Typical pure nonequilibrium steady states

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Abstract – We show that typicality holds for a class of nonequilibrium systems, i.e., nonequilibrium steady states (NESSs): almost all the pure states properly sampled from a certain Hilbert space well represent a NESS and characterize its intrinsic thermal nature. We clarify the relevant Hilbert space from which the pure states are to be sampled, and construct practically all the typical pure NESSs. The scattering approach leads us to the natural extension of the typicality for equilibrium systems. Each pure NESS correctly yields the expectation values of observables given by the standard ensemble approach. It means that we can calculate the expectation values in a NESS with only a single pure NESS. We provide an explicit construction of the typical pure NESS for a model with two reservoirs, and see that it correctly reproduces the Landauer-type formula for the current flowing steadily between the reservoirs.

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Introduction. – Recently, the typicality of pure states of large quantum systems has been attracting considerable attention for the foundations of statistical mechanics. It has been shown that the partially reduced states of the overwhelming majority of the pure states in an energy shell of a large quantum system look similar to each other, and well approximate the canonical state (“canonical typicality”), for which the importance of a large entanglement in each typical pure state of the whole system is stressed [1,2] (see also [3,4]). It has been also pointed out that a similar typicality already holds for the whole system: almost all the pure states in the energy shell of the whole system give the expectation values of an observable very close to that evaluated in the microcanonical state [5–7]. Such intrinsic thermal nature of typical pure states enables us to analyze mechanistic and thermodynamical quantities [8,9] and their fluctuations, especially the probability distributions [10], by only a single pure state. The equilibration/thermalization [11–16], the temporal fluctuation around equilibrium [17], and the relaxation time [18,19] have also been discussed for large quantum systems on the basis of the typicality arguments, which would be relevant to the experimentally observed emergence of thermal correlations in an isolated cold atomic gas [20]. Instead of the statistical ansatz such as a priori equal probabilities of energy eigenstates and the ergodicity hypothesis, the quantum spectral fluctuation provides alternative probabilistic properties necessary for the statistical mechanics.

These extraordinary achievements for typical pure states being at hand, it is natural to expect that the typicality holds also for nonequilibrium systems. As a first step, we are going to focus on nonequilibrium steady states (NESSs) [21–28]. Needless to say, the NESSs are of both practical and fundamental importance: they are of course relevant to the DC conductivity [29], and include interesting topics such as the long-range correlations in the NESSs [30]. On the other hand, the universal properties of the NESSs are less understood [23,30] compared with those of equilibrium systems. In addition, it is not clear whether the typicality holds for NESSs and how to construct typical pure states representing NESSs if any.

In this paper, we give an answer to this last question. We provide a construction of practically all typical pure NESSs. Our idea is to reduce the problem for the nonequilibrium situation to that for the equilibrium through the Lippmann-Schwinger scattering theory [31,32]; we “scatter” a typical pure state representing an equilibrium state to generate a typical pure NESS. We show that it actually gives the same expectation value as the standard ensemble approach. For concreteness, we investigate the simplest model for a quantum transport, and give an explicit construction of a typical pure NESS.

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Typicality for equilibrium systems. – Let us first recapitulate an aspect of the typicality for equilibrium systems, relevant to the following discussion. We consider a large quantum system, and an energy shell $\mathcal{H}_E$ spanned by the energy eigenstates $\{|E_i\rangle\}$ belonging to the energies between $E$ and $E + \Delta E$. The energy width $\Delta E$ is supposed to be small, but the system is so large that the energy shell $\mathcal{H}_E$ contains many energy eigenstates $\{|E_i\rangle\}$, i.e., $d = \dim \mathcal{H}_E$ is large. We then pick a pure state $|\psi\rangle = \frac{1}{\sqrt{d}}\sum_{i=1}^{d} c_i |E_i\rangle$ randomly from the energy shell $\mathcal{H}_E$, i.e., the complex coefficients $\{c_i\}$ are chosen from the uniform distribution on the surface of the $2d$-dimensional unit sphere $\sum_{i=1}^{d} |c_i|^2 = 1$, according to the Haar measure. Such a single pure state $|\psi\rangle$ typically well represents the microcanonical ensemble on the energy shell $\mathcal{H}_E$: almost all the pure states $|\phi\rangle$ on the energy shell $\mathcal{H}_E$ give the expectation value $\langle \phi | \hat{A} | \psi \rangle$ of an observable $\hat{A}$ close to the expectation value $\langle \hat{A} \rangle_{mc} = \text{Tr}\{\hat{A} \hat{\rho}_{mc}\}$ in the microcanonical ensemble $\hat{\rho}_{mc} = \frac{1}{|\mathcal{E}|} \sum_{i=1}^{d} |E_i\rangle\langle E_i|$, i.e.,

$$\langle \psi | \hat{A} | \psi \rangle \sim \langle \hat{A} \rangle_{mc}.$$  

More rigorously, the probability of $\langle \phi | \hat{A} | \psi \rangle$ deviating from $\langle \hat{A} \rangle_{mc}$ is bounded, for any positive $K$, by

$$P\left( |\langle \phi | \hat{A} | \psi \rangle - \langle \hat{A} \rangle_{mc}|^2 > K \frac{(\Delta \hat{A})^2_{mc}}{d + 1} \right) < \frac{1}{K},$$  

where $\Delta \hat{A}_{mc}^2 = \langle \hat{A}^2 \rangle_{mc} - \langle \hat{A} \rangle_{mc}^2$. Roughly, it means that the error is typically $\mathcal{O}(\Delta \hat{A}_{mc}/\sqrt{d})$ [10]. This is valid even for an unbounded operator $\hat{A}$ as long as the microcanonical variance $\Delta \hat{A}_{mc}^2$ is under control. Each typical pure state $|\psi\rangle$ on the energy shell $\mathcal{H}_E$ well describes the thermal equilibrium state of the system.

Note that we do not put the system in contact with an “environment”. Such an external agent is not necessary for the typicality and for the equivalence with the microcanonical state [5-8]. If we divide the system into two parts and take the partial trace over one of them, all the reduced states of the typical pure states in the energy shell $\mathcal{H}_E$ of the total system are very close to a canonical state. It is called “canonical typicality” [1,2] (see also [3,4]). We are not going to discuss this in this paper: we will not have an environment and will not take a partial trace.

The objective of the present paper is to extend this typicality argument to a nonequilibrium situation, i.e., to NESS. At first glance, it is not clear from which subspace we should sample pure states. Moreover, there is no clear clue whether the typicality holds also for nonequilibrium systems. For NESSs, nonetheless, we will clarify that the typicality actually holds: we will identify the relevant subspace and construct practically all pure NESSs.

Nonequilibrium steady state (NESS). – The simplest setup for discussing the NESS is shown in fig. 1(a) [21-29]. We have two reservoirs $L$ and $R$, one at temperature $T_L$ with chemical potential $\mu_L$ and the other at $T_R$ with $\mu_R$. Connecting them via a weak link, a current starts to flow between them. This can be described in the following natural way [21-29]: we let the whole system evolve from the initial state $\hat{\rho}_L \otimes \hat{\rho}_R$ by a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$, $\hat{H}_0 = \hat{H}_L + \hat{H}_R$, where $\hat{H}_L$ and $\hat{H}_R$ are the Hamiltonians of the reservoirs $L$ and $R$, respectively, with a weak local interaction $\hat{V}$ which transfers particles between the two reservoirs. $\mu_L$ and $\mu_R$ represent the thermal equilibrium states of the reservoirs $L$ and $R$, respectively, with the relevant temperatures and chemical potentials. Usually, the grand canonical ensembles $\beta_{gc}(\xi L \xi R) = e^{-\beta_{L}(\xi L \xi R) N_{L}(\xi L \xi R)}/\Xi_{L}(\xi L \xi R)$ are taken, with $\beta_{L}(\xi L \xi R)$ being the inverse temperature, $N_{L}(\xi L \xi R)$ the number of particles in reservoir $L(R)$, and $\Xi_{L}(\xi L \xi R)$ the grand canonical partition function.

If the two systems $L$ and $R$ are large but of finite size, the whole system eventually reaches an equilibrium state with the two systems at the same temperature. Here, instead, we are interested in infinitely large systems as $L$ and $R$, and the thermodynamic limit will be taken. Then, in the long-time limit, the system reaches a NESS, in which a current flows steadily. We are going to discuss such NESSs [21-29].

However, mathematically the state $e^{-i\hat{H}t}(\hat{\rho}_L \otimes \hat{\rho}_R)e^{i\hat{H}t}$ does not converge in general (more rigorously, the expectation values of observables in this state would not converge).

1We can easily generalize the following arguments to the systems with multiple reservoirs, but we focus on the two-reservoir case for simplicity.
in the long-time limit \( t \to \infty \). The mathematically well-defined construction of NESS instead is given by [21,23–26]

\[
\hat{\rho}_{\text{NESS}} = \hat{\Omega}(\hat{\rho}_L \otimes \hat{\rho}_R)\hat{\Omega}^\dagger
\]  

(5)

with the Moller wave operator [31,32]

\[
\hat{\Omega} = \lim_{t \to \infty} e^{-iH_0 t} e^{iH_0 t}.
\]  

(6)

The very rough idea is to remove the free oscillations by \( e^{iH_0 t} \) to ensure the convergence in the long-time limit. In the context of a scattering problem, the wave operator \( \hat{\Omega} \) transforms incident plane waves to the scattering states satisfying the Lippmann-Schwinger equation under the outgoing boundary condition. In the present context, the free state \( \hat{\rho}_L \otimes \hat{\rho}_R \) of \( H_0 \) as the incident state is transformed into a scattering state by \( \hat{\Omega} \), which is the NESS. We are interested, in particular, in the current between the two reservoirs. We compute the expectation value of the current operator (see the example below), which approaches a well-defined stationary value in the long-time limit: the current flows steadily, and this is a NESS.

There might exist some pathological system for which the long-time limit in (6) does not exist. In the following, we exclude such an exceptional case and assume the existence of a well-defined NESS.

**Construction of typical pure NESSs.** – Having seen the above approach to the NESS, we are led to the following natural way for constructing *typical pure NESSs*. The basic idea is to sample a typical pure state representing the thermal equilibrium states \( \hat{\rho}_L \otimes \hat{\rho}_R \) of the reservoirs, and “scatter” it by the wave operator \( \hat{\Omega} \).

More specifically, we take a subspace \( \mathcal{H}_{E_L,E_R} = \mathcal{H}_{E_L} \otimes \mathcal{H}_{E_R} \) in the Hilbert space of the total system, where \( \mathcal{H}_{E_{L(R)}} \) is the energy shell around the energy \( E_{L(R)} \) of reservoir \( L(R) \) with a small energy width \( \Delta E \), spanned by the energy eigenstates \( \{ |E_{L(R)}\rangle \} \) in the energy range (see fig. 1(b)). Its dimension is \( D = \dim \mathcal{H}_{E_L,E_R} = d_L d_R \) with \( d_{L(R)} = \dim \mathcal{H}_{E_{L(R)}} \) (see footnote 2). We then pick a pure state \( |\phi\rangle \) randomly from the subspace \( \mathcal{H}_{E_L,E_R} \) with respect to the Haar measure in \( \mathcal{H}_{E_L,E_R} \), and define

\[
|\phi\rangle_{\infty} = \hat{\Omega}|\phi\rangle.
\]  

(7)

Our main result is that the pure state \( |\phi\rangle_{\infty} \) constructed in this way is a typical pure NESS in the well-defined thermodynamical limit. That is, almost all the pure states \( |\phi\rangle_{\infty} \) sampled in this way give the expectation values \( \langle \phi|A|\phi\rangle_{\infty} \) close to the expectation value \( \langle A\rangle_{\text{NESS}} = \text{Tr}\{\hat{\rho}_{\text{NESS}}A\} \) evaluated with \( \hat{\rho}_{\text{NESS}} \) given in (5),

\[
\langle \phi|A|\phi\rangle_{\infty} \sim \langle A\rangle_{\text{NESS}}.
\]  

(8)

Note that \( |\phi\rangle_{\infty} \) is invariant under the time evolution up to a global phase, since \( e^{-iH_0 t}\hat{\Omega}|\phi\rangle = \hat{\Omega}^{-iH_0 t}|\phi\rangle \) holds for an arbitrary \( t \), \[32\] and \( |\phi\rangle \) is approximately an eigenstate of \( \hat{\Omega} \) due to the assumption of the small energy width \( \Delta E \). Thus, the expectation values in \( |\phi\rangle_{\infty} \) are stationary.

Before proving the typicality of \( |\phi\rangle_{\infty} \), it is important to point out the following fact. One distinguished characteristics of NESS, in contrast to equilibrium cases, is that it is endowed with multiple different temperatures and chemical potentials, or in other words, it is characterized by multiple different energy scales. We basically intend to take a typical pure state \( |\phi\rangle \) representing the product of the two thermal equilibrium states \( \hat{\rho}_L \otimes \hat{\rho}_R \) as the initial state, but our sampling is not performed separately for \( \mathcal{H}_{E_L} \) and \( \mathcal{H}_{E_R} \). Each initial state \( |\phi\rangle \) is sampled from \( \mathcal{H}_{E_L,E_R} \), which in general is not of the product structure, but rather entangled,

\[
|\phi\rangle = \sum_{i=1}^{d_L} \sum_{j=1}^{d_R} c_{ij} |E_i^{(L)}\rangle \otimes |E_j^{(R)}\rangle.
\]  

(9)

It still typically represents the product state \( \hat{\rho}_L \otimes \hat{\rho}_R \), as we will see below. This is an important point. We are exploring the whole of the subspace \( \mathcal{H}_{E_L,E_R} \) characterized by the two intrinsic energy scales \( E_L \) and \( E_R \). Then, through (7), which establishes an isometric construction of the pure NESSs \( |\phi\rangle_{\infty} \) expressed as scattering states, practically all pure NESSs are at our hand.

**Typicality of pure NESSs.** – The proof of the typicality of the pure NESSs \( |\phi\rangle_{\infty} \) consists of two steps. The first step is to show

\[
\mathbb{E}[\langle \phi|\hat{\Omega}^\dagger \hat{\Omega}\langle \phi\rangle] = \text{Tr}\{\hat{\rho}_{\text{nc}}^{(L)} \otimes \hat{\rho}_{\text{nc}}^{(R)} |\phi\rangle \langle \phi|\hat{\Omega}^\dagger \hat{\Omega}\langle \phi\rangle] = \langle \phi| \hat{\Omega}^\dagger \hat{\Omega}|\phi\rangle_{\text{nc}}
\]  

where \( \mathbb{E}[\cdots] \) represents the ensemble average over the uniformly sampled \( |\phi\rangle \) with respect to the Haar measure in \( \mathcal{H}_{E_L,E_R} \), and \( \hat{\rho}_{\text{nc}}^{(L(R))} = \frac{1}{d_{L(R)}} \sum_{i=1}^{d_{L(R)}} |E_i^{(L(R))}\rangle \langle E_i^{(L(R))}| \) is the microcanonical ensemble for the thermal equilibrium state of reservoir \( L(R) \). We abbreviate it to \( \hat{\rho}_{\text{mc}}^{(L)} \otimes \hat{\rho}_{\text{mc}}^{(R)} |\phi\rangle \langle \phi| \hat{\Omega}^\dagger \hat{\Omega} \rangle_{\text{nc}} \), which is the expectation value of the microcanonical average \( \langle \hat{\Omega}^\dagger \hat{\Omega}\rangle_{\text{mc}} \) well coincides with the grand canonical average \( \text{Tr}\{\hat{\rho}_{\text{gc}}^{(L)} \otimes \hat{\rho}_{\text{gc}}^{(R)} |\phi\rangle \langle \phi| \hat{\Omega}^\dagger \hat{\Omega} \rangle_{\text{gc}} \}. \)

We then see that the variance is bounded by

\[
\mathbb{V}[\langle \phi|\hat{\Omega}^\dagger \hat{\Omega}|\phi\rangle] \leq \frac{(\Delta \langle \hat{\Omega}^\dagger \hat{\Omega}\rangle_{\text{nc}})^2}{D + 1}
\]  

(11)

\footnote{The wave operator \( \hat{\Omega} \) is not unitary in the presence of non-decaying bound states \( \{|\phi_{B,i}\rangle\} \) [31,32]. Indeed, \( \hat{\Omega}\hat{\Omega}^\dagger = 1 - \sum_i |\phi_{B,i}\rangle \langle \phi_{B,i}| \). Equation (7) further shows that \( |\phi\rangle_{\infty} = (1 - \sum_i |\phi_{B,i}\rangle \langle \phi_{B,i}|) |\phi\rangle \). This means that the pure NESS \( |\phi\rangle_{\infty} \) constructed by (7) is necessarily a scattering state. For the discussion of NESSs, it is reasonable to exclude the superpositions of energetically separated scattering and bound states.}

\footnote{This is valid only in the absence of condensation [33,34]. We exclude cases with symmetry breaking, where the grand canonical catastrophe occurs. Such cases will be studied elsewhere.}
with \( V[A] = E[A^2] - E[A]^2 \), \( (\Delta \hat{A})^2_{\text{mc}} = \langle \hat{A}^2 \rangle_{\text{mc}} - \langle \hat{A} \rangle^2_{\text{mc}} \), and that it shrinks as \( D \to \infty \), ensuring the typicality (8).

The crucial observation is that, thanks to the introduction of the wave operator \( \hat{\Omega} \), the expectation value of \( \hat{A} \) in the NESS is translated into the expectation value of \( \hat{\Omega}^\dagger A \hat{\Omega} \) in the double thermal equilibrium state. Therefore, we can easily extend the standard arguments for equilibrium systems [5–7] to the present discussion for NESSs. One subtle nontrivial point is the entanglement in (9) to represent the product of the two thermal equilibrium states \( \hat{\rho}_L \otimes \hat{\rho}_R \). It is however not a difficult problem.

Here comes the proof of the typicality of the pure NESSs |\( \phi \rangle_{\infty} \). The key formulas are available by generalizing those for equilibrium cases with the single-index coefficients \{\( c_i \)\} in (1) to the multi-index coefficients \{\( c_{ij} \)\} in (9). The Haar measure is proportional to \( \delta(\sum_i d_i^L + \sum_i d_i^R) \) in the discussion of NESS is the current flowing between the reservoirs. The microcanonical variance of the current \( c_{ij} \) remains finite in the thermodynamical limit, since it is an integral over the dispersion relations and nonvanishing width in \( \omega \) and \( \omega' \), and it is a difficult problem.

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Here, we apply the typicality of \(|\phi\rangle\) proved by (13) with (14) and the equivalence between the microcanonical and the grand canonical ensembles for large systems:

\[
\langle \phi | \hat{b}_w^\dagger \hat{a}_w | \phi \rangle \sim 0, \quad \langle \phi | \hat{b}_w^\dagger \hat{a}_w \hat{b}_w^\dagger \hat{a}_w | \phi \rangle \sim 0, \quad (22)
\]

Equations (22)–(24) are written keeping the presence of fermions (upper signs) and bosons (lower signs). Even though the bosonic canonical operators \(a_w\) and \(b_w\) are unbounded operators, the typicality holds, since the relevant microcanonical variances are finite. Recall (14) (see footnote 6). Then, the expectation value of the current (21) is reduced to

\[
\sum_{\phi} \langle \phi | \hat{J} | \phi \rangle \sim 2 \pi \int d\omega |g_{w,w'}|^2 \left[ f_L(\omega) - f_R(\omega) \right] + \ldots, \quad (25)
\]

where we have taken the thermodynamical limit and used \(1/(x - i\eta) = P(1/x) + \pi i \delta(x)\). This reproduces the Landauer-type formula derived by the ensemble approach [29]. The current flows with the difference between the Fermi/Bose distributions \(f_L(\omega)\) and \(f_R(\omega)\) of \(L\) and \(R\).

**Summary.** – We have successfully constructed a class of typical pure states \(|\phi\rangle\) which describe a NESS. We just sample initial pure states randomly from \(\mathcal{H}_{E_L+E_R} = \mathcal{H}_{E_L} \otimes \mathcal{H}_{E_R}\) to represent \(\hat{\rho}_L \otimes \hat{\rho}_R\) and then “scatter” them to get a set of pure states, each of which describes the NESS, since the statistical error vanishes in the thermodynamical limit. In this way, the typicality of equilibrium states naturally amounts to the typicality of NESSs.

The thermodynamical structures of NESSs have been explored, e.g., by informational [30,37] and dynamical approaches [23,27]. The informational statistical mechanics suggests that NESSs can be characterized by the principle of maximization of an entropy under a constrained current [37]. However, its applicability is restricted due to the

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6 Note that the delta functions are written loosely, as mentioned before. They are actually Kronecker’s deltas for a finite volume of the system. In the thermodynamical limit, they become delta functions, but they accompany \(g_{w,w'}\) in the current (20). The microcanonical variances of the relevant operators integrated with \(g_{w,w'}\) are finite in the thermodynamical limit, and the typicality holds. Equations (22)–(24) are written keeping the presence of \(g_{w,w'}\) in mind.
omission of higher-order fluctuations. By using the Gibbsian state as the initial state, any higher-order fluctuations of current are fully taken into account [23,27,28,38,39]. The typicality of pure NESSs allows us to relax the assumption of the initial Gibbsian state. The equivalence (8) holds also for the variance and the higher-order fluctuations of the current. Note, however, that if we look at all the moments of the current at the same time, we acquire enough knowledge about the state to discriminate it from other pure NESSs and we lose the typicality: we should not look at too many moments. See [5–7]. It remains an important issue to be better clarified how many observables we can look at without losing the typicality.

Another interesting subject is the typicality under symmetry breaking. If we think of a generic many-body system, it might exhibit condensation at low temperatures. When a symmetry of a system is spontaneously broken, the naive random sampling from energy shells would not work, since in that way we might typically pick a superposition of states belonging to different phase sectors, which is not observed in real experiments. The typicality approach to statistical mechanics in the presence of symmetry breaking is an interesting and important future subject. An aspect relevant to this issue is discussed in [40].

Finally, the typicality of pure states would help reduce computational resources in evaluating thermodynamical quantities of large systems. Such an advantage is explored in [8,9] for equilibrium systems. We expect the same to hold also for the typical pure NESSs, and the practical utility of typicality deserves a detailed study.

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