situation (thermalization) can be further classified according to whether \( O(t) \) relaxes in an exponential way or in a power-law way, etc., by supposing different asymptotic behavior of \( f(\omega) \) in the limit \( \omega \to 0 \). Therefore, Eq.\,(13) serves as a benchmark for understanding the nonequilibrium dynamics of chaotic quantum systems.

III. NUMERICAL SIMULATION OF THE DIAGONAL PART OF DENSITY MATRIX

Next, we test NESSH (Eqs.\,(5) and\,(6)) in spin lattice models. We consider the two-dimensional (2D) transverse field Ising model (TFIM) and the one-dimensional (1D) disordered XXZ model. The Hamiltonian of TFIM is

\[
\hat{H}_{\text{Ising}} = -J \sum_{\langle i,j \rangle} \sigma_i^x \sigma_j^x + g \sum_i \sigma_i^z,
\]

where \( \sigma_i^x \) and \( \sigma_i^z \) are the Pauli matrices. We consider only the interaction between nearest-neighbor sites. The ferromagnetic coupling \( J \) is set to the energy unit and \( g \) denotes the transverse field. The total number of lattice sites in numerical simulation is set to \( N \). This model has already been studied for testing ETH, and found to be chaotic\cite{26,27}. We choose the natural states \( |s\rangle \) to be the eigenstates of \( \{\sigma_i^z\} \). After a straightforward calculation, we obtain \( \sigma_i^z = N g^2 \) which is a constant, thereafter, the fluctuation of energy density is \( \frac{\sigma_i^z}{N} = \frac{g^2}{N} \), which goes to zero in the thermodynamic limit \( N \to \infty \), as we expect.

The second model we study is the one-dimensional XXZ model:

\[
\hat{H}_{\text{XXZ}} = -J \sum_i \left( \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z \right) + \sum_i h_i \sigma_i^z,
\]

where \( h_i \in [-h, h] \) is a random number with uniform distribution and \( h \) is the disorder strength. Again \( J \) is set to unity. The XXZ model without disorder is integrable, but infinitesimal disorder destroys integrability. As is well known, the XXZ model is in the many-body localized phase in the case of strong disorder. In our study, we control \( h \) to be small enough for avoiding localization.

In order to obtain the density matrix elements, we first diagonalize the model Hamiltonians. For the 2D-TFIM, we choose a lattice of specific shape that breaks the geometric symmetries (see Ref.\,[27] for detail). Similarly, there is a symmetry in the XXZ model. Following previous literatures\cite{28}, we focus on a subspace of the Hilbert space associated with the operator \( \hat{\sigma}^z = \sum_i \hat{\sigma}_i^z \). Only the subspace \( \sigma_i^z = 0 \) is considered. After diagonalization, we calculate the density matrix elements \( \rho_{\alpha \beta} = \langle \alpha | s \rangle \langle s | \beta \rangle \).

According to our assumption, the diagonal element \( \rho_{\alpha \alpha} \) is a Gaussian function blurred by the fluctuation \( C_s R_{s s} \).

![FIG. 1. (Color online) The plot of \((\bar{D}_{\alpha \alpha}D)\) as a function of \( \bar{E} \) for (a) 2D-TFIM with \( g = 2 \), \( \bar{E} = 1 \) and \( N = 12 \), and (b) the disordered XXZ chain with \( h = 0.05 \), \( \bar{E} = 1 \) and \( N = 16 \). The black solid lines are the Gaussian functions of \( \mu_s = 4.58 \times 10^{-6} \), \( \sigma_z^2 = 61.3 \), and \( \mu_s = -0.18 \), \( \sigma_z^2 = 3.73 \), respectively.](image)
The width of the energy shell is set to $2\Delta E = 2$ in practice to contain enough number of eigenstates. But it is worth mentioning that $\Delta E$ can be made smaller and smaller as the system’s size increases, since the density of states increases. And in thermodynamic limit, $\Delta E$ can be made arbitrarily small, while there are still infinite number of states in the shell. Fig. 1 shows $\rho_{\alpha\alpha}$ for (a) 2D-TFIM at $g = 2$ and $N = 12$ and (b) the XXZ model at $h = 0.05$ and $N = 14$. We choose $E = 0$ and $\omega = 1$ as the center of the energy box whose sides are set to $\Delta E = 0.1$ and $\Delta \omega = 0.1$. The red lines are the stable distributions with the parameters $a = 0.99$, $b = 0.05$, $c = 5.78 \times 10^{-5}$ and $\delta = -2.37 \times 10^{-6}$ for panel (a), and $a = 0.51$, $b = -5.51 \times 10^{-4}$, $c = 1.67 \times 10^{-5}$ and $\delta = -1.96 \times 10^{-9}$ for panel (b).

Next let us study $\rho_{\alpha\beta}$ for $\alpha \neq \beta$, which should be expressed as $D^{-3/2}f R_{\alpha\beta}^s$ according to our assumption. $R_{\alpha\beta}$ is a random number of zero mean and unit variance, therefore, $\rho_{\alpha\beta}$ should be a random number of zero mean and the variance $D^{-3}f^2$. We consider the set of $\rho_{\alpha\beta}$ within a small rectangular energy box centered at $(\bar{E}, \bar{\omega})$ with the sides $2\Delta E$ and $2\Delta \omega$, that is $\alpha$ and $\beta$ satisfy $\bar{E} - \Delta E < (E_0 + E_\beta)/2 < \bar{E} + \Delta E$ and $\omega - \Delta \omega < E_\alpha - E_\beta < \omega + \Delta \omega$. We choose small $\Delta E$ and $\Delta \omega$ so that $f$ and $D$ are approximately constants within the energy box, and then obtain the statistics of $
abla$
\(\rho_{\alpha\beta}\). Fig. 3 plots the distribution of \(\rho_{\alpha\beta}\). It is clear that the distribution is symmetric with respect to zero, indicating that the mean of \(\rho_{\alpha\beta}\) is zero. And the distribution function has a similar shape for the TFIM and XXZ models. It is also quite similar to that in the fermionic models studied previously. Since the distribution of \(\rho_{\alpha\beta}\) is indeed determined by the random number \(R\), our finding suggests that \(R_{\alpha\beta}\) has a universal distribution in arbitrary chaotic system.

We fit the histogram of \(\rho_{\alpha\beta}\) to the stable distribution (the red lines in Fig. 3), which is defined as the Fourier transformation

\[
P (x) = \frac{1}{2\pi} \int dp e^{-ip(x-\delta)} \times e^{-c|p|^4[1+ib \text{sign}(p) \tan(\pi a/2)(|c|p|^{2a-1}-1)]}
\]

with the parameters \(a, b, c\) and \(\delta\). \(\text{sign}(p)\) denotes the sign of \(p\). \(\delta\) is the location parameter, which is almost zero, indicating that the distribution is symmetric to zero. \(c\) is the scale parameter, which is also small. The shape parameters \(a\) and \(b\) measure the concentration and the asymmetry of the distribution, respectively.

![FIG. 4. (Color online) The variance of \(\rho_{\alpha\beta}\) as a function of \(\omega\) is plotted for TFIM. (a) \(\Sigma(\omega)\) at different system's size. (b) The plateau of \(\Sigma(\omega)\) at small \(\omega\) is plotted as a function of the system's size. The dotted line is the function 0.21|p|^{-3.31N}, (c) The functions \(\Sigma(\omega)\) for different initial states \(|s_1\rangle\) and \(|s_2\rangle\), whose spin configurations are depicted in panel (d) with the circles and squares representing the spins up and down, respectively.](image)

We study the variance of \(\rho_{\alpha\beta}\), denoted by \(\Sigma(E, \omega) = D^{-3}(E) f^2(E, \omega)\). \(\Sigma\) is no more than the squared dynamical characteristic function weighted by a factor \(D^{-3}\), which is exponentially small as the system's size increases. We average \(\Sigma\) over \(E\), and then obtain a function of \(\omega\). The averaged \(\Sigma\) reflects how the dynamical characteristic function changes with \(\omega\). The results are plotted in Fig. 4. \(\Sigma(\omega)\) is a smooth function of \(\omega\), as we expect. And it develops a plateau at small \(\omega\), indicating that the system will thermalize in the long-time limit (see the discussion in the previous section). The thermalizing consequence agrees with previous studies. For large \(\omega\), the dynamical characteristic function decays exponentially to zero. This is believed to be a typical feature of \(f\).

For \(N = 11\), \(\Sigma(\omega)\) displays a peak before the exponential decay (see Fig. 4(a)), which should be attributed to the small value that \(N\) takes. This peak vanishes as we choose \(N = 12\). We also see that the value of \(\Sigma\) decreases with increasing \(N\). This is due to the factor \(D^{-3}\) in the expression of \(\Sigma\), which decays exponentially as \(N\) increases. We denote the value of \(\Sigma\) at the plateau as \(S_d\) and display it as a function of \(N\) in Fig. 4(b). As we expect, \(S_d\) does decay exponentially.

In general, the dynamical characteristic function should be dependent on the initial state \(|s\rangle\). Fig. 4(c) shows \(\Sigma(\omega)\) for two different initial states \(|s_1\rangle\) and \(|s_2\rangle\), which are depicted in Fig. 4(d). As we see, their dynamical characteristic functions differ from each other, but the difference is not significant, indicating that the real-time dynamics starting from \(|s_1\rangle\) and \(|s_2\rangle\) has similar properties.

In this section, we focus on the dependence of \(\Sigma\) or \(f\) on \(\omega\), but neglect their dependence on \(E\). The former is more important, since the time-dependent observable \(O(t)\) is a Fourier transformation with respect to the variable \(\omega\) (see Eq. 9). The real-time dynamics is then sensitive to the dependence of \(f\) on \(\omega\).

V. THE CONNECTION BETWEEN NESSH AND ETH

In this section, we try to connect ETH, i.e. the assumption about the matrix elements of an observable operator \(\hat{O}\), to our assumption about the density matrix \(\rho = |s\rangle \langle s|\). For this purpose, we notice that the natural state \(|s\rangle\) can be chosen to the eigenstate of some observable operators. Without loss of generality, we suppose that \(|s\rangle\) is the eigenstate of \(\hat{O}\). And all the natural states form a complete basis of the Hilbert space, satisfying \(\sum_s |s\rangle \langle s| = 1\). In this natural basis, \(O_{\alpha\beta} = |s\rangle \langle \alpha| \hat{O} |s\rangle\) is a diagonal matrix. The matrix elements of the observable in the eigenbasis of the Hamiltonian can then be expressed as

\[
O_{\alpha\beta} = \sum_s O_{ss} \rho_{\alpha\beta},
\]

where \(\rho_{\alpha\beta} = \langle \alpha|s\rangle \langle s|\beta\rangle\) denotes the element of the density matrix.

NESSH states that \(\rho_{\alpha\beta}\) has a universal expression in chaotic systems (see Eqs. 5 and 6). Therefore, our target is to use Eqs. 5 and 6 to prove that \(O_{\alpha\alpha}\) changes
smoothly with $E_{\alpha}$, which is the central idea of ETH for explaining thermalization. Substituting Eqs. 5 and 10 into Eq. (13), we obtain

$$O_{\alpha\alpha} = \sum_s D^{-1}(E_{\alpha})O_{ss}\rho(E_{\alpha})$$

$$= \sum_s D^{-1}O_{ss} \frac{1}{\sqrt{2\pi}\sigma_{ss}^2} e^{-\frac{(E_{\alpha}-\mu_s)^2}{2\sigma_{ss}^2}} + \sum_s O_{ss}D^{-1}C_s R_{\alpha\alpha}^s. \tag{16}$$

Our numerics has shown that $D^{-1}C_s R_{\alpha\alpha}^s$ goes to zero in thermodynamic limit (see Fig. 2 and the corresponding discussion). And since $R_{\alpha\alpha}^s$ is a random number of zero mean independent of $O_{ss}$, we have sufficient reason to believe that $\sum_s O_{ss} D^{-1} C_s R_{\alpha\alpha}^s \to 0$ in thermodynamic limit.

Next we use 2D-TFIM as an example to show that the first term in Eq. (16) changes smoothly with $E_{\alpha}$ in the limit $N \to \infty$. The observable operator is chosen to be $O = \hat{\sigma}_z^i$ with $i$ denoting the bottom site in Fig. 4(d). The first term of Eq. (16) is the sum of a series of Gaussian functions weighted by $O_{ss}$. $O_{ss}$ is usually bounded, and the sum of finite number of Gaussian functions must changes smoothly. In order to extend this conclusion to the limit $N \to \infty$, we compute the derivative

$$O'_{\alpha\alpha} = \sum_s O_{ss} \frac{d}{dE_{\alpha}} \left( D^{-1} \frac{1}{\sqrt{2\pi}\sigma_{ss}^2} e^{-\frac{(E_{\alpha}-\mu_s)^2}{2\sigma_{ss}^2}} \right). \tag{17}$$

And we define $O'_{\alpha\alpha}^{\text{max}}$ as the maximum of $|O'_{\alpha\alpha}|$ over $\alpha$. A scaling analysis of $O'_{\alpha\alpha}^{\text{max}}$ is given in Fig. 5 which clearly shows that $O'_{\alpha\alpha}^{\text{max}}$ converges in the limit $N \to \infty$. This means that $O_{\alpha\alpha}$ has a finite derivative at arbitrary energy, i.e., $O_{\alpha\alpha}$ changes smoothly with $E_{\alpha}$. We then reach the central idea of ETH and also the basis of thermalization - $O_{\alpha\alpha}$ does not fluctuate infinitely with $\alpha$ even in thermodynamic limit.

VI. SUMMARY

We summarize our results. NESSH assumes a universal form of the density matrix in the eigenbasis of the Hamiltonian of a quantum chaotic system. The main assumption of NESSH is given in Eq. (2). The diagonal element of the density matrix $\rho_{ss}$ is a Gaussian function, with the mean $\mu_s$ and the variance $\sigma_{ss}^2$ determined by the initial state. The off-diagonal elements $\rho_{s\bar{s}}$ are random numbers with a universal distribution. Its standard deviation is dubbed the dynamical characteristic function, which governs the real-time dynamics of the system according to Eq. (9). For a typical initial state that thermalizes in the long-time limit, the dynamical characteristic function exhibits a plateau at low frequencies but an exponential decay at high frequencies.

We provide the numerical evidence of NESSH in two chaotic spin models - the 2D transverse field Ising model and the 1D disordered XXZ model. The numerics for these two models is consistent with the prediction of NESSH, both for the diagonal and off-diagonal elements. Furthermore, we show how to reach ETH from the assumptions of NESSH by factorizing the observable matrix elements into the density matrix elements and the expectation value of observable in the natural basis. By using the assumptions of NESSH, we show that the diagonal element of the observable matrix changes smoothly with energy, which explains why thermalization happens.

ACKNOWLEDGEMENTS

This work is supported by NSF of China under Grant Nos. 11774315 and 11304280. Pei Wang is also supported by the Junior Associates programm of the Abdus Salam International Center for Theoretical Physics.

1 I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
2 A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, Rev. Mod. Phys. 83, 863 (2011).
3 J. Eisert, M. Friesdorf, and C. Gogolin, Nat. Phys. 11, 124 (2015).
4 M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, Phys. Rev. Lett. 98, 050405 (2007).

\text{wangpei@zjnu.cn}
5 M. Rigol, V. Dunjko, and M. Olshanii, Nature 452, 854 (2008).
6 J. von Neumann, Z. Phys. 57, 30 (1929).
7 S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, Eur. Phys. J. H 35, 173 (2010).
8 E. Wigner, Ann. Math. 62, 548 (1955).
9 E. Wigner, Ann. Math. 65, 203 (1957).
10 E. Wigner, Ann. Math. 67, 325 (1958).
11 N. Rosenzweig and C. E. Porter, Phys. Rev. 120, 1698 (1960).
12 T. A. Brody, J. Flores, J. B. French, P. Mello, A. Pandey, and S. S. Wong, Rev. Mod. Phys. 53, 385 (1981).
13 O. Bohigas, M.-J. Giannoni, and C. Schmit, Phys. Rev. Lett. 52, 1 (1984).
14 M. R. Schroeder, J. Audio. Eng. Soc. 35, 299 (1987).
15 T. Guhr, A. Müller-Groeling, and H. A. Weidenmüller, Phys. Rep. 299, 189 (1998).
16 M. V. Berry and M. Tabor, Proc. Roy. Soc. A 356, 375 (1977).
17 J. M. Deutsch, Phys. Rev. A 43, 2046 (1991).
18 M. Srednicki, Phys. Rev. E 50, 888 (1994).
19 M. Srednicki, J. Phys. A: Math. Gen. 32, 1163 (1999).
20 L. D’Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol, Adv. Phys. 65, 239 (2016).
21 K. R. Fratus and M. Srednicki, Phys. Rev. E 92, 040103 (2015).
22 I. V. Gornyi, A. D. Mirlin, and D. G. Polyakov, Phys. Rev. Lett. 95, 206603 (2005).
23 D. Basko, I. Aleiner, and B. Altshuler, Ann. Phys. 321, 1126 (2006).
24 P. Wang, J. Stat. Mech. 2017, 093105 (2017).
25 V. Kravtsov, arXiv preprint arXiv:0911.0639 (2012).
26 R. Mondaini and M. Rigol, Phys. Rev. E 96, 012157 (2017).
27 R. Mondaini, K. R. Fratus, M. Srednicki, and M. Rigol, Phys. Rev. E 93, 032104 (2016).
28 C. L. Bertrand and A. M. García-García, Phys. Rev. B 94, 144201 (2016).