Thermodynamics of quantum informational systems - Hamiltonian description

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It is often claimed, that from a quantum system of \(d\) levels, and entropy \(S\) and heat bath at temperature \(T\) one can draw \(kT(\ln d - S)\) amount of work. However, the usual arguments basing on Szilard engine, are not fully rigorous. Here we prove the formula within Hamiltonian description of drawing work from a quantum system and a heat bath, at the cost of entropy of the system. We base on the derivation of thermodynamical laws and quantities in [R. Alicki, J. Phys. A, 12, L103 (1979)] within weak coupling limit. Our result provides fully physical scenario for extracting thermodynamical work form quantum correlations [Oppenheim et al. Phys. Rev. Lett. 89, 180402 (2002)]. We also derive Landauer principle as a consequence of second law within the considered model.

I. INTRODUCTION

It is well known that thermodynamical work can be drawn at the expense of entropy. An obvious example is a container with ideal gas placed within thermal reservoir at temperature \(T\). Since the energy of ideal gas does not depend on volume, by expanding gas we draw work from reservoir solely at the expense of entropy. The drawn work is equal to \(T \Delta S\). A more sophisticated example is Maxwell demon in Szilard engine \[1\]. The engine consists of a box with one particle of gas. The demon measures where the particle is, puts the piston and by expansion draws \(kT \ln 2\) of work. The price is that entropy of demon increases by 1 bit, as was pointed out by Bennett \[2\] based on Landauer work \[3\]. The demon serves as entropy sink, which is needed to divide heat from the heat bath into entropy and work. Unlike the gas in container we deal here with microscopic objects: we have one molecule, and the demon is thought to be a small, microscopic being. Moreover, demon is not assumed to be necessarily in equilibrium state, so that thermodynamical quantities are not applicable. This gives rise to the following general view: if one has an \(d\)-level quantum system in a pure state \(\psi\) one can draw \(kT \ln d\) work out of heat bath of temperature \(T\). If a state of the system is a mixed state \(\rho\), then the amount of work would correspond to

\[ W = kT(\ln d - S(\rho)) \]  

(1)

where \(S\) is von Neumann entropy. The latter function can be viewed as information contents of a state.

Recently, the idea that one can draw work from heat bath and a system with non-maximal entropy was used to investigate quantum properties of compound systems \[4\]. The equivalence between work and information (see \[5\]) was used in definition of the so called work deficit, which was a difference between the work drawn when there is global access to the bipartite system, and when only local operations and classical communication is allowed \[6\]. As a result, a new paradigm of investigation of correlations of quantum compound system was obtained, in which quantum correlations manifest themselves through a loss of information during its concentration to local subsystems for the purpose of drawing work from local heat baths. The paradigm, though based on thermodynamical ideas, can be formulated solely by means of basic logical structure of thermodynamics, without the need of referring to the process of drawing work \[7\]. Yet, the connection with physical quantities such as energy, work and heat makes it even more interesting, especially in the context of more and more realistic proposals to implement thermodynamical quantum microengines \[8, 9, 10, 11\].

However, so far in the literature there is no rigorous Hamiltonian description of a process of drawing work from heat bath and additional quantum system, to show that we can change information into work according to formula \(1\). In this paper we provide such a description basing on derivation of phenomenological thermodynamical laws from theory of quantum open system \[12, 13\]. We will then provide a physical description of protocols considered in \[4\] for drawing work from local heat baths and compound systems by LOCC. We assume that the quantum system is coupled weakly to the bath. The assumption is needed to give rise to thermodynamical regime. If the system is instead strongly coupled to the reservoir (see e.g. \[14\]), our results do not apply, then however it is hard even to define work and heat, due to large fluctuations of energy of the system caused by interaction. In the paper we also show how Landauer principle follows from second law derived within the model we discuss (c.f. \[15\]).

II. PROTOCOL OF CONCENTRATION OF INFORMATION TO LOCAL FORM

In this section we will describe the idea of \[4\] which motivates the present work. There are two parties, that are situated in distant labs. In each lab there is heat bath with temperature \(T\). The parties Alice and Bob, possess subsystems \(A\) and \(B\) of a quantum system being in some state \(\rho_{AB}\). They can send particles to each other via fully decohering channel, i.e. the channel that removes off-diagonal terms of a density matrix of the sent system in a fixed basis. Locally, their actions are not con-
III. DRAWING WORK FROM HEAT BATH AND QUANTUM SYSTEM

A. Quantum system as a model of heat engine

In this section we recall the microscopic model for heat engine of 12 13. In particular, we will present thermodynamical quantities and laws within dynamical model, where the working body is quantum system, that is driven by external force, and can be coupled to reservoirs. The laws are not postulated, but derived. It should be noted here, that the second law derived for quantum reservoir, but without a system as working body was derived in $C^*$-algebraic context by Pusz and Woronowicz 10.

a. Quantum system and reservoirs. Consider a quantum system $S$ thermal reservoir $R_T$, and decohering reservoir $R_d$. The state of the system is denoted by $\rho(t)$. The system is coupled to thermal bath via coupling constant $\lambda$ and to the decohering reservoir via constant $\nu$. The constants are external parameters, that can be changed, so that the system can be coupled to reservoirs at our will. The self Hamiltonian of the system can be changed in time by external force. The whole setup is illustrated on figure 2.

$$H_{S+R_T+R_d} = H_S(t) + \lambda(t)H_{SR_T} + \nu(t)H_{SR_d}$$

(2) We can single out three time scales: (1) $\tau_H$ - characteristic scale of change of Hamiltonian $H_S$ and of coupling constants (2) $\tau_S \approx \lambda^2, \nu^2$ - relaxation time of the system and (3) $\tau_{R_d}, \tau_{R_T}$ - relaxation times of reservoirs (for our purpose, both times, as well as both coupling constants can be of the same order of magnitude). Assuming that $\tau_H, \tau_S \gg \tau_R$, the evolution of the system can be approximated by Markovian master equation 13 14 15 16.

$$\frac{d\rho}{dt} = i^{-1}[H(t), \rho] + \lambda^2(t)L(t)\rho + \nu^2(t)K(t)\rho$$

(3) where $L$ describes interaction with thermal reservoir while $K$ describes interaction with decoherence reservoir. The generators $L, K$ include the shifts of Hamiltonians. They depend on time through change of coupling constants, that can switch them on and off and also through the change of Hamiltonian. Both generators $L$ and $K$ depend functionally on Hamiltonian: $L$ it causes relaxation of the system to the Gibbs state $\rho(t) = Z^{-1}e^{-\beta H(t)}$ while the generator $K$ dephases state in basis of the self Hamiltonian $H(t)$. Thus the interaction with thermal reservoir can change energy of the system while the decohering reservoir does not change the energy, only destroys coherences between the eigenstates of self-Hamiltonian. Once the Hamiltonian is switched off, $K$ decoheres in some basis determined by interaction Hamiltonian.

Usually, it is not the case that there are two separate reservoirs. A typical reservoir which can be described by Markovian master equation is rare gas, and it causes both effects: The suitable generator can be divided into two parts, decohering one $K$ and $L$ inducing transitions between the levels. When the Hamiltonian is switched on, both parts are present, while for degenerated levels,
only the decohering part is present. In such case, one can control couplings as follows: in order to switch off the \( L \) part, one has to switch off the Hamiltonian. To effectively switch off both parts, one should simply use much faster changes of Hamiltonian than the time of decay induced by reservoir. It is not possible to have \( L \) but not \( K \), however it is not important in the present context.

b. Thermodynamical quantities and laws. Now one can define the thermodynamical quantities as follows. The thermodynamical energy of the system is identified with average energy of the system

\[ E(t) = \text{Tr} \rho(t) H(t) \quad (4) \]

Heat and work are defined as follows

\[ Q(t) = \int_0^t \text{Tr} \left[ \frac{d\rho(t)}{dt} H(t) \right] dt \quad (5) \]

\[ W(t) = \int_0^t \text{Tr} \left[ \rho(t) \frac{dH(t)}{dt} \right] dt. \]

They obviously satisfy the first law of thermodynamics

\[ dE = dW + dQ \quad (6) \]

It is convenient to require that the energy of the system does not change in time and thus can be set to be zero

\[ \text{Tr} \rho(t) H(t) = 0, \quad (7) \]

so that \( dW = -dQ \) in our case. The entropy is given by

\[ S(\rho) = -k \text{Tr} \rho \ln \rho \quad (8) \]

The variation of entropy can be divided into the part due to heat exchange, and the rest, called entropy production.

\[ \frac{dS}{dt} = \frac{1}{kT} \frac{dQ}{dt} + \sigma(t) \quad (9) \]

The first part can be negative or positive, while the second one, defined by the equation, is always nonnegative

\[ \sigma(t) \geq 0 \quad (10) \]

as follows from monotonicity of relative entropy under physical processes \([12, 21]\). This is actually a statement of the Second Law. From the above formulas one gets formula for work in any process

\[ W = kT [(S(t_2) - S(t_1)) - \int_{t_1}^{t_2} \sigma(t) dt]. \quad (11) \]

B. Elementary processes

To show that from pure qubit one can draw work equal to \( kT \ln 2 \), we have to show process that will change entropy from zero to maximal equal to \( \ln 2 \) with zero entropy production. To this end we will examine elementary processes which can be run.

Adiabatic change of Hamiltonian. In this process, the system is not coupled to the thermal bath, so that \( \lambda(t) = 0 \). Also it is not coupled to the decohering bath i.e. \( \nu(t) = 0 \). Since the operation is unitary, the entropy production \( \sigma(t) \) is zero. As mentioned, we allow only such changes that keep the energy to be zero. Thus, if the system initially had two degenerated levels, and it is in the state with populations \( p_1 \) and \( p_2 \) then we change Hamiltonian in such a way, that one of the level gets energy \( +E/2p_1 \) while the other \( -E/2p_2 \), so that the change produces energy difference \( E \), but the total energy is still zero. The Hamiltonian commutes with \( \rho \) all the time: \([H(t), \rho] = 0\). The process is shown on figure 3.

Isothermal and quasistatic contact with thermal bath. During the process, the state of the system is in equilibrium with thermal bath

\[ \rho(t) = Z^{-1} e^{-\frac{H(t)}{kT}} \quad (12) \]

In this process the system is coupled to the reservoir, so that \( \lambda(t) \neq 0 \). Still \( \nu = 0 \), as we do not couple the system to decohering reservoir. The process is quasistatic, which means that the time \( \tau_H \) is much longer than the time of system relaxation \( \tau_S \). This means that the changes of Hamiltonian are so slow, that the system is all the time approximately in equilibrium state. Therefore The entropy production is all the time zero while entropy production can be only due to either decohering reservoir or nonequilibrium processes. The process is illustrated on figure 4.
FIG. 5: Unitary c-not gate. When the qubit X is in ground state Y is unchanged, otherwise Y is flipped.

equal to 0:

\[ H(t_1) = H(t_2) = 0 \]  
(13)

Thus, the Hamiltonian is switched on to run required unitary operation, and then switched off. Thus the unitary gate is actually composed of two adiabatic changes of Hamiltonian. As it should be, the work performed during unitary gate is zero, as it is equal to heat exchange, so that

\[ W = \int_{t_1}^{t_2} \text{Tr} \left\{ \frac{\text{d}\rho(t)}{\text{d}t} H(t) \right\} \text{dt} = 0 \]  
(14)

The most common example of two-qubit unitary gate is c-not gate, which is defined by

\[ U_{XY} |0\rangle_X |0\rangle_Y = |0\rangle_X |0\rangle_Y \]  
(15)

\[ U_{XY} |0\rangle_X |1\rangle_Y = |0\rangle_X |1\rangle_Y \]  
(16)

\[ U_{XY} |1\rangle_X |0\rangle_Y = |1\rangle_X |1\rangle_Y \]  
(17)

The transformation if applied to standard basis does not change first qubit X. Second qubit Y is also untouched once the first qubit is in state |0\rangle and is flipped if the first qubit is in state |1\rangle (see Figure 5). The qubit X is called source, while the qubit Y - target. The gate can be realized by applying the following Hamiltonian

\[ H(t) = E(t) |1\rangle_X \langle 1| \otimes |-\rangle_Y \langle -|, \]  
(18)

with \( \int E(t) \text{dt} = \pi, |-\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \).

Irreversible pure decoherence. The system is coupled to the decohering reservoir only, so that \( \lambda = 0 \) but \( \nu \neq 0 \). The Hamiltonian is off i.e. \( H(t) = 0 \). Under such process, the off diagonal terms in a fixed basis disappear. Of course, to draw optimal work one will not use this process. It is useful to model communication via dephasing channel: Instead of sending qubit via the channel, Alice can first decohere it locally, and then send such decohered intact to Bob.

C. Drawing work by use of quantum system

Consider the following initial conditions: Hamiltonian is equal to zero, and the state is pure. As we know, to draw work without entropy production, one should apply isothermal process, which requires the system to be in equilibrium state. However the state is pure, and Gibbs state is always mixed. Nevertheless one can obtain almost Gibbs state. To this end one performs adiabatic switching on the Hamiltonian in such a way, that the state is ground state of the Hamiltonian and the obtained energy splitting must be much higher than \( kT \).

Then to a good approximation, the pure state is equal to Gibbs state. Subsequently, one switch on isothermal contact with reservoir, with the Hamiltonian adiabatically changed to zero. Therefore, since all the time state is in equilibrium, the final state is equally populated. The obtained work is then equal to \( kT \ln 2 \) (the initial entropy was 0, while the final one is \( ln 2 \)). The process is illustrated on Figure 6. If the initial qubit is not in pure state but in some mixed state \( \rho \) the amount of work is given by its information (or negentropy) contents

\[ W = T(S_{\text{max}} - S(\rho)) = kT \ln 2 - TS(\rho). \]  
(19)

FIG. 6: Drawing work by use of a pure qubit. Dotted line denotes energy 0 level. The initial state is pure, occupying ground level, while the final state has both levels equally populated.

IV. Deriving Landauer Principle

From the formula for work (11) implied directly by the second law (10), we can derive Landauer principle. Recall, that the latter says that erasure one bit of information in contact with heat reservoir with temperature \( T \) costs dissipation of \( kT \ln \text{of energy} \). The information is here considered in Shannon subjective sense, where information produced by a source is measured by the entropy of ensemble emitted by the source. Thus 1 bit of information is represented by a 1-bit register in maximally mixed state. Quantum mechanically, it is one qubit in maximally mixed state. The "erasure of the bit" means transformation of the state into some standard pure state |0\rangle. Such state represents zero information in Shannon sense, because it is apriori known. In terms of objective information understood as purity or negentropy, we
have the converse interpretation: the initial state, maximally mixed, hence with zero information contents, become transformed into pure state, containing 1 bit of information. Then we could say: creation of information costs dissipation of $kT \ln 2$ of energy. (of course the information of the total system: qubit plus reservoir is conserved, as the entropy of the reservoir increased).

Let us now prove the Landauer principle within Hamiltonian model. Assume that one has a maximally mixed qubit. Denote by $W_{eq}$ the work that needs to be dissipated into reservoir, while bringing the system to the pure state $|0\rangle$. If less than $kT \ln 2$ work would be dissipated, then we could draw work from system in maximally mixed state and heat bath, what is forbidden by formula (11). Indeed, one could start with maximally mixed state and heat bath, what is forbidden by (c.f. [4]). We assume that the levels are degenerated unless driven by external force being magnetic field. The state has maximally mixed subsystems, so that Alice and Bob cannot draw any work locally. Thus in first stage, Alice and Bob will aim to concentrate information to local subsystems. To this end, they take a third two-level quantum system $C$ which will be used for communication. The particle is prepared in pure state $|0\rangle$ and after the whole protocol it must be return in such state (thus it serves for a working body, for which the cycle has to be closed). Before and after the process, the system $C$ is in equilibrium with the bath, and its pure state is maintained by using potential with gap between ground and first excited state much greater than $kT$ as explained in sec. III C.

To start the process of localisation of information, Alice and Bob will switch off the potential, and the process the system $C$ is not coupled to the thermal reservoir. After the process, the qubit $C$ can be again put into high potential well, and put in contact with reservoir.

The process of localisation of information of the state (10) is the following.

1. The particle $C$ is coupled to the particle $A$ via Hamiltonian of equation (17) with source system $X = A$ and target $Y = C$. This realizes c-not gate between $A$ and $C$ which results in transition

$$|0\rangle_C \frac{1}{\sqrt{2}}(|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B) \rightarrow \quad (20)$$

The qubit $C$ (target) has measured the qubit $A$ (source).

2. In LOCC paradigm, $C$ is classical bit, therefore Alice will switch on the decohering reservoir for the qubit $C$. The state turns then into probabilistic mixture:

$$\frac{1}{\sqrt{2}} (|0\rangle_C |0\rangle_A |0\rangle_B + |1\rangle_C |1\rangle_A |1\rangle_B) \rightarrow \quad (21)$$

$$\rightarrow \frac{1}{2} |0\rangle_C |0\rangle_A |0\rangle_B |0\rangle +$$

$$+ \frac{1}{2} |1\rangle_C (|1\rangle_A \otimes |1\rangle_B)$$

3. The qubit $C$ is communicated to Bob. The state is now

$$\frac{1}{2} |0\rangle_A |0\rangle_B |0\rangle_A |0\rangle + \quad (22)$$

$$+ \frac{1}{2} |1\rangle_A (|1\rangle_B \otimes |1\rangle_B)$$

4. Bob applies Hamiltonian of (refeq:hamil-cnot) with $C$ being source and $B$ - target system. As a result the qubit $B$ uncouples from two other ones, and the total state is

$$\frac{1}{2} (|0\rangle_A |0\rangle_B |c\rangle + |1\rangle_A (|1\rangle_B \otimes |1\rangle_C |1\rangle) \otimes (23)$$

$\otimes |0\rangle_B |0\rangle$
The qubit $C$ is sent back to Alice. Alice applies the same Hamiltonian as at the beginning ($H_{XY}$ of eq. (17) with $X = A$, $Y = C$) to finish cycle by resetting the qubit $C$ to the standard state $|0\rangle$. The final state is:

$$|0\rangle_C |0\rangle \otimes \frac{1}{2} (|0\rangle_A \langle 0| + |1\rangle_A \langle 1|) \otimes |0\rangle_B \langle 0|$$

(24)

This was the stage of localization of information. During the process, the entropy increased by one bit. The Bob’s qubit is now pure, and $kT \ln 2$ work can be drawn from it by adiabatic quasistatic coupling to thermal reservoir. In this process next bit of entropy is produced. The initial pure state $\psi_{AB}$ becomes maximally mixed.

VI. CONCLUSIONS

In conclusion, we have presented a Hamiltonian model of drawing work from single heat bath and a quantum system. In the model the system is weakly coupled to the heat bath. In the process whole heat is changed into work; the second law is saved, because the quantum system increases its entropy. The overall process can be viewed as depleting entropy from the noisy energy contained in Gibbs state. The latter state contain both entropy. In the process of drawing work the entropy goes to qubit, while the energy is obtained in ordered form (it can be stored as potential energy.

We have pointed out how Landauer principle follows from the second law derived within the model: were it possible to erase qubit at lower cost than $kT \ln 2$, one could draw more work from pure qubit, which would violate second law.

Finally we have represented in Hamiltonian picture the process of drawing work from compound systems and local heat baths by local operations and classical communication of [4]. Such process consists of two stages: localisation of information (which is usually irreversible) and then drawing work locally. We have carried out energy balance of such process, and obtained that the process of localisation of information no energy needs to be spent. In the second stage, by use of our model, one can draw the amount of work determined by local information contents. Thus the localisable information of [4, 7] can be interpreted as the maximal amount of work drawn by use of quantum system distributed into distant labs and local heat baths operated by local operations and classical communication.

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