Heat-to-work conversion by exploiting full or partial correlations of quantum particles

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It is shown how information contained in the pairwise correlations (in general, partial) between atoms of a gas can be used to completely convert heat taken from a thermostat into mechanical work in a process of relaxation of the system to its thermal equilibrium state. Both classical correlations and quantum correlations (entanglement) are considered. The amount of heat converted into work is proportional to the entropy defect of the initial state of the system. For fully correlated particles, in the case of entanglement the amount of work obtained per particle is twice as large as in the case of classical correlations. However, in the case of entanglement, the amount of work does not depend on the degree of correlation, in contrast to the case of classical correlations. The results explicitly demonstrate the equivalence relation between information and work for the case of two-particle correlations.

The connection between work and information was first pointed out by Szilard\cite{szilard1929} in his analysis of Maxwell’s demon, and later by Landauer\cite{landauer1961} and Bennett\cite{bennett1982}. Using the setup of a “thought experiment” related to Gibbs’s paradox, it was shown\cite{levitin1966,levitin1968,levitin1969} that using a system of two gases of $N$ molecules each, with the molecules being in different (in general, nonorthogonal) quantum states $\rho^{(1)}$ and $\rho^{(2)}$, it is possible to convert completely into mechanical work an amount of heat, taken from a thermostat, which is proportional to the entropy defect\cite{levitin1970} of the system

$$W = 2NkT I_0,$$

where $W$ is work, $T$ the temperature of the thermostat, and $I_0$ the entropy defect (also called “quantum information” or “Levitin–Holevo bound”\cite{levitin1973,levitin1974}) of the system per molecule, which, in this particular case, is

$$I_0 = - \text{Tr} \rho \ln \rho + \frac{1}{2} \sum_{i=1}^{2} \text{Tr} \rho^{(i)} \ln \rho^{(i)}, \quad \rho = \frac{1}{2}(\rho^{(1)} + \rho^{(2)}).$$

Entropy defect has the meaning of information (about the microstate of the system) associated with the selection of a subensemble (in this example, $\rho^{(1)}$ or $\rho^{(2)}$) from the total ensemble $\rho$.

It was conjectured\cite{levitin1966,levitin1968,levitin1969} that there exists a general equivalence relation between information and work; namely, that by having any information $J$ about the state of a physical system, it is possible, by allowing the system to relax to its maximum-entropy state, to convert into mechanical work an amount of heat $W = kTJ$ without any entropy increase in the environment. (Of course, all information $J$ is lost in the process, since the system reaches the thermal equilibrium state that has the same energy and volume as the initial state.)

Since then, a number of papers (in particular,\cite{lloyd1993,lloyd1995,lloyd1996,lloyd1997,levitin1998,levitin1999,levitin2000,levitin2001,levitin2002}) has been devoted to various aspects of the connection between information and work. However, the general equivalence relation remains up to now unproven. (Part of the problem, in our opinion, is the still existing fuzziness of distinction between “mechanical work” and “heat.”) Moreover, all real-life examples of getting work from a non-equilibrium system (e.g., chemical reactions, separated electrical charges, compressed gas) by allowing it to relax to equilibrium are based on the information contained in one-particle distributions—as if all the particles comprising the system were independent. To the best of our knowledge, information stored in multi-particle distributions has never been used to extract mechanical work.

Here we address the problem of using information contained in two-particle correlations for converting heat into work. Our analysis is based on two important assumptions:

1. Since a unitary transformation of the system’s state does not change its entropy, it can be performed without any energy dissipation; and

2. Since orthogonal quantum states are perfectly distinguishable, there exist partitions which are permeable for one of such states but not for the other (a well-known example of such “partitions” is a light polarizer).

In order to avoid getting involved in definitional arguments—such as appear sometimes in the physics literature—concerning the distinction between work and heat, we shall consider an isothermal quasistatic process in which heat is taken from a thermostat and eventually transferred to another system in a form that is unequivocally mechanical work—namely, the lifting of a weight.

We shall treat in separate sections the case when the two particles are classically correlated and that dealing with quantum correlations, and conclude with a discussion of the overall results.

1 The case of classical correlations

Consider a gas of molecules that consist of two different atoms, $A$ and $B$. To each atom is associated a 2-dimensional Hilbert space of states with basis vectors $|0\rangle$ and $|1\rangle$ (a qubit\cite{nielsen2000}). The thermal equilibrium (maximum-entropy) state of a gas molecule is described by a density matrix

$$\rho = \frac{1}{2}(\rho_1 + \rho_2), \quad \text{with} \quad \rho_1 = \frac{1}{2}(|00\rangle \langle 00| + |11\rangle \langle 11|), \quad \rho_2 = \frac{1}{2}(|01\rangle \langle 01| + |10\rangle \langle 10|).$$
States $\rho_1$ and $\rho_2$ are orthogonal, and correspond to (classically) maximally correlated atoms $A$ and $B$. Each of these states has an entropy defect (in nats) $I_c = \ln 2$ per pair, or $J_c = N \ln 2$ for a gas of $N$ molecules. Note that the one-particle probabilities of states $|0\rangle$ and $|1\rangle$ of both atoms are the same in states $\rho_1$ and $\rho_2$ as at equilibrium. Therefore, it is impossible to distinguish between this state and the equilibrium state on the basis of one-particle measurements.

Without loss of generality, assume we know that the gas is in state $\rho_1$ (let us call it gas 1). Let the gas occupy a vessel of volume $2V$ divided by a partition into two equal parts of volume $V$, each occupied by $\frac{N}{2}$ molecules, and being in thermal contact with a thermostat at temperature $T$. To the gas on the right side of the partition apply a unitary transformation $U_1 = I_A \otimes U_B$, where $I_A$ is the identity operator in the Hilbert space of $A$ and $U_B$ the operator that interchanges states $|0\rangle$ and $|1\rangle$ of $B$—that is, the Pauli matrix $\sigma_z$. Transformation $U_1$ converts gas 1 into a gas with density matrix $\rho_2$ (gas 2).

Now, replace the partition by two movable semipermeable partitions such that the partition that faces gas 1 is permeable to gas 1 but not to gas 2, and vice versa for the other partition. Since the total pressure of the mixed gases is larger than the pressure of one of the gases, the two partitions will be pushed apart—and we can use the setup shown in Fig. 1 to lift weights $m_1$ and $m_2$.

![Figure 1: Scheme for obtaining work by mixing gases. The excess pressure of the gases between the semipermeable partitions pushes them apart and lifts weights $m_1$ and $m_2$.](image)

Consider the moment when the right partition has advanced to the right by a volume $V_1$ and the left partition to the left by a volume $V_2$. Gas 1 will then fill the volume $V + V_1$ and gas 2 the volume $V + V_2$. Let us assume that the gases are ideal and rarefied. Then the pressures of the gases to the left, to the right, and in between the partitions are, respectively,

$$P_1 = \frac{(N/2)kT}{V + V_1}, \quad P_2 = \frac{(N/2)kT}{V + V_2},$$

$$P_m = \frac{NkT}{2} \left( \frac{1}{V + V_1} + \frac{1}{V + V_2} \right).$$

The work produced by the gas by lifting masses of appropriate weights in this quasistatic isothermal process is

$$W_c = \int_0^V (P_m - P_2) dV_1 + \int_0^V (P_m - P_1) dV_2 = NkT \ln 2.$$

Note that the total energy of the system has not changed in the process. Thus, the amount of heat converted into mechanical work is proportional to the entropy defect of the system,

$$W_c = NkT I_c = kT J_c.$$

(1)

By the end of the process the entire vessel is occupied by a mixture of gas 1 and gas 2 with density matrix $\rho$. The initial information about the location of each pair of atoms, contained in the correlation of states of the two atoms in a molecule, is now erased, and this increase in entropy exactly compensates for the decrease of entropy of the thermostat.

Consider now the case of partial classical correlations, when each molecule is in a separable state

$$\rho_{1p} = p \langle 00 \rangle \langle 00 \rangle + \frac{1}{2} p \langle 01 \rangle \langle 01 \rangle + \frac{1}{2} (\langle 00 \rangle \langle 11 \rangle + \langle 11 \rangle \langle 00 \rangle),$$

where $\frac{1}{2} < p \leq 1$. (If $p = \frac{1}{2}$, the system is in the maximum-entropy—i.e., equilibrium—state, and no correlation exists.) The complementary state is

$$\rho_{2p} = \frac{1}{2} \rho_{1p} + \frac{1}{2} \rho_{2p},$$

so that the equilibrium state is $\rho = \frac{1}{2} (\rho_{1p} + \rho_{2p})$. Note that the marginal probabilities for each atom to be in state $|0\rangle$ or $|1\rangle$ are equal; thus, the deviation from equilibrium is entirely due to correlations.

The entropy defect (per molecule) of the system is now

$$I_{cp} = - \text{Tr} \rho \ln \rho + \frac{1}{2} \sum_{i=1}^2 \text{Tr} \rho_{ip} \ln \rho_{ip} = \ln 2 - h(p),$$

where $h(p) = -p \ln p - (1-p) \ln (1-p)$ is the binary entropy function.

Suppose the gas is in state $\rho_{1p}$ (gas 1p). Using the same experimental setup as in the case of maximally correlated atoms, we apply the unitary transformation $U_1$ to the gas on the right side of the partition. This transforms gas 1p into gas 2p with density matrix $\rho_{2p}$.

Now let us use exactly the same movable semipermeable partitions as before. Note that the partition that faces gas 1p performs in fact a measurement over the state $\rho_{1p}$, which results either in state $\rho_1$ (with probability $p$) or $\rho_2$ (with probability $1-p$). Similarly, the partition that faces gas 2p produces molecules in state $\rho_2$ (with probability $p$), or in state $\rho_1$ (with probability $1-p$). As a result, the gas between the partitions has the maximum-entropy density matrix $\rho$.

Initially, the total pressure of the mixed gases between the partitions is larger than the pressures of the gases to the left or to the right of both partitions. Hence the partitions are pushed apart as in the previous case, and the gases can produce work by lifting weights (Fig. 2). Note, however, that the compositions of the gases beyond the partitions are changing in the process, owing to the filtering action of the partitions (we denote changing mixtures by gases $1p'$ and $2p'$).

![Figure 2: Scheme for converting heat to work by mixing partially correlated gases.](image)
volume $V_2$. The pressures of the gases to the left, the right, and in between the partitions then become, respectively:

$$P_{1p} = \frac{NkT}{2} \left( \frac{p}{V + V_1} + \frac{1-p}{V - V_2} \right),$$

$$P_{2p} = \frac{NkT}{2} \left( \frac{p}{V + V_2} + \frac{1-p}{V - V_1} \right),$$

$$P_{mp} = \frac{pNkT}{2} \left( \frac{1}{V + V_1} + \frac{1}{V + V_2} \right).$$

The partitions will stop moving when the pressures on the two sides of the partitions become equal, i.e.,

$$P_{1p} = P_{mp} = P_{2p}.$$  

Solving these equations, one obtains

$$V_{1\text{max}} = V_{2\text{max}} = (2p-1)V.$$  

Hence, the total work produced by the gas from the heat taken from the thermostat is

$$W_{\text{cp}} = \int_0^{2p-1V} (P_{mp} - P_{2p})dV_1 + \int_0^{2p-1V} (P_{mp} - P_{1p})dV_2 = NkT(\ln 2 - b(p)) = NkTI_{\text{cp}}.$$  

Note that by the end of the process all three parts of the entire vessel are occupied by gas in the equilibrium state $\rho$. Thus, the initial information (equal to the entropy defect) is expended in the conversion of heat into work.

2 The case of quantum correlations (entanglement)

Consider now the case where atoms forming a molecule are in a maximally entangled state. There are four such states of two qubits, namely, the Bell states $|\Psi^+\rangle, |\Phi^+\rangle, |\Psi^-\rangle,$ and $|\Phi^-\rangle$, defined as follows:

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \quad |\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle).$$

These four states are orthogonal and form a basis in the 4-dimensional tensor-product Hilbert space of those two atoms. The entropy defect of the system in one of those states is $I_q = 2\ln 2$ per pair, or $J_q = 2N\ln 2$ for the whole gas (as before, we assume the gas to be ideal and the states of the molecules, independent).

Suppose that the gas is initially in state $|\Phi^+\rangle$. Then, by use of the same transformation $U_1$ as in the previous section, we can convert half of the gas molecules into state $|\Psi^-\rangle$. Using the same setup as in Fig.1, we obtain work $W_1 = NkT \ln 2$; the final state of the gas will be a mixture

$$\rho^{(1)} = \frac{1}{2}(|\Phi^+\rangle \langle \Phi^+| + |\Psi^-\rangle \langle \Psi^-|).$$

Now we can use a unitary transformation $U_2 = U_\Phi \otimes U_\Psi$, where $U_\Psi$ is the unitary transformation that permutes $\Phi^+$ and $\Phi^-$ in the subspace spanned by these orthogonal states, and $U_\Phi$ analogously permutes $\Psi^+$ and $\Psi^-$. Transformation $U_2$ converts $\rho^{(1)}$ into a mixed state

$$\rho^{(2)} = \frac{1}{2}(|\Phi^-\rangle \langle \Phi^-| + |\Psi^-\rangle \langle \Psi^-|).$$

Note that states $\rho^{(1)}$ and $\rho^{(2)}$ are orthogonal, and thus perfectly distinguishable.

Employing transformation $U_2$ and using the same setup as before, we can now repeat the mixing procedure. This will yield additional work $W_2 = Nk\ln 2$, bringing the system to the equilibrium state $\rho = \frac{1}{2} (\rho^{(1)} + \rho^{(2)})$. Hence, the total amount of heat converted into work is

$$W_q = W_1 + W_2 = 2NkT \ln 2 = NkTI_q = kTJ_q.$$  

Since the entropy defect of the entangled states is two times as large as that of classically correlated states, the amount of work $W_q$ is also larger than $W_c$ by a factor of 2.

Now assume that the gas molecules are initially in a pure partially entangled state

$$\psi = a |00\rangle + b |01\rangle + c |10\rangle + d |11\rangle,$$

where

$$|a|^2 = |d|^2 = \frac{1}{2}, \quad |b|^2 = |c|^2 = \frac{1}{2} - \frac{1}{2}p, \quad c = b^*, \quad d = -a^*.$$  

Conditions (11) ensure that the one-particle density matrices are the same as at equilibrium. (Entanglement vanishes when $p = \frac{1}{2}$.) State $\psi$ displays the same partial two-particle correlation as the mixed state $\rho_{1p}$. The important difference is that in this case the correlation is entirely due to the entanglement. Thus, the two-particle system is in a pure state and its entropy defect is $I_q = 2\ln 2$, independently of the parameter $p$. This leads to the paradoxical fact that the amount of work that can be obtained by the use of a gas in a partially entangled state is the same as in the case of maximally entangled state, namely,

$$W_q = 2NkT \ln 2 = NkTI_q.$$  

Indeed, state $\psi$ can be transformed by an appropriate unitary operator into state $|\Phi^+\rangle$, and the procedure described above can be applied to convert to work an amount of heat equal to $W_q$.

Expressions (11), (12), (13), and (14) present results related to the two extreme cases of entirely “classical” and entirely “quantum” correlations. One could consider a more general case of a mixed non-separable state, where the correlation is partially “quantum” (entanglement) and partially “classical.” The amount of work in this case should fall between the values given by (12) and (13).

3 Conclusions

The above results demonstrate the equivalence relation between information and work for the case when the information is contained only in two-particle probability distributions, and cannot be extracted from a mere one-particle distribution.
The situation with the equivalence between information and work in general remains unclear and, in a way, paradoxical. On one hand, many researchers are strongly convinced of it and express it in a very firm way, e.g., “Information has an energetic value: It can be converted into work” (Zureck [19]; but cf. [17]). (In fact, it is not information that can be converted into work, but heat that can be converted into work by use of information.) On the other hand, in our opinion, one still lacks a convincing general proof that any kind of information can be equally successfully used to convert heat into any kind of work, so that the general statement remains a sort of “folk theorem.” We believe that the root of this problem is the fact that, in spite of many unquestionable examples of “work” known to physicists, there is no general rigorous definition that would distinguish between these two forms of energy transfer—heat and work.

Informally speaking, work is an “informed” transfer of energy, i.e., a transfer such that we know exactly the change of the state of each degree of freedom, resulting from this transfer; while heat is energy transferred in such a way that we have no such knowledge. From that viewpoint, the equivalence between information and work becomes indeed a tautology. However, a rigorous formalization of these ideas has not yet been presented.

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