

Maxwell's Demon and Maxwell-Boltzmann Distribution

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In a simple model of Maxwell's demon endowed with a Turing-type memory tape, we present an operational derivation of the Maxwell-Boltzmann distribution in the equilibrium statistical mechanics. It is based solely on the combined gas law of the elementary thermodynamics for the model of the memory. Equilibrium is defined in terms of the stability of thermodynamic work F against noise, where F is the work surplus when resetting the gas system and the memory. This model can be applied to non-equilibrium processes, in principle, because of the universality of the Turing machine. We demonstrate the dissipation-fluctuation as a simple example.

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I. INTRODUCTION

In our previous paper [1], we investigated the relationship between the information theoretic and thermodynamic entropies, which was originally discussed by Brillouin in a general context [2, 3] and later clarified by Landauer and Bennett in the study of the physics of computation. In the resolution of the Maxwell's demon paradox based on the Szilard engine model [9], the link between the two entropies vividly manifested in the form of the information erasure principle [4–7]. Generalizing Landauer-Bennett's argument, we showed that the optimal work cost of information erasure for arbitrary probabilities is indeed exactly equal to the amount that keeps the second law of thermodynamics inviolated. In order to do so without relying on the second law, we made use of the optimality of Shannon's data compression, which is independent of physical laws. Namely, due to the optimal data compression, the minimum work cost of information erasure was shown to be

$$W_{\text{er}} = k_B T \ln 2 \cdot H(p), \quad (1)$$

where $H(p)$ is the information theoretic (Shannon) entropy [10] given by $H(p) = -p \log_2 p - (1-p) \log_2 (1-p)$ for a binary probability distribution $\{p, 1-p\}$. Also, k_B is the Boltzmann constant and T is the temperature of the heat bath with which the gas is in contact. The cost W_{er} is manifestly expressed in terms of $H(p)$, rather than the thermodynamic entropy $S(p)$, hence the clear equivalence between the two entropies [1].

In this paper, we pursue our information theoretic approach to thermodynamics further by enduing the demon with a Turing machine. To be specific, we derive the form of the Maxwell-Boltzmann distribution, which gives the

rate of particles possessing energy ϵ in an N particle system in equilibrium, i.e.,

$$p \propto \exp\left(-\frac{\epsilon}{k_B T}\right), \quad (2)$$

where T is the temperature of the heat bath that is in contact with the particles.

A significance of the present work is in showing that the Maxwell-Boltzmann distribution, which is a key ingredient of statistical mechanics, can in fact be seen as a consequence of the optimal reset of memory that records the particle states. The memory is modeled solely on the basis of the thermodynamic combined gas law. Our model of the particle-memory system can also be applied to generic non-equilibrium processes and we shall present a simple demonstration of the dissipation-fluctuation theorem without using statistical mechanics, unlike the original derivation [11].

This paper is organized as follows. In Sec. II, we recapitulate the resolution of the Maxwell's demon paradox in the case of biased probability distribution [1]. In Sec. III, we describe our *thermo-Turing machine*, in which the particles are manipulated by Maxwell's demon according to information in a Turing-machine-like apparatus. In Sec. IV, we derive the Maxwell-Boltzmann distribution in the scenario of the thermo-Turing when the system is in equilibrium. Section V is for the generalization of the previous section to systems of arbitrary number of energy levels. We shall consider an application of the model to non-equilibrium statistical mechanics by reproducing the dissipation-fluctuation theorem for a near equilibrium case in Sec. VI. Section VII is devoted to summary and discussions, mentioning an idea that our model essentially mimics a Markovian process and that universal gates on the Turing-memory side simulate the interactions of particles in the system. Appendices are for a note on the two entropies and for a comparison between our derivation of the Maxwell-Boltzmann distribution and that by Jaynes [12].

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II. ASYMMETRIC SZILARD ENGINE AND ERASURE OF COMPRESSED MEMORY

Let us recapitulate the resolution of the Maxwell's demon paradox with an asymmetric Szilard engine. The engine contains a single molecule gas in the cylinder and a partition is to be inserted to divide the whole volume V_0 into pV_0 and $(1-p)V_0$ with $0 < p < 1$ [1]. First, the demon inserts the partition into the cylinder and measures the position of the molecule. Second, he ties a weight at the side in which he found the molecule. The demon lets the gas expand isothermally at temperature T to push the partition to the end of the cylinder. This expansion provides the demon with $TS(p)$ of work, where $S(p) = -k_B\{p \ln p + (1-p) \ln(1-p)\}$ is the thermodynamic entropy. Finally, the demon removes the partition to close the cycle of the asymmetric Szilard engine. It looks as if the demon could extract work from a heat bath without leaving any trace in the state of the gas. This apparent violation of the second law of thermodynamics is called the Maxwell's demon paradox [7].

The key to the resolution of this paradox is in the fact that the demon keeps information on the molecule's position in his memory. The physical process of memory reset should also be taken into account to complete the cycle [4-6]. No costs are assumed for the actions of inserting and removing the partition, tying a weight, measuring the position of the molecule [5], and computing inside the memory [6]. It is most natural and judicious to consider a symmetric physical configuration for the (binary) memory, in terms of transparency of the discussion. Thus, the necessary amount of work to erase one bit of information is $k_B T \ln 2$ [7]. It is emphasized that only the combined gas law is used to evaluate the erasure work, avoiding the use of the second law, let alone statistical mechanics [8]. The demon operates the asymmetric Szilard engine for sufficiently many times to accumulate the data regarding molecule's positions. Then he carries out the optimal data compression, whose compression factor is equal to the Shannon information entropy $H(p) = -p \log_2 p - (1-p) \log_2(1-p)$. After compressing the data, Maxwell's demon resets the memory according to the model we introduced above.

Therefore, the difference between the work to reset the memory and the one extracted by the Szilard engine per cycle asymptotically approaches zero,

$$k_B T \ln 2 \cdot H(p) - TS(p) = 0, \quad (3)$$

as the length of the data sequence tends to infinity. That is, the second law remains intact and the Maxwell's demon paradox [1] is resolved. Note that the data cannot be compressed in the original case of the symmetric Szilard engine, i.e., the cylinder with a partition inserted at its center [4, 5]. Also, Eq. (3) strongly corroborates the equivalence between the thermodynamic and information theoretic entropies in the case of the optimal information processing and thermodynamical operation. See more details in Appendix. A.

III. THERMO-TURING MODEL

The primary components of our model are a set P of N particles with two energy levels $|0\rangle$ and $|1\rangle$, a long tape M , on which a sequence of N memory cells are embedded, and Maxwell's demon who are capable of manipulating the particles' states and the tape. We will denote the energy gap between the two levels of the particles ϵ , and assume that each particle is numbered to make a correspondence with a memory cell. The tape of memory cells can be thought of as the one we typically consider in the context of Turing machine. Each memory cell can store a binary information, either 0 or 1, and it can be modeled as a one-molecule gas with a partition at the center of cylinder. The whole system $P + M$ is supposed to be in contact with environment (heat bath) of the temperature T .

Suppose that initially the particles are all in their ground state $|0\rangle$ and the values stored in the memory are all 0. Some mechanism, whose detail is irrelevant to the present discussion, excites some of the particles to $|1\rangle$, and the demon changes the information in the tape, monitoring the state changes of the particles. Let p be the rate of the excited particles, i.e., pN particles are in the excited state, while $(1-p)N$ in the ground state.

Let us consider the amount of work F that the entire system ($P + M$) can potentially exert towards the outside, when we let it return to the original state, where all particles are in the ground state and the memory tape contains only a sequence of 0's. The energy stored in P contributes to F positively, and its amount is $E := pN\epsilon$. On the other hand, in order to make the data on the tape all 0, we need to consume some energy W_{er} , as a cost to erase information. As a result, we have

$$F = E - W_{\text{er}}. \quad (4)$$

Since we are naturally interested in the optimal (largest) value of F for a given p , W_{er} needs to be minimized. Thus, we have $W_{\text{er}} = NH(p)k_B T \ln 2$ [1], which leads to

$$F = pN\epsilon - NH(p)k_B T \ln 2. \quad (5)$$

We shall define the equilibrium to be the state whose F is stable against small noises on either the tape or the particles. Let us now describe a physical scenario that justifies the consideration of the stability of F as condition for equilibrium. Because we now focus on the stability of the equilibrated state, we imagine a process in which the state starts from equilibrium and a small number of errors occur. The condition of the equilibrium requires that the particle system stays in equilibrium under the repetition of this process. So, in the initial state, there are pN particles in the excited state and all the memory cells of the tape store 0.

For the following scenario, we need a Carnot engine C that is operated between two heat baths, i.e., those of two different temperatures, T_H and $T_L (< T_H)$. The engine C is used to pump up the energy level of particles by

providing work taken from heat baths. The temperatures are thus chosen so that the work by C is equal to ϵ . In other words, they should satisfy $T_H/T_L = Q_H/Q_L$ and $\epsilon = Q_H - Q_L$, where Q_H is the amount of heat flow from the heat bath of T_H to the engine and Q_L is that to the heat bath of T_L from the engine. For simplicity, we will assume that the expansion (compression) rate of the volume is 2 (1/2), thus $\epsilon = k_B(T_H - T_L) \ln 2$.

Another component is a work reservoir, which is a standard gadget in thermodynamics and typically modeled by a spring. It is a mechanism that can keep mechanical energy, and we can either extract energy from it or add extra energy to it when necessary. The net change in the stored energy in the work reservoir should be zero when a thermodynamic cycle is completed. (If an excess energy was still stored at the end of a cycle, it can be discarded as heat into the heat bath.)

We then consider the following cycle, consisting of steps (a)–(g) (see Fig. 1). The particles are initially in equilibrium with the heat bath of temperature T : pN of them are excited, and all of N memory cells contain 0. Since the particles should always be in a reasonable physical state when seen from the outside, all artificial manipulations in the cycle are designed to be performed on the memory tape; the tape is subject to only occasional (natural) errors. We also assume that the demon knows the value of p , having operated the system for a long time.

- (a) The demon lets $NH(p)$ memory cells expand to the end isothermally at temperature T . Each cell does $k_B T \ln 2$ of work, and the demon stores the energy of $W_1 = NH(p)k_B T \ln 2$ in the work reservoir.
- (b) The demon inserts a partition at the centre of the cylinder of those $NH(p)$ cells, so that a half of $NH(p)$ cells represent the value 0 and the other half have 1.
- (c) The demon applies data decompression, the inverse operation of Shannon's data compression, on all N cells. After the decompression, pN cells will be in 1 and the rest in 0. Since this operation is reversible, it can be designed so that no energy consumption is required.
- (d) The demon re-sorts the data sequence, according to the states of particles, so that if the k -th particle has the energy E_i ($i \in \{0, 1\}$) the k -th cell contains the value i . No energy consumption is needed.
- (e) During some fixed time Δt , a small number ($\ll N$) of errors would occur in the tape. An error can be modeled as a NOT operation applied on a randomly chosen cell.
- (f) Detecting the cells where an error occurred, the demon changes the states of the corresponding particles. He transfers energy from the particles to the work reservoir and vice versa, depending on the direction of the change.

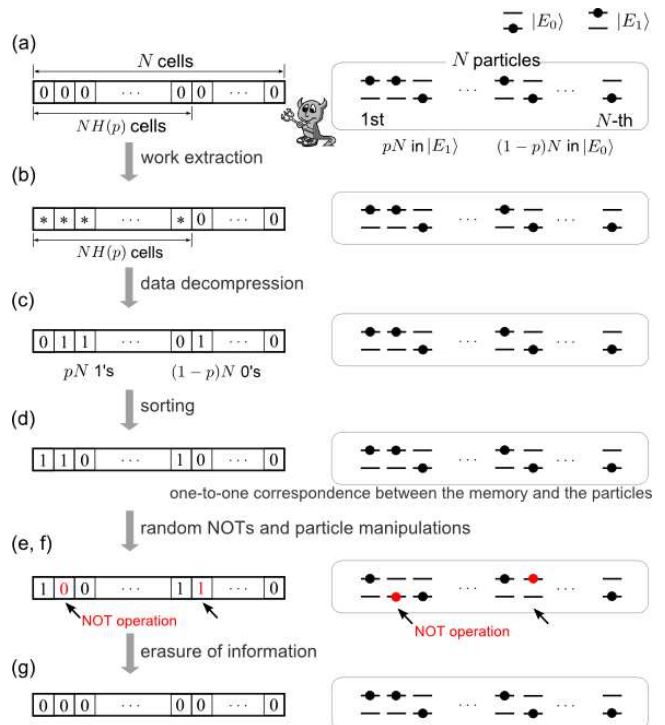


FIG. 1: (color online) The virtual process for which we consider the change of F . The '*' sign in (b) represents a randomized memory state with no physical distinction between 0 and 1; the molecule can move around in the whole configuration space of the cylinder. The demon operates both the memory tape and particles, sitting (standing) in between them.

- (g) The demon erases all data in the tape, which now stores $H(p')$ bits with p' being the new rate of 1's. The minimum work is $W_2 = NH(p')k_B T \ln 2$, a part (or all) of which would be supplied by the work reservoir.

The data sequence returns to $00\dots 0$, while $p'N$ particles are now in the excited state. The random NOT in the Step (e) may be a physical error to particle state, rather than a computational error to the memory state. Such a physical error can be triggered by thermal fluctuation, thus the energy for flipping the state is supplied by its environment in this case. In the above scenario (Steps (a)–(g)), on the other hand, a computational error occurred to the memory without energy supply, and then the demon changed the particle state accordingly by taking energy from the heat bath. So the net physical effect and the energy balance are the same.

The detection of errors in the Step (f) may seem to require an additional memory, which is as long as the tape, to keep the data in the previous cycle. If so, we would need to take another erasure cost as well, making the story cumbersome. Fortunately, the demon can detect errors simply by comparing the data stored in a cell and the state of the corresponding particle. The necessary number of memory registers is negligible compared with the length of the tape.

One might naively wonder why we do not simply encode the particle state to the tape without the steps (a)-(c). The point is the energy W_1 that we can extract from the heat bath exploiting the initial low entropy state. Although it may look unnecessarily complex, we believe that it is the most natural scenario in which the stability of F manifests as a condition for equilibrium.

IV. MAXWELL-BOLTZMANN DISTRIBUTION

There is a one to one correspondence between the physical state Π in the phase space of classical particles of P and the computational state Ψ of the tape of the Turing machine M . This correspondence is guaranteed in the two ways. That is, $\Pi \rightarrow \Psi$ by measurement of Π and its encoding in Ψ , and $\Psi \rightarrow \Pi$ by readout of Ψ of the Turing machine and a subsequent operation of the Carnot engine C .

Equilibrium is characterized by the balance between the energy income and expenditure in $P+M$ against small errors to Ψ , which we model by random operations. Arbitrary operations can be simulated by NOT and Toffoli gates, since any reversible computation can be executed by these two. Once a NOT or Toffoli operation occurs to a randomly chosen cell, the demon activates the Carnot engine C to change the state of the corresponding particle.

Let us start with an intuitive picture of equilibrium. Suppose there are more 0's than 1's. Then random NOTs tend to equalize the populations of 0's and 1's in the tape. As the number of 0's approaches that of 1's, the demon has to consume more energy to excite particles from $|0\rangle$ to $|1\rangle$. At the same time, the bit string on the tape becomes less compressible, thus larger information content, which means that more work would be needed to erase it. This energy for erasure can be paid by the particle system. So the whole system can be said to be in equilibrium, if these increases in energies for state excitation and for information erasure are equal.

The net energy balance in the process from (a) to (g) is simply a sum of the energy transfers in the Steps (a), (f), and (g). It is

$$W_1 + (p'N - pN)\epsilon - W_2 = \Delta p \cdot N\epsilon - N\Delta H(p) \cdot k_B T \ln 2, \quad (6)$$

where $\Delta p = p' - p$ and $\Delta H(p) = H(p') - H(p)$. The above cost is equal to the change ΔF of the function introduced in Eq. (5). Since the number of errors is small, i.e., $\Delta p \ll 1$, $\Delta H(p) = dH(p)/dp \Delta p \equiv H'(p)\Delta p$. When the system is in equilibrium, $\Delta F = 0$, thus

$$\epsilon - k_B T \ln 2 \cdot H'(p) = 0. \quad (7)$$

The same equation holds in the case where the NOT gate hits a cell of 1 to change it to 0.

Noting that $\ln 2 \cdot H'(p) = \ln[(1-p)/p]$, we see that Eq.

(7) reduces to

$$\frac{p}{1-p} = \exp\left(-\frac{\epsilon}{k_B T}\right), \quad (8)$$

which is nothing but the Maxwell-Boltzmann distribution. A similar calculation can be done for the case in which the Toffoli gate is considered as an error operation.

To sum up the Maxwell-Boltzmann distribution (8) has been operationally derived under the assumptions

- (1) the state preparation by the Turing machine and the device (Carnot engine) C to assign energy levels for the N -particles
- (2) Landauer-Bennett's principle for the erasure of memory
- (3) the equilibrium condition in terms of the work extractable from $P + M$.

as well as the combined gas law in elementary thermodynamics.

Let us now evaluate the second order effect. A straightforward calculation shows that the average change in the information-theoretic entropy due to a random NOT is

$$H(p) \rightarrow H(p) + H'(p)\frac{(1-2p)}{N} + H''(p)\frac{1}{2N^2} + \dots \quad (9)$$

noting that the transition $0 \rightarrow 1$ takes place with probability $1-p$, which increases p to $p + \frac{1}{N}$, while the transition $1 \rightarrow 0$ occurs with probability p , which decreases p to $p - \frac{1}{N}$. This makes a change of $H(p) \rightarrow (1-p)H(p + \frac{1}{N}) + pH(p - \frac{1}{N})$, each term of which can be expanded as in Eq. (9).

The total cost change by the random Toffoli gate is computed as

$$\Delta F(\text{Toffoli}) = -k_B T p^2 H''(p) \frac{\ln 2}{2N} + \mathcal{O}\left(\frac{1}{N^2}\right). \quad (10)$$

Note that the first order contributions, i.e., the terms having $H'(p)$, cancel out due to the equilibrium condition. The effect of the random Toffoli gate is essentially equivalent to that of the random NOT gate except for the overall probability factor p^2 for having two 1's in the control bits.

Therefore, the sum of the second order contribution of the random NOT and Toffoli gates is

$$\begin{aligned} \Delta F &= -k_B T [\#(\text{NOT}) + \#(\text{Toffoli})p^2] H''(p) \frac{\ln 2}{2N} \\ &+ \mathcal{O}\left(\frac{1}{N^2}\right) (> 0). \end{aligned} \quad (11)$$

That is, the change ΔF by the random NOT and Toffoli gates tends to strengthen the local stability of the cost function F near the equilibrium. This further supports our definition of equilibrium in the thermo-Turing model. It is also noted that the quantity in the square bracket is the effective computational complexity.

V. GENERALIZATION

The above argument to derive the Boltzmann distribution can be generalized to the case of *dits*. That is, the cells of the tape can store d values from 0 to $d-1$, and the particles have d energy levels from $|E_0\rangle$ to $|E_{d-1}\rangle$. Let p_i be the ratio of the number of cells storing the value i to the total number of cells on the tape. Suppose that the k -th particle is excited to the state $|E_i\rangle$ when the k -th cell stores the value i . This state preparation can be completed by a similar mechanism to the one above, where a Carnot engine C is operated depending on the data in cells. Here, we can think of $d-1$ engines, C_i ($i \in \{1, \dots, d-1\}$). The engine C_i is switched on when the measurement apparatus D finds i in a cell, and then C_i dispenses energy E_i to the corresponding particle. Each engine thus utilizes two heat baths of temperatures $T_H^{(i)}$ and $T_L^{(i)} (< T_H^{(i)})$ so that $E_i = k_B(T_H^{(i)} - T_L^{(i)}) \ln 2$ [13], where all engines are assumed to be operated between two volumes, V and $V/2$. We will use another notation C_i^{-1} to indicate the engine C_i operated in the reverse direction.

Instead of the random NOT studied in the previous section, let us suppose random SWAP operations that change the value in a single cell. Let SWAP_{ij} denote a SWAP between two values i and j , namely, SWAP_{ij} maps a value i of a randomly chosen cell to j and vice versa. Note that the NOT operation between two levels is effectively the same as the SWAP between them. Once such a SWAP_{ij} is applied to the k -th cell, which stores the value i (assume $i < j$ without loss of generality), the mechanism D activates C_i^{-1} and then C_j to change the state of the k -th particle: C_i^{-1} retrieves energy E_i from the particle and discard it to the heat bath at $T_L^{(i)}$, and C_j gives E_j of energy to it.

Suppose that a SWAP_{ij} has occurred to one of the cells. The SWAP_{ij} changes the value stored in the cell if it retains either i or j , otherwise nothing happens. The probability of such a ‘successful’ SWAP_{ij} is $p_i + p_j$. If it was i the corresponding particle is excited from $|E_i\rangle$ to $|E_j\rangle$, and if it was j the particle loses energy to become $|E_i\rangle$. Thus once the SWAP_{ij} hits a single cell on the tape, the energy change in the particle system is $(E_j - E_i)(p_i - p_j)/(p_i + p_j)$ on average.

The change in the erasure entropy times temperature after the single SWAP_{ij} is

$$\begin{aligned} & Nk_B T \ln 2 \left[\frac{p_i}{p_i + p_j} H\left(p_i - \frac{1}{N}, p_j + \frac{1}{N}\right) \right. \\ & \left. + \frac{p_j}{p_i + p_j} H\left(p_i + \frac{1}{N}, p_j - \frac{1}{N}\right) \right] - Nk_B T \ln 2 \cdot H(p) \\ & \simeq k_B T \ln 2 \frac{p_i - p_j}{p_i + p_j} \ln \frac{p_i}{p_j}, \end{aligned} \quad (12)$$

where $H(p_i \pm \frac{1}{N}, p_j \mp \frac{1}{N})$ are $-\sum_k p_k \log_2 p_k$ with the replacement of p_i and p_j with $p_i \pm \frac{1}{N}$ and $p_j \mp \frac{1}{N}$, respectively.

Making the change in F equal to zero as in the case of bits and two-level particles, we arrive at the desired relation:

$$\begin{aligned} (E_j - E_i) \frac{p_i - p_j}{p_i + p_j} - k_B T \frac{p_i - p_j}{p_i + p_j} \ln \frac{p_i}{p_j} &= 0 \\ \frac{p_j}{p_i} &= \exp\left(-\frac{E_j - E_i}{k_B T}\right). \end{aligned} \quad (13)$$

This relation holds for any pairs of i and j , hence $p_i \propto \exp(-E_i/k_B T)$ for all i .

VI. DISSIPATION-FLUCTUATION THEOREM

In principle, our thermo-Turing model can be applied to generic non-equilibrium processes. Here, we will present a modest step to this direction, choosing a particular model which exhibits a characteristic feature of dissipation-fluctuation theorem.

The maximal work F we can obtain from $P+M$ to let it return to the standard state $00\dots 0$ is given by

$$F = pN\epsilon - Nk_B T \ln 2 \cdot H(p) \quad (14)$$

as in Eq. (5).

Let the change of the maximal work F by an operation ω be

$$\Delta_\omega F = \Delta_\omega p N \epsilon - Nk_B T \ln 2 \cdot H'(p) \Delta_\omega p. \quad (15)$$

Suppose that this change is caused by an external energy supply u ;

$$\Delta_\omega F = u. \quad (16)$$

The solution to this equation gives a non-equilibrium steady state distribution

$$p_0(u) = \left[1 + \exp\left(\frac{\epsilon - u}{k_B T}\right) \right]^{-1}, \quad (17)$$

for $\Delta_\omega p = 1/N$ which corresponds to the transition $0 \rightarrow 1$. The distribution becomes $p_0(-u)$ for $\Delta_\omega p = -1/N$, i.e., the transition of the opposite direction, $1 \rightarrow 0$.

Now consider a spatially fluctuating potential u_n where n ($n = 1, 2, \dots, N$) represents a site location, and we assume $\sum_n u_n = 0$ [14]. We then evaluate the average work $\langle W \rangle$ done by a NOT gate under this potential. Suppose a set of sites m such that $p_0(u_m) > p_{eq}$, where p_{eq} is the probability distribution for equilibrium. For such sites, an incoming energy $u_n > 0$ ($n \in \{m\}$) causes the change $0 \rightarrow 1$, and the rate of transition should be proportional to the non-equilibrium distribution (the occupation probability) $1 - p_0(u_n)$. So the average work done is $\sum_{\{n|u_n>0\}} [1 - p_0(u_n)] u_n$. If $u_n < 0$, then the induced transition is $1 \rightarrow 0$ and the average work is $\sum_{\{n|u_n<0\}} p_0(-u_n) u_n$. Together with a similar consideration for the set $\{m'|p_0(u_{m'}) < p_{eq}\}$, we have

$$\langle W \rangle = \sum_n [1 - p_0(u_n)] u_n + \sum_n p_0(-u_n) u_n. \quad (18)$$

To simplify the computation, consider the case in which the external potential u_n is weak. Using the approximation $p_0(u) \approx p_{eq} + p'_0(0)u$, we obtain

$$\langle W \rangle = -\frac{2}{k_B T} \left[1 + \exp\left(\frac{\epsilon - u}{k_B T}\right) \right]^{-2} \mathcal{F}, \quad (19)$$

where $\mathcal{F} = \sum_n u_n^2$ is the sum of squared values of the fluctuating potential. Equation (19) means that the NOT gate does negative work, $\langle W \rangle < 0$, thus it makes energy dissipate to the external space (environment). Further, it is proportional to the fluctuation of the potential. It is a simple expression of the dissipation-fluctuation theorem in the linear approximation of the fluctuating potential u_n .

The readers who are familiar with the standard dissipation-fluctuation theorem would feel more comfortable with the fluctuation in time rather than the spatial one of the external potential. In that case, one can reorder the site numbers according to the order of occurrence of the NOT gate. Then, the n can be interpreted as time, and the average $\langle \cdot \rangle$ can be understood as that over a long time.

VII. SUMMARY AND DISCUSSIONS

We have presented an operational derivation of the Maxwell-Boltzmann equilibrium distribution in the statistical mechanics by a simple model of Maxwell's demon endowed with the Turing machine only on the basis of thermodynamics. The crux of the argument is in the thermodynamic work needed to reset the memory of the Turing-type tape. This model can also be applied to non-equilibrium processes. We have demonstrated the dissipation-fluctuation using a simple example.

Our operational derivation can be contrasted with the standard one based on the micro-canonical ensemble, in which the entropy S is given by the Boltzmann formula $S = k_B \log \Omega(E)$ with $\Omega(E)$ being the number of states under a given energy E . Clearly, we did not rely on the micro-canonical statistical mechanics. Instead, the notion of entropy comes in from information theory, and that of temperature is from Landauer-Bennett's erasure principle. Jaynes' derivation summarized in Appendix B is information theoretic, however, its connection to thermodynamics is rather hypothetical.

Assuming that the interaction of the particles is mathematically described, e.g., by Hamilton's equations, we can say from the universality of the Turing machine that the equations of motion are mapped to the operations of the machine. This means that the physical interaction can be simulated by the gates ω , consisting of NOT and Toffoli gates. The relaxation process is simulated by the reset of memory (a brute-force Markovian process). Note that the memory is also physically modeled on the basis of the combined gas law in the elementary thermodynamics.

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Appendix A: Note on thermodynamic and information-theoretic entropies

In our previous paper [1], we showed in the scenario of Maxwell's demon that the thermodynamic entropy coincides with the information theoretic entropy in the optimal case of the memory reset. In this Appendix we attempt to look at the same problem from a different perspective going back to the basic thermodynamics.

Let us recall how the thermodynamic entropy was introduced on the basis of Carnot's theorem. Let the work exerted towards the outside be $W(i \rightarrow f)$ for an isothermal state change $i \rightarrow f$, which is different from the change of the internal energy $U_i - U_f$, in general. An invisible energy flow that contributes to the energy balance is called heat Q exchanged between the system and the heat bath. Thus, the energy conservation is written as

$$W(i \rightarrow f) = U_i - U_f + Q. \quad (A1)$$

Carnot's theorem claims that the maximal heat flow from the heat bath in isothermal process is proportional to the temperature T of the heat bath,

$$Q_{max} = T S_{th}, \quad (A2)$$

where the maximization is made over all possible intermediate processes between the initial and the final states [15]. The coefficient S_{th} is defined as the increase of the thermodynamic entropy.

Now go back to our thermo-Turing model. Clearly, our F in Eq. (4) is the negative of the work that can be exerted outwards,

$$F = -W(i \rightarrow f). \quad (A3)$$

Letting the minimum of F in Eq. (A3) be equal to Eq. (5),

$$\begin{aligned} F_{min} &= -W_{max} = -U_i + U_f - Q_{max} \\ &= p\epsilon N - NH(p)k_B T \ln 2. \end{aligned} \quad (A4)$$

Since $-U_i + U_f = p\epsilon N$ in our model, we arrive at the equivalence between the thermodynamic and the information-theoretic entropies;

$$S_{th} = NH(p)k_B \ln 2. \quad (A5)$$

It is interesting to see that both the thermodynamic and the information theoretic entropies are defined as a limit, while the former is physically realized in the quasi-static

limit and the latter is achieved by the optimal limit of the data compression. The quasi-static processes means that the operation has to be slow enough compared with microscopic processes. This can be viewed as an aspect of the Markovian process, in which the information on the earlier configuration is lost due to, e.g., the multiple-scattering of particles by the cylinder wall. The corresponding process in our model is the erasure of information, which occurs when the partition in the memory cell is removed. To lose the information on the molecule's position, we need to wait for a while until it becomes impossible to infer the molecule's trajectory.

As a byproduct, we can see that the extensivity of the thermodynamic entropy follows from that of the Shannon entropy. Note also that Eq. (A5) can be viewed as the Boltzmann formula $S_{th} = k_B \ln W$, where $W = 2^{NH(p)}$ is the number of possible states under a given total energy.

Appendix B: A comparison with Jaynes' Work

In the work on the relation between information theory and statistical mechanics, Jaynes derived the corresponding equilibrium state (13) in the following way [12]. The plausible probability distribution is determined by the requirement that the estimator function $\text{Est}(p_1, p_2, \dots, p_n)$

is maximized under a given average energy $\langle E \rangle = \sum_i p_i E_i$ with $\sum_i p_i = 1$. Following Shannon [10], he required the mathematical properties for the estimator $\text{Est}(p_1, p_2, \dots, p_n)$: (i) $\text{Est}(p_1, p_2, \dots, p_n)$ is a continuous function of p_i , (ii) $f(n) := \text{Est}(1/n, 1/n, \dots, 1/n)$ is a monotonic increasing function of n , and (iii) $\text{Est}(p_1, p_2, \dots, p_n)$ satisfies the composition law. From these mathematical requirements (i)-(iii), the estimator is uniquely determined to be equal to the Shannon entropy, i.e., $\text{Est}(p_1, p_2, \dots, p_n) = -\sum_i p_i \log p_i$. Maximizing the Shannon entropy under the constraints that $\langle E \rangle$ is fixed and $\sum_i p_i = 1$, the plausible probability distribution is obtained to be the one in Eq. (13). Note that the temperature does not come in from the physical assumption but is defined so that the free energy thereby obtained coincides with the Helmholtz free energy.

In the present work, we have devised a model consisting of a memory tape (information theoretic object) and a set of particles (physical system), both of which are in contact with a heat bath of temperature T and are operated by the demon. Then, we have defined the equilibrium state operationally and subsequently derived the Maxwell-Boltzmann distribution. Thus, the temperature dependence of the distribution was naturally obtained, whereas it was not so in Jaynes' mathematical work.

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 - [13] Naturally, either of two heat baths can be a common one among as many engines as we like. For instance, all heat baths of lower temperature can be a single one at T_L , irrespective of the value in the cell, as far as the engine does a right amount of work.
 - [14] Since the formal definition of p is the ratio between the ground and excited states, strictly speaking, the site $n = 1, 2, \dots, N$ should be taken as a block, which consists of sufficiently many sites to define the locally non-equilibrium steady distribution. However, this does not affect our result.
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