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The second law of thermodynamics under unitary evolution and external operations

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ABSTRACT

The von Neumann entropy cannot represent the thermodynamic entropy of equilibrium pure states in isolated quantum systems. The diagonal entropy, which is the Shannon entropy in the energy eigenbasis at each instant of time, is a natural generalization of the von Neumann entropy and applicable to equilibrium pure states. We show that the diagonal entropy is consistent with the second law of thermodynamics upon arbitrary external unitary operations. In terms of the diagonal entropy, thermodynamic irreversibility follows from the facts that quantum trajectories under unitary evolution are restricted by the Hamiltonian dynamics and that the external operation is performed without reference to the microscopic state of the system.

1. Introduction

The thermodynamic entropy must be consistent with all empirical facts on a macroscopic scale, and should therefore satisfy the second law of thermodynamics, which dictates that, upon an external operation on an isolated system, entropy stays constant if the operation is quasi-static and otherwise increases [1]. The von Neumann entropy (vN-entropy) $S_{\mathrm{vN}}(\hat{\rho}) \equiv -\mathrm{tr}(\hat{\rho}\ln\hat{\rho})$, where $\hat{\rho}$ is the density

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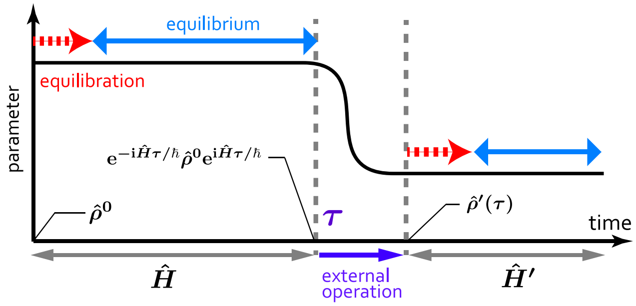

Fig. 1. (Color Online) A schematic picture of our setup. The initial state $\hat{\rho}^0$ evolves in time according to $\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\hat{\rho}^0\mathrm{e}^{\mathrm{i}\hat{H}t/\hbar}$ from $t = 0$ to τ, during which the system approaches a stationary state. At time $t = \tau$, by changing a parameter in the Hamiltonian, we perform an external operation described by a unitary operator $\hat{V}$ [20] to obtain $\hat{\rho}'(\tau) = \hat{V}\mathrm{e}^{-\mathrm{i}\hat{H}\tau/\hbar}\hat{\rho}^0\mathrm{e}^{\mathrm{i}\hat{H}\tau/\hbar}\hat{V}^\dagger$, which becomes stationary under unitary evolution with $\hat{H}'$.

operator of the system (the Boltzmann constant is set to unity throughout this paper), has been adopted as the microscopic definition of the thermodynamic entropy, because it is consistent with thermodynamics when applied to equilibrium states represented by the statistical ensembles such as the microcanonical and canonical ensembles.

Recently the notion of equilibrium states has been generalized and even a single pure state has been shown to typically represent an equilibrium state [2,3]. A great majority of pure states in a microcanonical energy shell, or typical pure states, have been shown to represent thermal equilibrium states [4–7]. Furthermore, it has also been shown that, during a long-time unitary evolution of a pure state with a time-independent Hamiltonian $\hat{H}$, a stationary state is seen at almost all times, or typical times, under appropriate assumptions (see Assumptions 1 and 2 below) [8–14]. The reason the stationary state is seen at typical times is that non-stationary states appear recurrently in unitary evolution [15] with the recurrence time growing exponentially with the number of particles in the system. We note that all the information about the stationary state is encoded in the diagonal elements ρ_{nn} of the density operator $\hat{\rho}$ in the energy eigenbasis at each instant of time, because the off-diagonal elements $\rho_{nm} (n \neq m)$ oscillate at different frequencies and do not contribute to the stationary state [9,10]. Those generalized equilibrium states have experimentally been realized in ultracold atomic systems [16–18].

The vN-entropy cannot represent the thermodynamic entropy of those generalized equilibrium states because it vanishes for any pure states and stays constant under any unitary evolution involving non-quasi-static external operations [1]. Thus we need to generalize it as to be applicable to generalized equilibrium states. We define the diagonal entropy (d-entropy) [19] as

$$S(\hat{\rho}) \equiv -\sum_n \rho_{nn} \ln \rho_{nn}, \tag{1}$$

which can be nonzero for pure states unlike the vN-entropy. If $\hat{\rho}$ is a density matrix which is diagonal in the energy eigenbasis such as the canonical ensemble $e^{-\beta\hat{H}}$, the d-entropy coincides with the vN-entropy. The d-entropy has been shown to be consistent with the second law under the assumption that an external operation is performed on a state represented by a density matrix that is diagonal in the energy eigenbasis [19]. However, this assumption excludes external operations on the generalized equilibrium states including pure states which have recently attracted much attention [4–7]. In addition, the argument cannot be applied to a sequence of external operations because the density matrix after an external operation is not necessarily diagonal in the energy eigenbasis.

In this paper, we show that the d-entropy is consistent with the second law when an arbitrary external operation is performed on equilibrium states which are pure or mixed. As shown in Fig. 1, we consider as a variable the timing τ at which the operation is performed and show that the d-entropy is increased on average over τ (Theorem 1 and Corollary 1). Furthermore, we show that the d-entropy increases for almost all τ in the thermodynamic limit (Theorem 2 and Corollary 2). In Section 5, we geometrically interpret how the asymmetry between increase and decrease in the d-entropy arises