Finite-Size Scaling Analysis of the Eigenstate Thermalization Hypothesis in a One-Dimensional Interacting Bose gas

Tatsuhiko N. Ikeda1, Yu Watanabe2, and Masahito Ueda1

1Department of Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
2Yukawa Institute for Theoretical Physics, Kyoto University, Kitashirakawa Oiwake-Cho, 606-8502 Kyoto, Japan

(Dated: December 4, 2012)

By calculating correlation functions for the Lieb-Liniger model based on the algebraic Bethe ansatz method, we conduct a finite-size scaling analysis of the eigenstate thermalization hypothesis (ETH) which is considered to be a possible mechanism of thermalization in isolated quantum systems. We find that the ETH in the weak sense holds in the thermodynamic limit even for an integrable system although it does not hold in the strong sense. Based on the result of the finite-size scaling analysis, we compare the contribution of the weak ETH to thermalization with that of yet another thermalization mechanism, the typicality, and show that the former gives only a logarithmic correction to the latter.

PACS numbers: 05.30.-d, 03.65.-w

Introduction. — Recently, there has been a resurgence of interest in understanding thermalization from quantum mechanics [1, 2] due in part to experimental techniques in ultracold atomic gases which enable one to prepare, control, and measure isolated quantum systems [3, 4], and also due to several theoretical advances [5–10]. Among possible mechanisms for thermalization, the eigenstate thermalization hypothesis (ETH) has attracted much attention [8, 13, 10]. The ETH states that the expectation value of an observable stays the same over many-body eigenstates having close eigenenergies in the thermodynamic limit. The validity of the ETH has been examined by using the numerical diagonalization of the Hamiltonian [6, 15, 10]. It has been claimed that the ETH holds for the case in which the system is non-integrable or chaotic [6, 13, 20]. These studies focus on the dependence on the characteristics of the system such as geometrical configurations and parameter sets, whereas the size of the system cannot be changed sufficiently due to an exponential growth of the numerical cost. However, since the ETH concerns the thermodynamic limit, it is essential to analyze the finite-size scaling of the ETH.

In this Rapid Communication, we identify the finite-size scaling properties of the ETH by calculating the correlation functions over each many-body eigenstate for the Lieb-Liniger model [21] in which the Bethe ansatz method allows us to obtain the exact many-body eigenstates and thus to circumvent the numerical difficulty in diagonalizing the Hamiltonian. We show the ETH holds in the weak sense but does not hold in the strong sense. (The definitions of weak and strong will be given below [22].) In particular, the weak ETH becomes better satisfied for larger systems according to the power law in the number of particles of the system. This suggests that there exist situations in which the microcanonical ensemble is applicable to integrable systems in the thermodynamic limit, while the generalized microcanonical or Gibbs ensemble leads to better predictions in such systems including the Lieb-Liniger model [23, 32]. Then, by using the result of the finite-size scaling of the weak ETH, we discuss the quantitative relation between the ETH and the typicality [6, 11–13], the latter being yet another possible mechanism of thermalization in isolated quantum systems. We find that the ETH contributes to thermalization at most as a logarithmic correction to the typicality.

Formulation of the Problem. — We consider an isolated quantum many-body system whose Hamiltonian is $H$. We denote each eigenstate of $H$ with eigenenergy $E_i$ as $|E_i\rangle$ and expand the initial state $|\psi_0\rangle$ in terms of them: $|\psi_0\rangle = \sum_i C_i |E_i\rangle$. Then, the state at time $t$ is given by $|\psi_t\rangle = \sum_i C_i e^{-iE_i t/\hbar} |E_i\rangle$. Here, we assume the condition of non-degenerate energy gaps [14] which states that if $E_i - E_j = E_k - E_l \neq 0$, then $E_i = E_k$ and $E_j = E_l$. Then, according to the study of equilibration [6, 14], if the inverse participation ratio $Q^{-1} = \sum_i |C_i|^2$ is sufficiently large, the time-dependent expectation value of an observable $A$ relaxes to its long-time average:

$$\langle \psi_t | A | \psi_t \rangle \longrightarrow \langle A \rangle_{LT} \equiv \lim_{T \to \infty} \int_0^T dt \frac{dT}{T} \langle \psi_t | A | \psi_t \rangle \quad (1)$$

which means that the fluctuation of $\langle \psi_t | A | \psi_t \rangle$ around $\langle A \rangle_{LT}$ becomes negligible in the long run [6]. We note that the long-time average of $A$ can be rewritten as $\langle A \rangle_{LT} = \sum_i |C_i|^2 \langle E_i | A | E_i \rangle$ unless the Hamiltonian $H$ has degeneracy (see Ref. [14] for the generalization to the case in which $H$ has degeneracies). This is because the relative phases of the eigenstates become random and off-diagonal contributions in $\langle \psi_t | A | \psi_t \rangle$ vanish.

Thus, the microcanonical ensemble is applicable if $\langle A \rangle_{ME} = \langle A \rangle_{LT}$, where the microcanonical ensemble average is defined as follows:

$$\langle A \rangle_{ME} = N_{\text{state}}^{-1} \sum_{E_i \in [E - \delta, E + \delta]} \langle E_i | A | E_i \rangle . \quad (2)$$

Here, $E \equiv \langle \psi_0 | H | \psi_0 \rangle$ is the total energy of the system, $\delta$ is a macroscopically small energy width, and $N_{\text{state}}$ is the number of the eigenstates in the microcanonical window $[E - \delta, E + \delta]$. For the sake of convenience, we assume that the initial state has no weight
Because outside the microcanonical window, \( i.e., C_i = 0 \) if \( E_i \not\in [E - \delta, E + \delta] \). To find the underlying mechanism for \((A)_{\text{ME}} = (A)^{\text{LT}}\), we must clarify the behavior of the eigenstate expectation value (EEV), \( (E_i | A | E_i) \). The ETH states that the EEV stays constant over a microcanonical window in the thermodynamic limit. However, since numerical analyses can only address finite-size systems, there always exist some fluctuations in the EEV which we call the ETH noise. To quantify how well the ETH holds, we consider the variance of the ETH noise \( \sigma_A^2 = N_{\text{state}}^{-1} \sum E_i \in [E - \delta, E + \delta] \left( (E_i | A | E_i) - (A)_{\text{ME}} \right)^2 \) and the support \( s_A \equiv \max_{E_i \in [E - \delta, E + \delta]} \langle E_i | A | E_i \rangle - \min_{E_i \in [E - \delta, E + \delta]} \langle E_i | A | E_i \rangle \). The ETH can then be interpreted in the weak and the strong sense as \( \sigma_A \rightarrow 0 \) and \( s_A \rightarrow 0 \) in the thermodynamic limit, respectively [22].

The weak ETH allows an infinitesimal fraction of eigenstates, called rare states [22], that make EEV’s deviate from their local averages. Since the difference between \((A)_{\text{ME}}\) and \((A)^{\text{LT}}\) is bounded from above by \( s_A \), the strong ETH ensures \((A)_{\text{ME}} = (A)^{\text{LT}}\) for any initial state. On the other hand, the weak ETH ensures \((A)_{\text{ME}} = (A)^{\text{LT}}\) for initial states satisfying \( Q = O(N_{\text{state}}) \) because the difference between \((A)_{\text{ME}}\) and \((A)^{\text{LT}}\) is bounded through the Schwarz inequality as

\[
\langle (A)_{\text{ME}} - (A)^{\text{LT}} \rangle \leq s_A \sqrt{N_{\text{state}}} Q - 1. \tag{3}
\]

Because \( Q^{-1} \) represents an effective number of manybody eigenstates in the initial state, this assumption states that the initial state includes a large number of manybody eigenstates. This condition is satisfied for quantum quench systems in nonintegrable systems [33] and suggested to be satisfied for those from nonintegrable to integrable systems [32]. However, this is not satisfied for quench systems within integrable systems; the microcanonical description actually breaks down for this case [32, 33]. In this case, the generalized microcanonical or Gibbs ensemble are known to better predict the long-time average than the microcanonical ensemble [23, 32].

Model. — We analyze the finite-size scaling of the ETH noise by invoking the Lieb-Liniger model, which describes a one-dimensional Bose gas with a delta-function interaction. The Hamiltonian is given in units of \( \hbar = 2m = 1 \) as

\[
H = \int_0^L dx \left[ \partial_x \Psi^\dagger(x) \partial_x \Psi(x) + c \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x) \right], \tag{4}
\]

where \( \Psi(x) \) is the bosonic field operator, \( L \) the linear dimension of the system, \( c \) the strength of the contact interaction, and the periodic boundary condition is assumed. The \( N \)-body eigenstates are constructed from the monodromy matrix [33] given by

\[
\begin{pmatrix}
A(\lambda) \\
B(\lambda) \\
C(\lambda) \\
D(\lambda)
\end{pmatrix}
\equiv P \exp \left[ -i \int_0^L dx \left( -\frac{\lambda/2}{\sqrt{\sigma(x)}} \frac{\sqrt{\sigma(x)}}{-\lambda/2} \right) \right] .
\tag{5}
\]

where \( P \) and \( \cdots : \) denote path ordering and normal ordering of bosonic field operators, respectively. The \( N \)-body eigenstate can be obtained by operating \( B(\lambda) \) \( N \)-times on the Fock vacuum \( |0\rangle \), \( \langle \{ \lambda_j \} N \rangle = \prod_{j=1}^N B(\lambda_j) |0\rangle \), provided that the set of parameters \( \{ \lambda_j \}_{j=1}^N \) satisfy the Bethe equations

\[
e^{i\lambda_j L} = -\prod_{k=1}^N \frac{\lambda_j - \lambda_k + ic}{\lambda_j - \lambda_k - ic} \quad (j = 1, 2, \ldots, N). \tag{6}
\]

Since the energy and momentum of this state are given by \( E = \sum_{j=1}^N \lambda_j^2 \) and \( P = \sum_{j=1}^N \lambda_j \), the set of parameters \( \{ \lambda_j \}_{j=1}^N \) may be interpreted as representing the momenta of the dressed noninteracting particles.

Correlation Function. — We consider the real and imaginary parts of the EEV of the quantity \( \Psi^\dagger(x) \Psi(0) \), \( i.e., \langle \{ \lambda_j \} | \Psi^\dagger(x) \Psi(0) | \{ \lambda_j \} \rangle \). These correspond to the EEVs of Hermitian operators \( \Psi^\dagger(x) \Psi(0) \)/2 and \( | \Psi^\dagger(x) \Psi(0) \rangle/2i \), respectively. They have also been measured experimentally [36]. These quantities are of great importance because they reflect the off-diagonal long-range order. Substituting \( \Psi^\dagger(x) = e^{-i P x} \Psi(0) e^{i P x} \) and inserting the completeness relation for the \((N - 1)\)-body eigenstates, we obtain

\[
\langle \{ \lambda_j \} | \Psi^\dagger(x) \Psi(0) | \{ \lambda_j \} \rangle
\]

\[
= \sum_{\{ \mu_k \}_{N-1}} e^{-i \sum_{j=1}^N \lambda_j - \sum_k \mu_k x} | \langle \{ \mu_k \} | \Psi^\dagger(0) | \{ \lambda_j \} \rangle |^2 , \tag{7}
\]

where the summation is taken over all the \((N - 1)\)-body eigenstates. The form factor \( \langle \{ \mu_k \} | \Psi(0) | \{ \lambda_j \} \rangle \) is reduced to \( N \) scalar products \( \langle \{ \mu_k \} | \lambda_j \rangle \neq i \) \( (i = 1, 2, \ldots, N) \) [37], which are represented by the determinants of \((N - 1) \times (N - 1)\) matrices [38]. The crucial observation is that these determinants can be summed up, giving a single determinant of an \( N \times N \) matrix [33]. This algebraic manipulation greatly reduces the computational task, enabling us to conduct a finite-size scaling for \( N \) as large as 35.

By increasing \( N \) and \( L \) with their ratio held fixed, we calculate the real and imaginary parts of the quantities \( \langle \{ \lambda_j \} | \Psi^\dagger(x) \Psi(0) | \{ \lambda_j \} \rangle \), as plotted in Fig. 1. We set the parameters as \( c = 10 \) and \( x = 1/2 \), where the unit of length is taken to be the mean distance between particles \( L / N \). The energy window is taken as \([E_g, E_g + 10]\), where, \( i.e., E_g \) is the ground-state energy which depends on the size of the system [40]. The summation on the RHS of Eq. (7) is taken over the \((N - 1)\)-body eigenstates with energy up to 25. Then, all the data have
been obtained with accuracy over 97%. We have plotted all energy eigenstates in the energy window. The analyses of the ETH based on these data go as follows.

First, we consider the support of the ETH noise to examine the strong ETH. We fit each data with the least-squares method and subtract the fitted line from the data. Then, we define the support of the ETH noise, $s$, by the difference between the maximum and minimum of the subtracted data [41]. The support is plotted against the number of particles in Fig. 2. The data shows that, for both of the real and imaginary parts, there exist jumps between $N = 15$ and $N = 16$, which prevent the supports from decreasing monotonically. The origin of the jumps can be seen in the EEV’s for $N = 20$ shown in Fig. 1, where a pair of side branches indicated by circles emerge. Such branches begin to appear at $N = 16$ which explains a sudden jump in Fig. 2. We may expect similar side branches to appear as we increase the system size. These additional branches, which are constituted from what are called rare states [22], invalidate the strong ETH.

Second, we consider the variance of the data to examine the weak ETH. Since both the real and imaginary parts distribute around lines, we identify the variance of the data $\sigma$ as the residual error of the least-squares method [41]. The dependence of $\sigma$ on the size of the system is illustrated in Fig. 3, which shows that the ETH noise decays as $\sigma \propto N^{-\alpha}$, where the exponent $\alpha$ is determined by the least-squares fit to be $\alpha = 1.43 \pm 0.04$ and $0.786 \pm 0.008$ for the real and imaginary parts, respectively. These results show that the weak ETH becomes better satisfied as we approach the thermodynamic limit, despite the fact that the Lieb-Liniger model is integrable, whereas previ-
ous studies [8, 18, 20] showed that the ETH holds worse in integrable systems than in non-integrable chaotic systems at a fixed size of the system. Our result implies that, if the inverse participation ratio of the initial state is sufficiently large, the microcanonical ensemble is applicable also to integrable systems in the thermodynamic limit. It is known that we can construct a special class of initial states which give near-thermal distributions in integrable systems but conserved quantities do not become arbitrarily close to thermal expectation values even in the thermodynamic limit [34, 43]. On the other hand, our results show that expectation values of non-conserved quantities converge to the thermal expectation values as we increase the system size.

Interplay between ETH and Typicality.— Now that we have identified the power-law scaling of the ETH noise, we can discuss which of the weak ETH and the typicality [6, 11–13] dominantly contributes to thermalization. The typicality concerns the universal statistical-mechanical properties that are shared by randomly generated quantum states. Here, we follow the typicality argument and show that the long-time average is close to the microcanonical ensemble average for almost all initial states. We assume that the initial state is a linear combination of the many-body eigenstates in an energy window: \( |\psi\rangle = \sum_{i=1}^{N_{\text{state}}} C_i |E_i\rangle \), where the set of the coefficients \( \{C_i\}_{i=1}^{N_{\text{state}}} \) satisfy the normalization condition \( \sum_{i=1}^{N_{\text{state}}} |C_i|^2 = 1 \). Namely, \( 2N_{\text{state}} \) parameters \( \text{Re} C_i \) and \( \text{Im} C_i \) (\( i = 1, 2, \ldots, N_{\text{state}} \)) can be represented as a point on the \( (2N_{\text{state}} - 1) \)-dimensional sphere whose radius is 1. We denote the average over the uniform measure on the high-dimensional sphere as an orbit. For example, \( C_i = 0 \) and \( |C_i|^2 = 1/N_{\text{state}} \). Then, the initial-state average of a long-time-averaged quantity is given by \( \langle A \rangle_{\text{LT}} = \langle A \rangle_{\text{ME}} \), and the variance is obtained as

\[
V_A = \frac{\langle A \rangle_{\text{LT}} - \langle A \rangle_{\text{ME}}^2}{N_{\text{state}} + 1},
\]

where \( \sigma_A^2 \equiv N_{\text{state}}^{-1} \sum_{E_i \in E} \langle E_i | A | E_i \rangle - \langle A \rangle_{\text{ME}}^2 \).

Thus, the typical magnitude of the difference between the long-time average and the microcanonical ensemble average is given by \( \sqrt{V_A} \sim \sigma_A N_{\text{state}}^{-1/2} \). Since \( \sigma_A \propto N^{-\alpha} \) and \( N_{\text{state}} \sim e^{N^\gamma} \), the scaling of the typical magnitude of the difference turns out to be

\[
\exp \left( -\frac{1}{2} N - \alpha \ln N \right).
\]

The first and second terms in the exponent describe the contributions from the typicality and the ETH, respectively. In this sense, the ETH contributes to thermalization at most as a logarithmic correction to the typicality.

Conclusions and Discussions.— In this Letter, we have conducted a finite-size scaling analysis of the ETH by applying the algebraic Bethe ansatz method to the Lieb-Liniger model, and shown that the weak ETH holds in the sense that the variance of the ETH noise vanishes as a power law in the number of particles of the system. The weak ETH does not necessarily mean the applicability of the microcanonical ensemble for any initial state due to rare states [22]. We have shown that the microcanonical ensemble is applicable even in integrable systems if the inverse participation ratio of the initial state is sufficiently large. The thermalization problem for the case in which the inverse participation ratio is not that large remains an open question.

The finite-size scaling analysis has enabled us to study the quantitative relations between the ETH and yet another scenario for thermalization, the typicality. We find that the contribution of the ETH to thermalization is at most a logarithmic correction to that of the typicality. This originates from the fact that the ETH is the effect of the order of some powers of the degree of freedom of the system, whereas the typicality argument utilizes the immense dimensionality of the Hilbert space that grows exponentially with increasing the degrees of freedom. The scaling relation (9), which includes the ETH as a small correction to other factors is obtained by invoking the properties of energy eigenstates. However, the fact that it has been derived by the typicality (see Eq. (9)), which relies only on the immense dimensionality of the Hilbert space with a uniform Haar measure, strongly suggests that the obtained relation holds quite generally. This finding merits further study.

Acknowledgements.— This work was supported by KAKENHI 22340114, a Grant-in-Aid for Scientific Research on Innovation Areas “Topological Quantum Phenomena” (KAKENHI 22103005), a Global COE Program “the Physical Sciences Frontier”, and the Photon Frontier Network Program, from MEXT of Japan. T. I. acknowledges the JSPS for financial support (Grant No. 248408).

[1] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, Rev. Mod. Phys. 83, 863 (2011).
[2] V. I. Yukalov, Laser Phys. Lett. 8, 485 (2011).
[3] T. Kinoshita, T. Wenger, and D. S. Weiss, Nature 440, 900-903 (2006).
[4] S. Trotzky, Y.-A. Chen, A. Flesch, I. P. McCulloch, U. Schollwöck, J. Eisert, and I. Bloch, Nature Physics 8, 325 (2012).
[5] H. Tasaki, Phys. Rev. Lett. 80, 1373 (1998).
[6] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghi, Phys. Rev. Lett. 96, 050403 (2006).
[7] P. Reimann, Phys. Rev. Lett. 101, 190403 (2008).
[8] M. Rigol, V. Dunjko, and M. Olshanii, Nature (London) 452, 854 (2008).
[9] C. Gogolin, M. P. Müller, and J. Eisert, Phys. Rev. Lett. 106, 040401 (2011).
[10] T. N. Ikeda, Y. Watanabe, and M. Ueda, Phys. Rev. E 84, 021130 (2011).
[11] S. Popescu, A. J. Short, and A. Winter, Nature Physics 2, 754 (2006).
[12] A. Sugita, RIMS Kokyuroku (in Japanese) 1507, 147 (2006).
[13] P. Reimann, Phys. Rev. Lett. 99, 160404 (2007).
[14] A. J. Short, New Journal of Physics 13, 053009 (2011).
[15] J. M. Deutsch, Phys. Rev. A 43, 2046 (1991).
[16] M. Srednicki, Phys. Rev. E 50, 888 (1994).
[17] M. Horoi, V. Zelevinsky, and B. A. Brown, Phys. Rev. Lett. 74, 5194 (1995).
[18] M. Rigol, Phys. Rev. Lett. 103, 100403 (2009).
[19] M. Rigol and L. F. Santos, Phys. Rev. A 82, 011604(R) (2010).
[20] L. F. Santos and M. Rigol, Phys. Rev. E 82, 031130 (2010).
[21] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605-1616 (1963); E. H. Lieb, Phys. Rev. 130, 1616-1624 (1963).
[22] G. Biroli, C. Kollath, and A. M. Läuchli, Phys. Rev. Lett. 105, 250401 (2010).
[23] M. Rigol, A. Muramatsu, and M. Olshanii, Phys. Rev. A 74, 053616 (2006).
[24] M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, Phys. Rev. Lett. 98, 050405 (2007).
[25] A. C. Cassidy, C. W. Clark, and M. Rigol, Phys. Rev. Lett. 106, 140405 (2011).
[26] T. Barthel and U. Schollwöck, Phys. Rev. Lett. 100, 100601 (2008).
[27] M. A. Cazalilla, Phys. Rev. Lett. 97, 156403 (2006).
[28] A. Iucci and M. A. Cazalilla, Phys. Rev. A 80, 063619 (2009).
[29] P. Calabrese and J. Cardy, J. Stat. Mech., P06008 (2007).
[30] M. Eckstein and M. Kollar, Phys. Rev. Lett. 100, 120404 (2008).
[31] M. Kollar and M. Eckstein, Phys. Rev. A 78, 013626 (2008).
[32] J. Mossel and J. -S. Caux, New J. Phys. 14 075006 (2012).
[33] L. F. Santos, A. Polkovnikov, and M. Rigol, Phys. Rev. Lett. 107, 040601 (2011).
[34] M. Rigol and M. Srednicki, Phys. Rev. Lett. 108, 110601 (2012).
[35] V. E. Korepin, N. M. Bogoliubov, and A. G. Izergin, Quantum inverse scattering method and correlation functions, Cambridge (1997).
[36] I. Bloch, T. W. Hänsch, and T. Esslinger, Nature 403, 166 (2000).
[37] A. G. Izergin, V. E. Korepin, and N. Y. Reshetikhin, J. Phys. A 20, 4799-4822 (1987).
[38] N. A. Slavnov, Theor. Math. Phys. 79, 502-508 (1989).
[39] T. Kojima, V. E. Korepin, and N. A. Slavnov, Commun. Math. Phys. 188, 657-689 (1997).
[40] We set the microcanonical window not by energy per particle but by energy itself for the following two reasons. First, the energy window is closely related to the finiteness of the resolution of experimental apparatuses to measure energy which is evaluated by the absolute value of energy. Second, it is not taken as energy per particle in most of the references, for example Ref. [8]. However, the essential results are not changed whichever notation is used.
[41] The microcanonical window should, in principle, be chosen so small that the microcanonical average is almost independent of the width, but our choice, $[E_g, E_g + 10]$, does not satisfy this condition. The width is chosen for a mathematical trick which enables us to utilize more data points. After subtracting the systematic linear behaviors as we do in the manuscript, we can address a decent number of data points to obtain the variance of the EEV’s. This trick does not essentially change our results.
[42] M. Rigol and M. Fitzpatrick, Phys. Rev. A 84, 033640 (2011).
[43] M. -C. Chung, A. Iucci and M. A. Cazalilla, New Journal of Physics 14 075013 (2012).