Relaxation to equilibrium in macroscopic quantum systems

— foundation of statistical mechanics —

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1 Introduction

The relaxation to equilibrium is a fundamental irreversible process. It is our experience that isolated thermodynamic systems would eventually relax to a stationary state called equilibrium[1, 2]. In thermodynamics, this statement is regarded as requirements for the relevant choice of the model and its macroscopic descriptions. Recently, it is shown that equilibrium states are very popular in the extremely large Hilbert space of state vectors for macroscopic quantum systems[3, 4, 5, 6, 7, 8, 9, 10]. The expectation values with respect to a randomly sampled pure state are typically well described by equilibrium ensembles[3, 8, 10]. And it is expected that initial nonequilibrium state approaches to the typical state of equilibrium. Then it is reasonable to explore a dynamical explanation for the macroscopically observed behavior of the relaxation to equilibrium[4, 5, 7]. Indeed the coarsgrained macroscopic quantities typically yield a decomposition of the total Hilbert space with a subspace of overwhelming dimension which represents equilibrium[4, 5]. Based on this property, arbitrary state approaches and stays near equilibrium[4, 5], which is a version of quantum ergodic theorem[11].

Professor S.Tasaki regarded the microscopic justification of the relaxation processes as an important unsolved problem. He also emphasized that the definition of the typical state or the choice of relevant measure for random sampling is crucial. Typical states are macroscopically entangled and role of entanglement would be also important[8, 10]. As he pointed out, the issue on the relaxation is also important in the context of nonequilibrium theorems[15, 16], which relies on the use of thermodynamic ensembles. For the isolated system, the relaxation is not guaranteed for the total density matrix itself. Indeed the total density matrix does not actually relax to a thermal state in the course of unitary time evolution. Also, for classical systems, there exist exceptional integrable systems which do not reach an equilibrium state even after a long waiting time due to the conserved quantities. For isolated quantum systems, there are

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always conservative quantities such as projection operators on a specific energy eigenstates[7, 10, 9, 13, 14]. Thermalization would not occur for the expectation values of these microscopic quantities, however, our interest lies in the expectation values of quantities consists of a sum of local quantities such as the magnetization of a long spin chain, the energy or number of particles in a certain part of a box, and other extensive quantities of thermodynamics.

We insist that the expectation values of macroscopic quantities typically show relaxation to the equilibrium values. Especially, it is pointed out that the off-diagonal elements of the density matrix does not contribute to the expectation values. In this article, we explain how the statement is made quantitative for the time-dependent unitary time evolution. And the explanation is numerically verified for a spin chain with a magnetic field. This article is organized as follows. In Sec.2, we present our model with the precise external forcing procedure. In Sec.3, the relaxation of the expectation values are explained. In Sec.4, we show that the entropy at final state is well-defined. Sec.5 is devoted to a summary.

2 Macroscopic systems

Let us consider a macroscopically large but finite initially isolated system. After initial time $t = 0$, an external forcing acts on the system, and the total Hamiltonian $H(t)$ depends on time. Until $t = 0$, the density matrix describing the initial state is assumed to be microcanonical specified by an energy E

$$\rho(0) = \frac{1}{\Omega(0)}\delta(E - H(0)), \tag{1}$$

where $\Omega(0)$ is the density of the states. In actual, the energy scale is specified with a finite precision $[E, E+\delta E]$, and we assume that sufficiently many eigenenergies belong to the interval. In the course of time evolution, the external work is done on the system through the time dependence of $H(t)$.

The deterministic external forcing acts during the time interval $0 \leq t \leq T_0$, and switched off for $t > T_0$. It is expected that after a sufficiently long waiting time, i.e. at $t = T \gg T_0$, the density matrix reaches a state which yields approximately the same expectation values as the microcanonical ensemble $\rho(T) = \frac{1}{\Omega(T)}\delta(E + \Delta E - H(T))$ with an energy shift ΔE due to the work done.

3 Relaxation of the expectation values

It is our statement that the microcanonical ensemble well approximates actual expectation value of macroscopic quantity A whose maximum eigenvalue polynomially depends on the system size and contains various matrix elements with respect to the eigenenergy

$$\mathrm{Tr}U\rho(0)U^{+}A \cong \mathrm{Tr}\rho(T)A. \tag{2}$$

This evaluation shows that the relaxation to equilibrium is explained as the property of the expectation values instead of the density matrix.

The actual final state is reached by a unitary time evolution

$$\begin{aligned} & U\rho(0)U^{+} \\ = \; & e^{-\frac{i}{\hbar}H(T)(T-T_0)}U(T_0)\rho(0)U(T_0)^{+}e^{\frac{i}{\hbar}H(T)(T-T_0)} \\ = \; & \sum_{n,m} c_{n,m}|E_n\rangle\langle E_m|, \end{aligned} \tag{3}$$

where we presented the eigenstate of $H(T)$ as $H(T)|E_n\rangle = E_n|E_n\rangle$, $c_{n,m} = e^{-\frac{i}{\hbar}(E_n-E_m)(T-T_0)}\langle E_n|U(T_0)\rho(0)U(T_0)^{+}|E_m\rangle$, and $U(T_0) = T\{e^{-\int_0^{T_0}\frac{i}{\hbar}H(t)dt}\}$. After $t = T_0$, the total system is isolated, and evolves by the Hamiltonian $H(T)$. On the other hand, the off-diagonal elements of the physical quantity A is negligible compared to the diagonal elements:

i) The off-diagonal matrix element $\langle E_n|A|E_m\rangle$ is typically negligible in the macroscopic limit. Physically, this would be reasonable since it means that transition amplitudes between macroscopically different states due to the perturbation A are extremely small[17]. We shall give a quantitative explanation of this statement. The analysis is based on the high-dimensionality of the Hilbert space as in Refs.[3, 6, 8, 10]. Let us diagonalize the quantity A as

$$A = \sum_n A_n|A_n\rangle\langle A_n|, \tag{4}$$

and define its square root

$$B = \sum_n \sqrt{A_n}|A_n\rangle\langle A_n|. \tag{5}$$

Here the spectrum $\{A_n\}$ is assumed to be nonnegative. Without loss of generality, the operators bounded below such as energy and number of particles can be made into this form. We also define state vectors $\{|\Phi_n\rangle = B|E_n\rangle\}$ so that the matrix element is expressed as the inner product

$$\langle E_n|A|E_m\rangle = \langle\Phi_n|\Phi_m\rangle. \tag{6}$$

The states $\{|\Phi_n\rangle\}$ are chosen from the extremely large Hilbert space $\mathcal{H}$ with various directions. Thus we assume that the sequence of the normalized vectors $\{\frac{|\Phi_1\rangle}{\sqrt{\langle\Phi_1|\Phi_1\rangle}}, \frac{|\Phi_2\rangle}{\sqrt{\langle\Phi_2|\Phi_2\rangle}}, ...\}$ is regarded as a *uniformly random sampling* from $\dim\mathcal{H}$ dimensional unit sphere as we will confirm for the case of a spin chain. It is then straightforward to show that the mean square of the inner product is smaller than $\frac{\|A\|^2}{\dim\mathcal{H}}$[3], which we will show later. Here $\|A\|$ is the maximum of the eigenvalues of A.

Let us derive the inequality for the inner product

$$\langle|\langle\Phi_n|\Phi_m\rangle|^2\rangle \leq \frac{\|A\|^2}{\dim\mathcal{H}}, \tag{7}$$

where the bracket shows the average with respect to the uniform random sampling of $\frac{|\Phi_n\rangle}{\sqrt{\langle\Phi_n|\Phi_n\rangle}}$ from the unit sphere. Uniform random sampling is expressed by the vector representation of $\frac{|\Phi_n\rangle}{\sqrt{\langle\Phi_n|\Phi_n\rangle}}$ in an orthogonal complete basis as $\vec{d_n} = (\cos\theta_1, \sin\theta_1\cos\theta_2, \sin\theta_1\sin\theta_2\cos\theta_3, ..., \sin\theta_1\sin\theta_2\cdots\sin\theta_{d-1})$ with $d = \dim\mathcal{H}$. Hereafter we use the abbreviated notation for the dimension d. The angles θ_i are uniform random variables on the real axes. We are interested in particular cases where $\|A\|$ polynomially depends on the system size. On the other hand, the dimension $\dim\mathcal{H}$ grows exponentially as the system size increases. Then inequality (7) shows that the off-diagonal elements Eq.(6) is extremely small for the macroscopic system. We numerically show that Eq.(7,12) actually holds and hence random sampling assumption is reasonable for a quantum spin chain. The spin chain is regarded as a nice example, since it provides macroscopic quantities, which is a sum of the local quantities. The Hamiltonian of the spin chain is chosen as

$$H = -J\sum_{j=1}^{N-1}\sigma_j^z\sigma_{j+1}^z + \alpha\sum_{j=1}^{N}\sigma_j^x + \gamma\sum_{j=1}^{N}\sigma_j^z, \tag{8}$$

where J stands for the exchange interaction between neighboring sites, and a constant magenetic field $\mathbf{B} = (\alpha, 0, \gamma)$ is applied. σ_j^i is the $i = x, y, z$ component of the Pauli matrix at the site j. As a macroscopic quantity, we consider the square of the x component of the total magnetization

$$A = (\sum_{j=1}^{N}\sigma_j^i)^2. \tag{9}$$

Other choices of A are possible, but we use Eq.(9) which guarantees a well-defined square root $B = \sum_{j=1}^{N}\sigma_j^i$. For example, if we choose A as i component of the total magnetization, we still observe behavior resembles to Fig.1. The system sizes $6 \leq N \leq 11$ are explored. Note that the dimension of the total Hilbert space is 2^N and can be large for relatively small N. By diagonalizing the Hamiltonian matrix H, numerical eigenvectors $|E_n\rangle$ are obtained, and the absolute values of all the matrix elements $|\langle E_m|A|E_n\rangle|$ are shown in Fig.1. The data are shown only for parameters $J = 1$, $\alpha = 1$, and $\gamma = 0.5$, however, we have confirmed similar behavior for various values of γ. To verify that Eq.(7,12) is satisfied quantitatively, we also show the matrix elements $|\langle E_{1000}|A|E_n\rangle|$ with a fixed value of $m = 1000$ for $N = 11$. The statistical mean value of the off-diagonal elements agrees with the theoretical estimation $\frac{\langle A\rangle}{\sqrt{d}} \cong \frac{\|A\|}{\sqrt{d}}$ as shown in Fig.2. This estimation is considered as a generic property of macroscopic observables A, since it is expressed only by the typical value of A and the dimension d. Thus for large $d = 2^N$, the directions of $|\Phi_n\rangle$ are orthogonal to each other, and are considered to be distributed on the $\dim\mathcal{H} - 1$

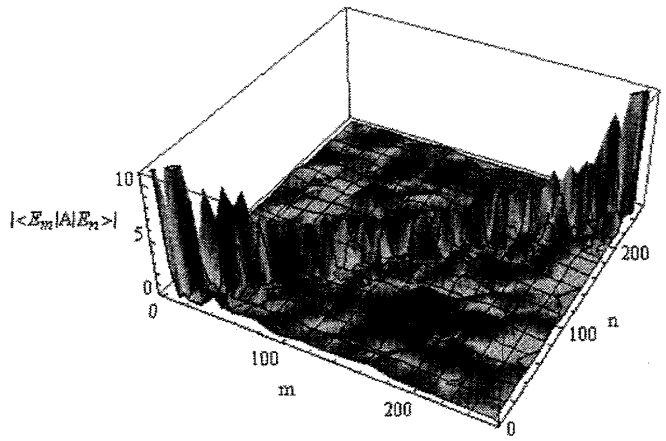

Figure 1: The absolute values of matrix elements $|\langle E_m|A|E_n\rangle|$ of $A = (\sum_{j=1}^{N} \sigma_j^x)^2$. The average of the off-diagonal elements is the same order as the average of the diagonal elements divided by $\sqrt{d}$. The system size is $N = 8$. We have confirmed qualitatively similar results for $6 \leq N \leq 11$.

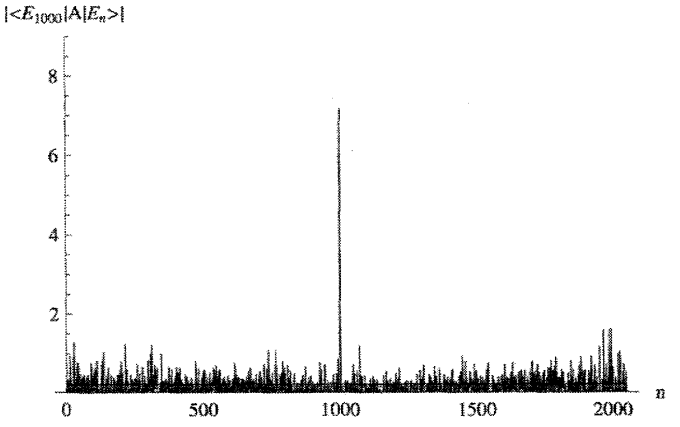

Figure 2: The absolute values of matrix elements $|\langle E_{1000}|A|E_n\rangle$ of $A = (\sum_{j=1}^{N} \sigma_j^x)^2.y$ and z components give similar results. The lines show average of the off-diagonal elements $\langle|\langle E_{1000}|A|E_n\rangle|\rangle = 0.173$, and the average of the diagonal elements divided by $\sqrt{2^N}$, 0.138. These two lines are mutually very close.

dimensional unit sphere without any bias to a specific direction.

$$\frac{\langle|\langle\Phi_m|\Phi_n\rangle|^2\rangle}{\sqrt{\langle\Phi_m|\Phi_m\rangle\langle\Phi_n|\Phi_n\rangle}} = \frac{1}{d} \tag{10}$$

is immediately derived, since the expectation values of each component are the same and their sum should be unity. For concreteness, we also show the Eq.(10) in an alternative way. The square inner product is calculated as

$$\begin{aligned}
&\frac{\langle|\langle\Phi_n|\Phi_m\rangle|^2\rangle}{\langle\Phi_n|\Phi_n\rangle\langle\Phi_m|\Phi_m\rangle} \\
= \;& N\int_0^{\frac{\pi}{2}}\cdots\int_0^{\frac{\pi}{2}}\cos^2\theta_1\left|\frac{\partial(r\cos\theta_1,...,r\sin\theta_1\cdots\sin\theta_{d-1})}{\partial(\theta_1,...,\theta_{d-1},r)}\right|_{r=1}d\theta_1\cdots d\theta_{d-1} \\
= \;& N\int_0^{\frac{\pi}{2}}\cdots\int_0^{\frac{\pi}{2}}(1-\sin^2\theta_1)\sin^{d-2}\theta_1\sin^{d-3}\theta_2\cdots\sin\theta_{d-2}d\theta_1\cdots d\theta_{d-1} \\
= \;& 1-\frac{(d-2)\Gamma(\frac{d-2}{2})}{\Gamma(\frac{d-1}{2})}\frac{\Gamma(\frac{d+1}{2})}{\Gamma(\frac{d}{2})d} \\
= \;& \frac{1}{d},
\end{aligned} \tag{11}$$

where $N=\prod_{n=1}^{d-2}\frac{n\Gamma(\frac{n}{2})}{\Gamma(\frac{n+1}{2})}$ is the normalization factor.

Since $|E_n\rangle$ and $|E_m\rangle$ are normalized,

$$\begin{aligned}
&\langle\Phi_n|\Phi_n\rangle\langle\Phi_m|\Phi_m\rangle \\
=\;& \langle E_n|A|E_n\rangle\langle E_m|A|E_m\rangle \\
\le\;& \|A\|^2.
\end{aligned} \tag{12}$$

The inequality (7) derives from Eqs.(10,12). From Eq.(7), the coefficient $c_{n,m}$ of Eq.(3) is safely replaced by $\langle E_n|U\rho(0)U^+|E_m\rangle\delta_{n,m}$ in the evaluation of $\mathrm{Tr}U\rho(0)U^+A$. The off-diagonal elements of $U\rho(0)U^+$ does not contribute to the expectation value of macroscopic quantity A. More quantitatively, the error caused by neglect of the off-diagonal elements is indeed negligible by random phase approximation, since there are d^2 terms of $O(\frac{1}{d^2})$ with various phases.

ii) The diagonal elements of the density matrix $U\rho(0)U^+$ is well-approximated by those of a microcanonical state with respect to $H(T)$. It is important to note that the initial microcanonical state specifies an energy scale E. Indeed the diagonal elements are expressed as

$$\begin{aligned}
&\langle E_n|U\rho(0)U^+|E_n\rangle \\
=\;& \frac{1}{\Omega(E(0))}\langle E_n|\delta(UH(0)U^+-E)|E_n\rangle \\
=\;& \frac{1}{\Omega(E(0))}\sum_m\delta(\tilde{E}_m-E)|\langle E_n|\tilde{E}_m\rangle|^2,
\end{aligned} \tag{13}$$

where we introduced the normalized eigenstates of $UH(0)U^+$ as $UH(0)U^+|\tilde{E}_n\rangle = \tilde{E}_n|\tilde{E}_n\rangle$, i.e. $U|E_n(0)\rangle = |\tilde{E}_n\rangle$ with an eigenstate of $H(0)$, $|E_n(0)\rangle$. The set of states $\{|E_n\rangle\}$ and $\{|\tilde{E}_n\rangle\}$ are related by a unitary transformation $\sum_n |E_n\rangle\langle\tilde{E}_n|$. In the presence of perturbation, $|\langle E_n|\tilde{E}_m\rangle|^2 = |\langle E_n|U|E_m(0)\rangle|^2$ would be non negligible only when the conservation of the energy is well-satisfied after the long waiting time, i.e. $E_n \cong \tilde{E}_m + \Delta E$ with the energy change ΔE from the initial to final times caused by external perturbation during $0 \leq t \leq T_0$.

We show a quantitative estimation of ΔE. The matrix element $\langle E_n|\tilde{E}_m\rangle$ is evaluated as $\delta_{nm} + \frac{\langle\tilde{E}_m|H(T)|\tilde{E}_n\rangle}{\tilde{E}_m - \tilde{E}_n}(1-\delta_{nm})$ up to the first order of the perturbation $H(T) - UH(0)U^+$, where the factor $\langle\tilde{E}_m|H(T)|\tilde{E}_n\rangle$ would be of order $\sqrt{\frac{\|H(T)\|^2}{d}}$ as in Eq.(7). Then it is immediately shown that $\tilde{E}_m$ contributes to $\langle E_n|\tilde{E}_m\rangle$ only when $\tilde{E}_m$ and $\tilde{E}_n$ are sufficiently near $|\tilde{E}_m - \tilde{E}_n| \leq \frac{E}{\sqrt{d}}$, otherwise the ratio $\frac{\langle\tilde{E}_m|H(T)|\tilde{E}_n\rangle}{\tilde{E}_m - \tilde{E}_n}$ is negligible. Such $|\tilde{E}_m\rangle$ is expanded as $|\tilde{E}_m\rangle = \sum_n d_{n,m}|E_n\rangle$, where the coefficient $d_{n,m}$ is non negligible for $\tilde{E}_n$ sufficiently near $\tilde{E}_m$. The energy change ΔE is determined as

$$\begin{aligned} & \Delta E = \langle\tilde{E}_m|(H(T) - UH(0)U^+)|\tilde{E}_m\rangle \\ = & \sum_k |d_{km}|^2 E_k - \tilde{E}_m \\ \cong & E_n - E, \end{aligned} \tag{14}$$

which is almost independent of the suffix n, and does not depend on the quantity of interest A. Here we evaluated as $\sum_k |d_{k,m}|^2 E_k \cong E_m \cong E_n$ and $\tilde{E}_m = E$ from the Dirac delta in Eq.(13). The important property used here is a continuity of the mapping, i.e. when $|\tilde{E}_n - \tilde{E}_m|$ is small enough compared to $\sqrt{\frac{E^2}{d}}$, $|E_n - E_m|$ is also sufficiently small.

Therefore the third line of Eq.(13) has a sharp peak at $E_n = E + \Delta E$ as a function of E_n and is proportional to the function $\delta(E_n - E - \Delta E)$ as

$$\begin{aligned} & \langle E_n|U\rho(0)U^+|E_n\rangle \\ \cong & \frac{1}{\Omega(T)}\delta(E_n - E - \Delta E) \\ = & \langle E_n|\frac{1}{\Omega(T)}\delta(H(T) - E - \Delta E)|E_n\rangle, \end{aligned} \tag{15}$$

where the density of the states at $t = T$ is determined uniquely from the normalization, and $H(T)|E_n\rangle = E_n|E_n\rangle$ is used. The diagonal elements is thus given by the microcanonical ensemble.

Then as far as the expectation value is concerned, the state $U\rho(0)U^+$ should be well-described by the microcanonical ensemble $\rho(T)$.

4 Entropy at final state

Given the relaxation to equilibrium, the equilibrium entropy at final time $S(T)$ is well-defined.

Since the microcanonical and canonical ensembles are quantitatively equivalent in the macroscopic limit due to the specification of the energy scale, we consider the canonical ensemble $\rho(s) = \frac{1}{Z(s)} e^{-\beta H(s)}$ at $t = s$. At time $t = s$, the nonequilibrium entropy is defined as the energy minus the free energy calculated from the canonical ensemble with the Hamiltonian $H(s)$ and the partition function $Z(s)$. The nonequilibrium entropy at final time is written as

$$\begin{aligned} \frac{S(T)}{k_B} &= \beta(E(T) - F(T)) \\ &= \mathrm{Tr} U\rho(0)U^+ \log \frac{e^{-\beta H(T)}}{Z(T)} \\ &\cong -\mathrm{Tr}\rho(T)\log\rho(T), \end{aligned} \tag{16}$$

where $E(T)$ and $F(T) = -\frac{1}{\beta}\log\Omega(T)$ are the internal and free energies, respectively. Then the nonequilibrium entropy at $t = T$ is equal to the equilibrium value due to the relaxation of the expectation value of $A = \log\rho(T)$.

5 Summary

In conclusion, by assuming that the initial state is prepared as a microcanonical ensemble, the actual state at time $t = T$ can be replaced by another microcanonical ensemble in the evaluation of macroscopic quantities. The derivation is based on the high dimensionality of the Hilbert space, and restrictions for the system size dependence of observables as well as the perturbative treatment of the unitary transformation of the energy eigenstates. The validity of the uniformly random sampling assumption for $\frac{|\Phi_n\rangle}{\sqrt{\langle\Phi_n|\Phi_n\rangle}}$ is numerically verified for a nonintegrable spin chain. It is also remarked that the initial state can be out of equilibrium, i.e. the initial density matrix is $\rho(0) = U_0 \frac{1}{\Omega(0)}\delta(E - H(0))U_0^+$ with a unitary transformation U_0, since this can be regarded as the state evolved from an actual initial state $U_0^+\rho(0)U_0 = \frac{1}{\Omega(0)}\delta(E - H(0))$.

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Here I would like to acknowledge the advises and collaborations when I was a student. In 2002, he showed me a stimulating paper on an experimental verification of transient fluctuation theorem and therefore negative entropy production for an externally dragged Brownian particle. And we were successful to interpret how the negative entropy production occurs in which time scale yet within the realm of fluctuation dissipation relation of the second kind. Then we proceeded to the quantum analogue of the above-mentioned negative entropy production. In particular, we showed an existence of quantum correction to the fluctuation theorem for the spectral statistics of accumulated work operator. Also it turned out that twice measurements of initial and final energies yields no corrections, and described by the so-called modular operator. These are what we have done in the beginning of my carrier 2002-2004. Then I pursued fundamental issues of statistical mechanics somehow independently. But in 2006, I defended my thesis under his supervision. He was not at all satisfied with the first several versions of the draft, since the relation between the chapters were incoherent. Just before the deadline, we finally agreed upon the publication of final version.

When I was an assistant Professor, I again learned much from him not only on the specialty but also how to teach. In September 2011, I met researchers in the field of social network, and they were taught by him at Nara Women's University. They remembered and admired his clear and well-organized way of teaching mathematical physics. In this way, his outstanding activities still afford us spiritual nourishment.

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