technical note

Inevitable irreversibility in a quantum system consisting of many non-interacting “small” pieces

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Abstract

We review the recent result of Sato, Sekimoto, Hondou, and Takagi [1] (cond-mat/0008393) on the irreversibility inevitably observed in systems consisting of many non-interacting “small” pieces. We focus on quantum models, and supply an explicit lower bound for the work required to complete a cyclic process.

1 Introduction

In statistical physics textbooks, one often encounters systems which consist of macroscopic numbers of identical small parts which do not interact with each other. This is not too unrealistic since there are many physical systems (such as certain spin systems, including nuclear spin systems) which are well approximated by such non-interacting models in some ranges of temperature and time.

The question that we wish to examine here is the following: Does a system which consists of many non-interacting pieces behave as a “healthy” thermodynamic system? It is evident from exercises in statistical physics that the answer is “yes” when only equilibrium properties are concerned. If one focuses on certain non-equilibrium aspects, however, the situation may be different. In fact Sato, Sekimoto, Hondou, and Takagi recently proved that, in a system which consists of many non-interacting small parts, a simple quasi-static process involving contacts with two heat baths can never be reversible in general. It is remarkable that such a system fails to provide us with reversible processes, which are among the building blocks of conventional thermodynamics. Sato, Sekimoto, Hondou, and Takagi then raise an interesting question whether one can develop a new thermodynamic framework which is capable of describing these unavoidable irreversible processes.

The basic idea of Sato, Sekimoto, Hondou, and Takagi is indeed quite simple. Suppose that a small piece (whose identical copies form the whole system) is a quantum system with \( n \) energy levels \( \varepsilon_1, \ldots, \varepsilon_n \). We first assume that the whole system is in equilibrium with a heat bath at inverse temperature \( \beta \). Then the probability of finding the small system in the \( i \)-th state is \( p_i = e^{-\beta \varepsilon_i}/z(\beta) \) where \( z(\beta) \) is the partition function for the small system. We then gently decouple the system from the bath in such a way that the small system is still described by the same probability \( p_i \). Then we change a parameter in the model Hamiltonian very slowly, modifying the energy levels to \( \varepsilon'_1, \ldots, \varepsilon'_n \). The adiabatic theorem tells us that, if the parameter change is sufficiently slow, the probability of finding the small system in the \( i \)-th state is still given by the same \( p_i \). But this \( p_i \) cannot be represented

1 The comparison hypothesis as in [2] is also violated, if we include a contact with a heat bath (whose temperature is chosen carefully so that no net energy is exchanged) at the end of each “adiabatic process.”

3 We number the states so that \( \varepsilon_i \leq \varepsilon_{i+1} \) and \( \varepsilon'_i \leq \varepsilon'_{i+1} \).
in the Gibsian form \( p_i = e^{-\beta' \varepsilon'_i / \beta'} \) for any \( \beta' \) unless the two energy levels \( \varepsilon_1, \ldots, \varepsilon_n \) and \( \varepsilon'_1, \ldots, \varepsilon'_n \) satisfy a special condition. (See (2.14).) Therefore if the system is brought into a contact with a heat bath after the operation, something nontrivial (which turns out to be a jump in the entropy) must take place, no matter how carefully one chooses the temperature of the bath.

Of course such a mechanism applies to any quantum systems, including truly macroscopic ones. But it is wellknown that this kind of deviation from a certain equilibrium distribution is irrelevant in thermodynamic limits. A crucial observation of Sato, Sekimoto, Hondou, and Takagi’s is that the smallness of each non-interacting piece makes this deviation thermodynamically observable.

If one regards non-interacting systems as models of more realistic weakly-interacting systems, then the above irreversibility of Sato, Sekimoto, Hondou, and Takagi should be observed only for operations which take place in a time interval which is not long enough for the system to redistribute its energy between the small parts. If the operation is slow enough and such a redistribution takes place, then the probability distribution for each part at the end of operation becomes essentially Gibbsian, and the process may be reversible.

\section{Setup and main results}

We consider a quantum system which consists of \( N \) identical “small” quantum systems which do not interact with each other. A single small system has an \( n \)-dimensional Hilbert space, and the whole system has an \( nN \)-dimensional Hilbert space.

The initial Hamiltonian of the system is

\[ H = \sum_{i=1}^{N} h_i, \quad (2.1) \]

where, for all \( i \), \( h_i \) is identical to a certain Hamiltonian \( h \) for the small system. Initially the system is in touch with a heat bath, and hence in the Gibbs state

\[ \langle \cdots \rangle^\text{Gibbs}_1 = \text{Tr}[\cdots | \rho^\text{Gibbs}_1], \quad (2.2) \]

with

\[ \rho^\text{Gibbs}_1 = \frac{e^{-\beta H}}{\text{Tr}[e^{-\beta H}]]. \quad (2.3) \]

We gradually decouple the system from the heat bath, making it thermally isolated. We assume that the state of the system is unchanged from (2.2).

We then perform a “classical” operation on the system. This corresponds to an adiabatic process in thermodynamics. We model the operation by a time dependent Hamiltonian

\[ H(t) = \sum_{i=1}^{N} h_i(t), \quad (2.4) \]

\footnote{Note that the word “adiabatic” means that no “heat” is exchanged between the system and the outside world, and does not mean anything like “slow and gentle.”}
Figure 1: Sato, Sekimoto, Hondou, and Takagi considered the following cycle; (a) A macroscopic system is in touch with a heat bath at inverse temperature $\beta$. The state of the system is described by a density matrix $\rho_1$. (b) One gently decouples the system from the heat bath, without changing its state. (c) An external agent performs an operation on the system, changing its Hamiltonian from $H$ to $H'$. The state changes to $\rho_2$, which may not be Gibbsian. (d) The system is put into contact with a heat bath at inverse temperature $\beta'$. Here $\beta'$ is carefully chosen so that there is no net exchange of energy between the system and the bath. Note that this is a very innocent thermal contact, which causes no observable effects in normal thermodynamic systems. (e) Again one gently decouples the system from the heat bath, without changing its state. (f) The external agent performs an operation on the system, bringing back its Hamiltonian from $H'$ to $H$, thus completing a cycle.

Let $W_{\text{cyc}}$ be the total work done to the system by the external agent during the above cycle. Conventional thermodynamics tells us that $W_{\text{cyc}}$ can be made arbitrarily small by performing the operation slowly and gently. When the system in consideration consists of many "small" parts which do not interact with each other, however, Sato, Sekimoto, Hondou, and Takagi proved that $W_{\text{cyc}}$ is always greater than a finite value. This means that the above thermodynamic cycle is inevitably irreversible.
where all \( h_i(t) \) are identical. After the operation, the Hamiltonian settles to

\[
H' = \sum_{i=1}^{N} h'_i, \quad (2.5)
\]

where all \( h'_i \) are identical to \( h' \). We denote by \( U \) the unitary operator which describes the quantum mechanical time evolution during the whole operation\(^5\). Since the system is thermally isolated, its state after the operation is simply given by

\[
\langle \cdots \rangle_2 = \text{Tr}[\langle \cdots \rangle \rho_2], \quad (2.6)
\]

with

\[
\rho_2 = U \rho_{1\text{Gibbs}} U^{-1}. \quad (2.7)
\]

Note that in general this is not a Gibbs state.

Next we put the system into a contact with another heat bath with the inverse temperature \( \beta' \). After equilibration, the state of the system becomes another Gibbs state

\[
\langle \cdots \rangle_{3\text{Gibbs}} = \text{Tr}[\langle \cdots \rangle \rho_{3\text{Gibbs}}], \quad (2.8)
\]

with

\[
\rho_{3\text{Gibbs}} = \frac{e^{-\beta' H'}}{\text{Tr}[e^{-\beta' H'}]} \quad (2.9)
\]

Here the inverse temperature is (carefully) chosen so that

\[
\langle H' \rangle_2 = \langle H' \rangle_{3\text{Gibbs}} \quad (2.10)
\]

holds. This means that there is no net exchange of heat between the system and the second heat bath\(^6\). This thermal contact thus looks quite innocent. We stress that for a normal thermodynamic system, such a thermal contact without energy exchange produces no observable effects. It is a peculiar nature of systems which consist of non-interacting small pieces that such a contact inevitably leads to irreversibility.

Finally we repeat the same process backwards. We first gently decouple the system from the heat bath (without changing the state of the system), and then make an arbitrary operation which brings back the Hamiltonian from \( H' \) to the initial \( H \). By denoting \( U' \) the unitary operator for this time evolution, we can write the final (generally non-Gibbsian) state as

\[
\langle \cdots \rangle_4 = \text{Tr}[\langle \cdots \rangle \rho_4], \quad (2.11)
\]

with

\[
\rho_4 = U' \rho_{3\text{Gibbs}} U'^{-1}. \quad (2.12)
\]

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\(^5\) The unitary operator \( U \) is formally defined as follows. Suppose that the operation is done during \( t = t_0 \) and \( t_1 \). Let \( U(t) \) be the solution of the Schrödinger equation \( i\partial U(t)/\partial t = H(t) U(t) \) with the initial condition \( U(t_0) = 1 \). Then \( U = U(t_1) \). In what follows, however, we only use the fact that \( U \) is unitary.

\(^6\) Because the Hamiltonian (2.5) is a sum of mutually commuting pieces, the fluctuation of the energy is \( O(\sqrt{N}) \) in the states \( \langle \cdots \rangle_2 \) and \( \langle \cdots \rangle_{3\text{Gibbs}} \). Since the expectation values of the energy itself is \( O(N) \), this means that the fluctuation of energy is simply negligible for large enough \( N \).
From the energy conservation law, one sees that the difference $\langle H \rangle_4 - \langle H \rangle_{\text{Gibbs}}$ is the total energy supplied to the system during the operation. In sufficiently large systems where the energy exchange between the second heat bath and the system is negligible, this difference is the total work done to the system by the outside agent (who performs the operation). Note that, from a thermodynamic point of view, the two operations together form a cycle because the Hamiltonian finally returns to the initial one. One of the basic assumptions in conventional thermodynamics is that the work during such a cycle can be made as small as possible by performing the operation slowly. The limiting operation in which the total work is vanishing is usually called a “reversible” cycle.

But the following theorem due to Sato, Sekimoto, Hondou, and Takagi clearly shows that a reversible cycle is never realized in a system which consists of non-interacting small pieces.

**Theorem** (Sato, Sekimoto, Hondou, and Takagi) For any unitary operators (which are consistent with the given initial and the final Hamiltonians) $U$ and $U'$, one has

$$\langle H \rangle_4 - \langle H \rangle_{\text{Gibbs}} \geq N \Delta \varepsilon(\beta; h, h'),$$

(2.13)

where $\varepsilon(\beta; h, h')$ depends only on $\beta$ and the energy levels $\varepsilon_1, \ldots, \varepsilon_n$ and $\varepsilon'_1, \ldots, \varepsilon'_n$ of the Hamiltonians $h$ and $h'$, respectively. The quantity $\varepsilon(\beta; h, h')$ is nonnegative in general, and is strictly positive unless

$$\varepsilon_i - \varepsilon_1 = A(\varepsilon'_i - \varepsilon'_1),$$

(2.14)

for any $i$ with a constant $A$.

For an explicit form of $\Delta \varepsilon(\beta; h, h')$, see (4.40).

### 3 Example

Simple (and probably realistic) examples are paramagnetic spin system. Note, however, that we do not expect the irreversibility due to the “smallness” in a paramagnetic $S = 1/2$ system, where the small system has only two levels.

The simplest example is the $S = 1$ model under external magnetic field $\vec{H}$ with a crystal field anisotropy $D$, whose Hamiltonian is

$$H = \sum_{i=1}^{N} \left\{ -\vec{H} S_i^{(z)} - D(S_i^{(z)})^2 \right\}.$$

(3.1)

Here $S_i^{(z)}$ is the spin operator with three eigenvalues $+1$, $0$, and $-1$. Thus each small system has three energy levels $-\vec{H} - D$, $0$, $\vec{H} - D$.

As in the standard adiabatic cooling experiments, we thermally isolate the spin system, and change the external magnetic field $\vec{H}$. We find that the condition (2.14) is satisfied when $D = 0$. Thus we expect that the irreversibility due to the smallness of non-interacting pieces is observable when $|D/\vec{H}|$ is sufficiently large.

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Footnote 5: See footnote 4.
4 Proof

4.1 Proof of the main theorem

We prove the main theorem by applying the ideas of Sato, Sekimoto, Hondou, and Takagi to quantum models. We stress that our argument is a straightforward implementation of that of Sato, Sekimoto, Hondou, and Takagi's. The main points in the proof are the use of Gibbs-like entropy (4.2), (4.3), and the representation (4.13) of the entropy increase as a relative entropy.

Throughout the present section, we only treat a special (and unphysical) case with \( N = 1 \), i.e., a single small system. Since the small systems do not interact with each other, results for \( N = 1 \) immediately implies the corresponding results for general \( N \).

For \( i = 1, \ldots, n \), let \( |\varphi_i\rangle \) and \( |\varphi'_i\rangle \) be the normalized eigenstates of \( h \) and \( h' \), respectively. We denote by \( \varepsilon_i \) and \( \varepsilon'_i \) the corresponding energy eigenvalues. We number the eigenstates so that \( \varepsilon_i \leq \varepsilon_{i+1} \) and \( \varepsilon'_i \leq \varepsilon'_{i+1} \) hold.

Let us define a unitary operator \( U \) by

\[
U|\varphi_i\rangle = |\varphi'_i\rangle, \tag{4.1}
\]

for all \( i = 1, \ldots, n \). The adiabatic theorem in quantum mechanics guarantees that the time evolution is described by this unitary operator when the operation is executed infinitely slowly (and if one tunes the phases of the basis states properly). We note that, in usual macroscopic quantum systems, an operation must be unphysically slow for the adiabatic theorem to be relevant. In the present case of systems consisting of non-interacting small systems, however, the slowness required by the theorem may be physically realized since each small system evolve independently.

Once we prove the desired bounds for the special unitary transformation \( U \), the same bounds for arbitrary \( U \) (and \( U' \)) follow immediately. This is because for given \( h \), \( h' \), and \( \beta \), the energy \( \langle h' \rangle_2 \) after the first operation for arbitrary \( U \) (consistent with the Hamiltonians \( h \) and \( h' \)) does not exceed the same quantity obtained from the unitary operation (4.1). (This is nothing but the minimum work principle.) The same is true for the second operation which brings back the Hamiltonian from \( h' \) to \( h \). Therefore we shall only concentrate on \( U \) defined by (4.1).

Let us define the Gibbs-like entropy with respect to Hamiltonian \( h \) as

\[
S_h[\rho] = -k \sum_{i=1}^{n} \langle \varphi_i | \rho | \varphi_i \rangle \log \langle \varphi_i | \rho | \varphi_i \rangle, \tag{4.2}
\]

and the entropy with respect to \( h' \) as

\[
S_{h'}[\rho] = -k \sum_{i=1}^{n} \langle \varphi'_i | \rho | \varphi'_i \rangle \log \langle \varphi'_i | \rho | \varphi'_i \rangle. \tag{4.3}
\]

Note that the present definition of entropy depends on the choice of Hamiltonian \( h \), while the Gibbs entropy (and the von Neuman entropy) does not depend on Hamiltonians. In this sense, the present definition is closer (in spirit) to the Boltzmann entropy, which depends on the way of characterizing the system from a macroscopic view point (e.g., by using energy).
Since the initial state $\langle \cdot \cdot \cdot \rangle_{1}^{\text{Gibbs}}$ is Gibbsian, we write down the density matrix explicitly as
\[ \rho_{1}^{\text{Gibbs}} = \frac{e^{-\beta h}}{\text{Tr}[e^{-\beta h}]} = \sum_{i=1}^{n} |\varphi_{i}\rangle p_{i} \langle \varphi_{i}|, \] (4.4)
where
\[ p_{i} = \frac{e^{-\beta \varepsilon_{i}}}{z(\beta)}, \quad z(\beta) = \sum_{i=1}^{n} e^{-\beta \varepsilon_{i}}. \] (4.5)

Thus, from the definition (4.2) of entropy, we find
\[ S_{h}[\rho_{1}^{\text{Gibbs}}] = -k \sum_{i=1}^{n} p_{i} \log p_{i} = k \beta \langle h \rangle_{1} + k \log z(\beta). \] (4.6)

By using (4.4) and (4.1), we find that the density matrix after the first operation is simply written as
\[ \rho_{2} = U \rho_{1}^{\text{Gibbs}} U^{-1} = \sum_{i=1}^{n} |\varphi'_{i}\rangle p_{i} \langle \varphi'_{i}|, \] (4.7)
with the same $p_{i}$ as in (4.5). We therefore find from (4.3) that
\[ S_{h'}[\rho_{2}] = -k \sum_{i=1}^{n} p_{i} \log p_{i} = S_{h}[\rho_{1}^{\text{Gibbs}}]. \] (4.8)

Our entropy is invariant under slow operation.

We then examine the next Gibbs state $\langle \cdot \cdot \cdot \rangle_{3}^{\text{Gibbs}}$ obtained by letting the system interact with the second heat bath. Its density matrix is simply
\[ \rho_{3}^{\text{Gibbs}} = \frac{e^{-\beta' h'}}{\text{Tr}[e^{-\beta' h'}]} = \sum_{i=1}^{n} |\varphi'_{i}\rangle p'_{i} \langle \varphi'_{i}|, \] (4.9)
where
\[ p'_{i} = \frac{e^{-\beta' \varepsilon'_{i}}}{z'(\beta')}, \quad z'(\beta') = \sum_{i=1}^{n} e^{-\beta' \varepsilon'_{i}}. \] (4.10)

Recall that the inverse temperature $\beta'$ is determined from the condition
\[ \langle h' \rangle_{2} = \langle h' \rangle_{3}^{\text{Gibbs}}. \] (4.11)

From the definition (4.3) of the entropy, we have
\[ S_{h'}[\rho_{3}^{\text{Gibbs}}] = -k \sum_{i=1}^{n} p'_{i} \log p'_{i} \]
\[ = k \beta \langle h' \rangle_{3}^{\text{Gibbs}} + k \log z'(\beta') \]
\[ = k \beta \langle h' \rangle_{2} + k \log z'(\beta') \]
\[ = k \beta \sum_{i=1}^{n} \varepsilon'_{i} + k \log z'(\beta') \}
\[ = -k \sum_{i=1}^{n} p_{i} \log p_{i}, \] (4.12)
where we used (4.11) and (4.7). Combining this with (4.6), we find that the difference of the two entropies can be represented in a remarkable manner as

\[
S_h'[^3\rho_{Gibbs}] - S_h[^1\rho_{Gibbs}] = -k \sum_{i=1}^{n} p_i \log \frac{p'_i}{p_i},
\]

where the right-hand side is nothing but the relative entropy. From the well-known property of relative entropies, we find

\[
S_h'[^3\rho_{Gibbs}] - S_h[^1\rho_{Gibbs}] \geq 0.
\]

Here the equality holds only when \( p_i = p'_i \) for all \( i \). By examining the explicit formulas (4.5) and (4.10) of \( p_i \) and \( p'_i \), respectively, one finds that this is possible only when the energy levels satisfy the condition (2.14).

As for the second operation (which brings back the Hamiltonian from \( h' \) to \( h \)), we assume that the time evolution is described by the unitary operator \( U^{-1} \). We repeat the same argument to show

\[
S_h[^4\rho_{Gibbs}] = S_h'[^3\rho_{Gibbs}].
\]

As a theoretical reference, we define yet another Gibbs state \( \langle \cdot \cdot \cdot \rangle_{Gibbs}^5 \) with the density matrix

\[
[^5\rho_{Gibbs}] = \frac{e^{-\beta''h}}{\text{Tr}[e^{-\beta''h}]},
\]

where \( \beta'' \) is determined by the condition

\[
\langle h \rangle_{Gibbs}^5 = \langle h \rangle_{Gibbs}^4.
\]

Then exactly the same argument as before shows

\[
S_h[^5\rho_{Gibbs}] - S_h'[^3\rho_{Gibbs}] \geq 0.
\]

From (4.14) and (1.18), we finally get

\[
S_h[^5\rho_{Gibbs}] - S_h[^1\rho_{Gibbs}] \geq 0,
\]

where the equality holds only when the condition (2.14) is satisfied. Since \( \langle \cdot \cdot \cdot \rangle_{Gibbs}^1 \) and \( \langle \cdot \cdot \cdot \rangle_{Gibbs}^5 \) are the Gibbs states for the same Hamiltonian \( h \) with the inverse temperatures \( \beta \) and \( \beta'' \), respectively, (4.19) implies that

\[
\beta'' \leq \beta,
\]

and hence

\[
\langle h \rangle_4 \geq \langle h \rangle_5 \geq \langle h \rangle_1.
\]

\[\text{Proof:}\] Since \( \log x \leq x - 1 \), one finds (L.H.S.) \( \geq -k \sum_{i=1}^{n} p_i \{ (p'_i/p_i) - 1 \} = k \sum_{i=1}^{n} \{ p_i - p'_i \} = 0 \). To show that the equality holds only when \( p_i = p'_i \) for all \( i \), it suffices to note that \( \log x < x - 1 \) whenever \( x \neq 1 \).
Again the equality holds only when the condition (2.14) is satisfied\(^ {10} \). This proves the desired theorem since, for the present choice of unitary operator \(U\), the quantity \(\langle h\rangle_4 - \langle h\rangle_1^{\text{Gibbs}}\) clearly depends only on \(\beta, \varepsilon_1, \ldots, \varepsilon_n\), and \(\varepsilon'_1, \ldots, \varepsilon'_n\), and has been shown to be strictly positive unless (2.14) holds\(^ {11} \).

4.2 Explicit lower bound of the work

We stress that the argument of Sato, Sekimoto, Hondou, and Takagi presented in the previous subsection indeed proves the strict inequality

\[
\langle h\rangle_4 - \langle h\rangle_1^{\text{Gibbs}} > 0, \tag{4.22}
\]

for any \(h\) and \(h'\) which do not satisfy the condition (2.14). But it might be desirable to have an explicit positive lower bound for the required work \(\langle h\rangle_4 - \langle h\rangle_1^{\text{Gibbs}}\). Let us construct a simple lower bound here.

We start from the representation (4.13) of the entropy difference, and rewrite it as

\[
S_{h'}[\rho_3^{\text{Gibbs}}] - S_h[\rho_1^{\text{Gibbs}}] = -k \sum_{i=1}^{n} p_i \log \frac{p'_i}{p_i} = k \sum_{i=1}^{n} p_i \left\{ \left( 1 - \frac{p'_i}{p_i} \right) + \frac{p'_i}{p_i} - 1 - \log \frac{p'_i}{p_i} \right\} = k \sum_{i=1}^{n} p_i g\left( \frac{p'_i}{p_i} \right), \tag{4.23}
\]

where

\[
g(x) = x - 1 - \log x. \tag{4.24}
\]

Note that \(g(x) \geq 0\) for any \(x > 0\) and \(g(x) > 0\) if \(x \neq 1\).

Let us first treat the simplest nontrivial case with \(n = 3\), i.e., a three level system. Let

\[
d_1 = \varepsilon_3 - \varepsilon_1, \quad d_2 = \varepsilon_3 - \varepsilon_2, \quad d'_1 = \varepsilon'_3 - \varepsilon'_1, \quad d'_2 = \varepsilon'_3 - \varepsilon'_2. \tag{4.25}
\]

Then for \(p_i\) and \(p'_i\) as in (4.5) and (4.10), we have

\[
\frac{p_3 p'_1}{p'_3 p_1} = \exp[-\beta d_1 + \beta' d'_1], \quad \frac{p_3 p'_2}{p'_3 p_2} = \exp[-\beta d_2 + \beta' d'_2]. \tag{4.26}
\]

It can be shown easily that the equality indeed holds when we have the condition (2.14) and the time evolution is described by the special \(U\) and \(U^{-1}\) defined by (4.1). For a general time evolution, the equality may be violated for any Hamiltonians, but this is of course the usual irreversibility.

\(^{11}\) We note that the above proof can be directly applied to classical systems. To do this, we fix a constant \(\delta > 0\), and (as in \([3]\)) decompose the whole phase space into slices with the same volume \(\delta\). The slices are determined so that the points in the \(i\)-th slice have initial energies between \(\varepsilon_i\) and \(\varepsilon_{i+1}\). We prepare similar decomposition for the final energy as well. Then we let \(p_i\) be the probability that the initial state is found in the \(i\)-th slice. If we perform the operation slowly, one finds that, in the final state, the probability that the state is in the \(i\)-slice (in the decomposition according to the final energy) is still given by \(p_i\). (We only use the adiabatic theorem.) Then we can simply repeat the above proof. By taking the limit \(\delta \to 0\) finally, the desired proof for classical systems follow.
Introducing vectors $\mathbf{d} = (d_1, d_2)$ and $\mathbf{d}' = (d'_1, d'_2)$, we observe that
\[
\min_{\beta'} |\beta \mathbf{d} - \beta' \mathbf{d}'| = \beta D(\mathbf{d}, \mathbf{d}'),
\tag{4.27}
\]
where
\[
D(\mathbf{d}, \mathbf{d}') = |\mathbf{d}| \sqrt{1 - \frac{(\mathbf{d} \cdot \mathbf{d}')^2}{|\mathbf{d}|^2 |\mathbf{d}'|^2}}.
\tag{4.28}
\]
Note that $D(\mathbf{d}, \mathbf{d}')$ is vanishing if $\mathbf{d}$ and $\mathbf{d}'$ are proportional, and is strictly positive otherwise. From (4.27) we see that
\[
|\beta d_i - \beta' d'_i| \geq \frac{\beta D(\mathbf{d}, \mathbf{d}')}{\sqrt{2}}
\tag{4.29}
\]
for at least one of $i = 1$ or 2. From this bound we can show that, at least for one of $i = 1, 2, 3$, we have
\[
\left| \log \frac{p'_i}{p_i} \right| \geq \frac{\beta}{2\sqrt{2}} D(\mathbf{d}, \mathbf{d}').
\tag{4.30}
\]
To see this, suppose the contrary, i.e., $|\log(p'_i/p_i)| < \beta D(\mathbf{d}, \mathbf{d}')/(2\sqrt{2})$ for all $i$. Then for $i$ in (4.29)
\[
\left| \log \frac{p'_i}{p_i} \right| = \left| \log \frac{p_3 p'_i}{p_3 p_i} + \log \frac{p'_3}{p_3} \right|
= \left| -\beta d_i + \beta' d'_i + \log \frac{p'_3}{p_3} \right|
\geq |\beta d_i - \beta' d'_i| - \left| \log \frac{p'_3}{p_3} \right|
\geq \frac{\beta}{2\sqrt{2}} D(\mathbf{d}, \mathbf{d}'),
\tag{4.31}
\]
which is a contradiction. We have here used (4.26), (4.29), the triangular inequality, as well as the assumption (4.30).

Let $i$ be such that (4.30) is valid. Since $g(x)$ is increasing in $x$ for $x > 1$ and decreasing in $x$ for $x < 1$, we find that $g(p'_i/p_i)$ is bounded from below by the smaller of $g(\exp[\beta D(\mathbf{d}, \mathbf{d}')/(2\sqrt{2})])$ and $g(\exp[-\beta D(\mathbf{d}, \mathbf{d}')/(2\sqrt{2})])$. Since the latter is smaller, we have
\[
g\left(\frac{p'_i}{p_i}\right) \geq \frac{\beta}{2\sqrt{2}} D(\mathbf{d}, \mathbf{d}') + \exp \left[ -\frac{\beta}{2\sqrt{2}} D(\mathbf{d}, \mathbf{d}') \right] - 1 > 0.
\tag{4.32}
\]
By using the representation (4.23), we can bound the total entropy difference as
\[
S_{\rho'_3[Gibbs]} - S_{\rho'_1[Gibbs]} \geq k p_i g\left(\frac{p'_i}{p_i}\right) \geq k p_3 g\left(\frac{p'_3}{p_3}\right).
\tag{4.33}
\]
By combining this with (4.18) and using (4.32), we get an explicit bound for the entropy increase\(^{12}\)

\[
S_h[\rho_5^{\text{Gibbs}}] - S_h[\rho_1^{\text{Gibbs}}] \geq \frac{k e^{-\beta \varepsilon_3}}{z(\beta)} \left\{ \frac{\beta}{2 \sqrt{2}} D(d, d') + \exp \left[ -\frac{\beta}{2 \sqrt{2}} D(d, d') \right] - 1 \right\} > 0. \tag{4.34}
\]

We can use the same estimate to treat models with general \(n\). Let \(M\) be the smallest integer which does not exceed \(n/3\). For each \(m = 1, \ldots, M\), we choose three integers \(1 \leq \ell_1(m) < \ell_2(m) < \ell_3(m) \leq n\), in such a way that each \(i = 1, \ldots, n\) is chosen at most once\(^{13}\).

Then by using the previous estimate for the levels \(\varepsilon_i, \varepsilon'_i\) with \(i = \ell_1(m), \ell_2(m), \ell_3(m)\), we get

\[
S_h[\rho_5^{\text{Gibbs}}] - S_h[\rho_1^{\text{Gibbs}}] \geq \sum_{m=1}^{M} \frac{k e^{-\beta \varepsilon_{\ell_3(m)}}}{z(\beta)} \left\{ \frac{\beta}{2 \sqrt{2}} D(d_m, d'_m) + \exp \left[ -\frac{\beta}{2 \sqrt{2}} D(d_m, d'_m) \right] - 1 \right\} > 0,
\tag{4.35}
\]

where

\[
d_m = (\varepsilon_{\ell_3(m)} - \varepsilon_{\ell_1(m)}, \varepsilon_{\ell_3(m)} - \varepsilon_{\ell_2(m)}), \tag{4.36}
\]

and

\[
d'_m = (\varepsilon'_{\ell_3(m)} - \varepsilon'_{\ell_1(m)}, \varepsilon'_{\ell_3(m)} - \varepsilon'_{\ell_2(m)}). \tag{4.37}
\]

It is clear that whenever the energy levels \(\varepsilon_i, \varepsilon'_i\) do not satisfy the condition (2.14), one can choose \(\ell_i(m)\) in such a way that \(D(d_m, d'_m) > 0\) for at least one \(m\).

Finally, we note that the entropy and the energy in the Gibbs state for the Hamiltonian \(h\) at a general inverse temperature \(\tilde{\beta}\) satisfies the wellknown relation

\[
\frac{\partial}{\partial \beta} S_h[\rho_{\tilde{\beta}, h}^{\text{Gibbs}}] = k \tilde{\beta} \frac{\partial}{\partial \beta} \langle h \rangle_{\tilde{\beta}, h}^{\text{Gibbs}}.
\tag{4.38}
\]

Dividing this relation by \(-k \tilde{\beta}\), and integrating it from \(\beta''\) to \(\beta\), one finds that

\[
\langle h \rangle_{5}^{\text{Gibbs}} - \langle h \rangle_{1}^{\text{Gibbs}} = \int_{\beta''}^{\beta} d\tilde{\beta} \frac{1}{k \tilde{\beta}} \left\{ -\frac{\partial}{\partial \beta} S_h[\rho_{\tilde{\beta}, h}^{\text{Gibbs}}] \right\} \geq \frac{1}{k \beta} \int_{\beta''}^{\beta} d\beta \left\{ -\frac{\partial}{\partial \beta} S_h[\rho_{\beta, h}^{\text{Gibbs}}] \right\} = \frac{1}{k \beta} \{ S_h[\rho_5^{\text{Gibbs}}] - S_h[\rho_1^{\text{Gibbs}}] \}. \tag{4.39}
\]

\(^{12}\) Although we can construct a lower bound for \(S_h[\rho_5^{\text{Gibbs}}] - S_h[\rho_1^{\text{Gibbs}}]\) in the same manner, it will depend on \(\beta''\) and won’t be an explicit bound as it is. Therefore we simply use the weak inequality (4.18) for the second operation.

\(^{13}\) If one prefers a bound which include only simple functions, one may use

\[
S_h[\rho_5^{\text{Gibbs}}] - S_h[\rho_1^{\text{Gibbs}}] \geq \frac{k e^{-\beta \varepsilon_3}}{z(\beta)} \times \begin{cases} \frac{\beta^2}{2} (D(d, d'))^2 & \text{if } \beta D(d, d')/(2 \sqrt{2}) \leq (4/3) \\ \frac{\beta}{2 \sqrt{2}} D(d, d') - 1 & \text{if } \beta D(d, d')/(2 \sqrt{2}) \geq (4/3), \end{cases}
\]

which is obtained from (4.34) through elementary estimate.

\(^{14}\) A simple choice is \(\ell_i(m) = 3(m - 1) + i\).
By substituting (4.35) and recalling (4.17), we get our final estimate for the irreversible work

\[ \langle h \rangle_4 - \langle h \rangle_1^\text{Gibbs} \geq M \sum_{m=1}^M \frac{e^{-\beta \epsilon_{\ell_2(m)}}}{\beta z(\beta)} \left\{ \frac{\beta}{2\sqrt{2}} D(d_m, d'_m) + \exp \left[ -\frac{\beta}{2\sqrt{2}} D(d_m, d'_m) \right] - 1 \right\}. \quad (4.40) \]

We stress that the bound (4.40) is far from optimal. In the crucial estimate (4.27), for example, we are simply looking for \( \beta' \) which minimizes the distance between \( \beta d \) and \( \beta' d' \). But the true \( \beta' \) is determined from the condition (4.11) about the balance of energy, which condition is not taken into account in our bound.

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