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# On the Computational Power of Molecular Heat Engines

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A heat engine is a machine which uses the temperature difference between a hot and a cold reservoir to extract work. Here both reservoirs are quantum systems and a heat engine is described by a unitary transformation which *decreases* the average energy of the bipartite system. On the molecular scale, the ability of implementing a (good) unitary heat engine is closely connected to the ability of performing logical operations and classical computing. This is shown by several examples:

(1) The most elementary heat engine is a SWAP-gate acting on 1 hot and 1 cold two-level systems with different energy gaps.
(2) An optimal unitary heat engine on a pair of 3-level systems can directly implement OR and NOT gates, as well as copy operations. The ability to implement this heat engine on each pair of 3-level systems taken from the hot and the cold ensemble therefore allows universal classical computation.
(3) Optimal heat engines operating on one hot and one cold oscillator mode with different frequencies are able to calculate polynomials and roots approximately.
(4) An optimal heat engine acting on 1 hot and $n$ cold 2-level systems with different level spacings can even solve the NP-complete problem KNAPSACK. Whereas it is already known that the determination of ground states of interacting many-particle systems is NP-hard, the optimal heat engine is a thermodynamic problem which is NP-hard even for *n non-interacting* spin systems. This result suggests that there may be complexity-theoretic limitations on the efficiency of molecular heat engines.

**KEY WORDS:** Second law; complexity theory; molecular computing; nanoscopic machines.

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## 1. INTRODUCTION

One of the most important consequences of the second law of thermodynamics is the statement that the heat energy of a bath with *uniform* temperature cannot be converted into other forms of energy. Instead, systems with different temperatures are needed. Machines using temperature differences between two or several heat reservoirs are called *heat engines*. Here we consider hypothetical heat engines on the quantum scale that "extract" energy from a collection of elementary quantum systems with different temperatures. An appealing feature of thermodynamic machines on the quantum scale is that their relation to information processing devices become more obvious. This is already seen in cooling algorithms which have been proposed in the context of NMR quantum computing [(1)], where the analogy between *initialization of bits* and *cooling* is apparent.[2] Another *Gedankenexperiment* which shows that a memory of a computing device can play the role of a thermodynamic reservoir is Szillard's hypothetical engine [(3)] which extracts work from a reservoir with uniform temperature for the cost of writing on an initialized memory (the 'cold' reservoir). From a modern point of view, it is natural to replace hot and cold reservoirs with quantum registers. In quantum computing (QC) (see e.g. [(4)]) every unitary operation on such a register is interpreted as a *logical gate*. Therefore, the QC point of view offers a clear language for analyzing the complexity of physical processes in the sense of computer science.

By identifying the bits of the quantum register ('qubits') with physical two-level systems one obtains well-defined thermal equilibrium states allowing the proper definition of 'hot' and 'cold' qubits. After having represented hot and cold reservoirs by quantum memories, heat engines which transfer entropy from the hot to the cold reservoir are *quantum operations* and it is straightforward to ask for the complexity of these operations compared to the complexity of *computing* steps. This shall be our subject. As the article will show, one can construct many instances of molecular systems where heat engines are close to logical operations and computing devices.

First we state more clearly what we mean by "extracting energy" from a physical system.

*Definition 1.* (Energy Gain of a Unitary) Given a quantum system with Hilbert space $\mathcal{H}$ with Hamiltonian $H$, i.e., a self-adjoint operator $H : \mathcal{H} \to \mathcal{H}$, and the state be a density operator $\rho : \mathcal{H} \to \mathcal{H}$. Then we say that a unitary $U$ extracts energy if and only if

$$E_{\text{gain}} := tr(\rho H) - tr(U\rho U^{\dagger} H) > 0\,. \tag{1}$$

[2] This analogy is a basic insight for the thermodynamics of computation [(2)] and Landauer's principle saying that the erasure of a bit of information 'wastes' the energy $\ln 2\; kT$, where $k$ is Boltzmann's constant and $T$ the reference temperature of the bath which absorbs the erased information.

Similar formal settings for energy extraction from molecular systems are considered in [5–7], whereas the authors in [8] describe cycles in which the energy levels, i.e., the Hamiltonians, of the quantum systems are changed adiabatically. Systems where no energy extraction in the sense above is possible are called *passive* in [5].

Below we will consider "unitary heat engines" where $\rho$ is the product state $\rho = \rho_A \otimes \rho_B$ of a bipartite system $A$, $B$ and $\rho_A$ and $\rho_B$ are thermal equilibrium states with different temperatures $T_A$, $T_B$, respectively.

Definition 1. requires some clarification. First of all one has to ask where the energy goes. If it is transferred to the environment, the energy extraction will in general not perform any useful work. However, we assume that it is transferred to some *target* system which is not explicitly included into the model. Consider, for instance a two level system with energy gap $E$ in the excited state $|1\rangle$. Transferring it to its lower level $|0\rangle$ releases the energy $E$. If the process would be implemented by stimulated emission, for instance, the energy would be absorbed by the stimulating field mode. We will not consider the problem how the released energy could really perform some *useful* work, instead, we only demand that the unitary process $U$ in ineq. (1) *lowers* the average energy of the system. It should be emphasized that we only allow unitary transformations here instead of general completely positive (CP) trace-preserving operations [9], since it is commonly believed that all processes are unitary provided that a sufficiently large environment is taken into account. By allowing general CP-operations one would therefore implicitly allow *information* transfer between the system and its environment. The fact that the operation on the *whole system* involves information processing would then be obscured by the restriction to a *non-informationally* complete subsystem.

One may be surprised why the target system, i.e., the energy sink (like the field mode in the example above), does not explicitly occur in the description. From the fundamental point of view one would expect a unitary operation on a system which includes the target. The problem is that the thermodynamics in such a model depends strongly on the assumptions on the physics of the target system. If the latter acts not only as an energy sink but also as an *entropy* sink, the *free energy*, i.e., the thermodynamically valuable energy, is not necessarily increased since the latter is a difference between energy and entropy multiplied by the Boltzmann constant and a given reference temperature. The latter temperature determines therefore the gain of usable energy.

In [10] we have considered thermodynamic models consisting of a hot and a cold system as well as a target system which is driven to a non-equilibrium state by an energy conserving transformation on the whole *tripartite* system. The question, which resources are sufficient to prepare a desired non-equilibrium state in the target system has extensively been studied in [10] in the context of a quasi-order of thermodynamic resources. We will show in the appendix that energy conserving transformations on the tripartite system can approximately lead to

unitary transformations by restriction to the hot and cold reservoir if the target system starts in a superposition of many energy eigenstates (as a coherent state in quantum optics). This should be considered as justification of our model.

In this paper, we do not consider the question of which physical interactions could implement the desired unitaries. It is clearly far away from present technology to implement a unitary heat engine in such a way that the energy consumption of the implementation is less than the thermodynamic energy yield. The interesting question is whether this is a matter of principle or not; if there are fundamental bounds on the energy consumption of the required unitaries one should expect similar lower bounds for logical operations. At the moment, no fundamental lower bounds are known on the energy consumption of a computer [11–16]; likewise we do not know of any such bound for heat engines. Nevertheless molecular heat engines extracting the *full amount* of thermodynamically available work from a hot and a cold reservoir could involve logical transformation too complex to be feasible.

The paper is organized as follows. In Section 2 we introduce the mathematical model of molecular heat engines and recall some properties of Gibbs states. Section 3 shows that basic logical operations give examples of simple heat engines. Sections 4 and 5 give examples of molecular heat baths where every good heat engine must necessarily solve some computation problems. In Section 6 we introduce heat engines on collections of two-level systems which are interpreted as quantum bits. In this setting we ask for the number of elementary logical operations which are necessary for implementing heat engines and show that it increases for small temperature differences. In Section 7 we show that an optimal heat engine on $2n$ hot and 1 cold two-level systems is the inverse of the MAJORITY gate and argue that this implies lower bounds on the number of elementary quantum gates required. Section 8 shows that optimal heat engines on two 3-level systems are logical transformations which are universal for classical computation. In order to suggest that it is unlikely to find a general algorithm for the implementation of optimal heat engines Section 9 shows that this would provide an algorithm for solving an NP-complete problem. The appendix tries to justify the model used in this article a bit deeper than it is done in the introduction.

## 2. UNITARY HEAT ENGINES

In order to see that unitary processes on molecular systems with different temperatures could extract some work we first want to recall thermodynamics of quantum systems with discrete energy levels. We will also recall another characterization of thermal equilibrium states as the only states which do not allow any energy extraction even if arbitrarily many copies are available.

First we state the usual definition of thermal equilibrium ("Gibbs state"):

*Definition 2.* (Thermal Equilibrium) Let $H := \sum_j E_j |j\rangle\langle j|$ be the Hamiltonian with energy levels $E_j$ and energy eigenstates $|j\rangle$. Whenever $tr(\exp(-H/T))$ is finite, the thermal equilibrium state $\gamma_T$ for some $T > 0$ is given by

$$\gamma_T := e^{-H/T}/tr(e^{-H/T}) = \sum_j e^{-E_j/T}|j\rangle\langle j| \Big/ \sum_l e^{-E_l/T},$$

where we have dropped Boltzmann's constant. For $T = \infty$ the density matrix $\gamma_T$ is the maximally mixed state and for $T = 0$ a uniform mixture over all ground states, i.e., energy eigenstates with minimal energy.

One can check easily that $\gamma_T$ does not allow any energy extraction since the states with lower energy are more likely than the states with larger energy. Note that the converse statement is not true, i.e., there are states $\rho$ which differ from all temperature states $\gamma_T$ for $T \in [0, \infty]$ but for which no unitary lowering the energy exists. However, Theorem 7 in[5] shows[3] that a weaker form of the converse is true: a state $\rho$ is called 'completely passive' if all states $\rho^{\otimes n}$ are passive. Then it is showed that completely passive states are either Gibbs states or some ground states. In our language we have:

**Theorem 1.** *(Copies of Non-Equilibrium States are Energy Sources) Let $\rho$ be a state with $\rho \neq \gamma_T$ for all $T \in [0, \infty]$ which has the additional property that not all the probability is concentrated in the ground states. Then there is an $n \in \mathrm{N}$ such that an appropriate unitary extracts energy from $\rho^{\otimes n}$.*

We give an alternative proof to that one in [5] which makes the geometric origin of the Gibbs distribution more obvious.

**Proof:** As already stated in Theorem 2 in [5] $U$ can only minimize $tr(U\rho U^\dagger H)$ if $U\rho U^\dagger$ commutes with $H$ since the minimum $tr(UAU^\dagger B)$ for any two self-adjoint matrices $A, B$ is always attained if $UAU^\dagger$ and $B$ commute [18]. We may therefore assume that $\rho$ commutes with $H$. Let $p_0, \ldots, p_{d-1}$ be the eigenvalues of $\rho$ corresponding to the energy levels $E_0, \ldots, E_{d-1}$. An eigenbasis of $\rho^{\otimes n}$ is clearly given by all products of $n$ eigenvectors of $H$. We characterize these basis states by vectors $l \in \mathbb{Z}^d$ with $l = (l_1, \ldots, l_d)$ and $\tilde{l} = (\tilde{l}_1, \ldots, \tilde{l}_d)$ where $l_j$ and $\tilde{l}_j$ are the number of components being in level $j$. Their energy difference can be written as an inner product in $\mathbb{R}^n$:

$$\sum_j (l_j - \tilde{l}_j)E_j = (l - \tilde{l}|E)\,.$$

[3] see also [17] for a generalization to infinite dimensional systems.

Assume first that $p_j \neq 0$ for all $j = 1, \ldots, d$. The logarithm of the probability ratio of the two states can also be written as an inner product;

$$\sum_j (l_j - \tilde{l}_j) \ln p_j = (l - \tilde{l} | \ln p) ,$$

where '$\ln p$' denotes the vector obtained by taking the logarithm of each entry of $p$. Assume that $p$ is not the equilibrium distribution. Then there exists, by definition, no $T > 0$, $\mu \in \mathbb{R}$ such that

$$p_j = e^{-E_j/T + \mu} \quad \forall j ,$$

which would be equivalent to

$$\ln p = -\frac{1}{T} E + \mu a ,$$

if we define $a \in \mathbb{R}^d$ as the vector having only 1 as entries. Let $R$ be the projection onto the space $a^\perp$. Then we have

$$R \ \ln p \neq -\frac{1}{T} R\, E$$

for all $T > 0$. Since not all levels have the same energy we have $R\, E \neq 0$. Furthermore, not all entries of $\ln p$ are equal because this would be the $T = \infty$ state. Elementary geometry shows that there is an $x$ in $a^\perp$ such that

$$(x | \ln p) > 0$$

and

$$(x | E) > 0 .$$

Of course $x$ can be chosen with rational entries and therefore, by multiplication with the least common multiple of their denominators, also as a vector $x \in \mathbb{Z}^d$. With such an $x$ there exist vectors $l, \tilde{l} \in \mathbb{N}_0^d$ such that $x = l - \tilde{l}$. By defining

$$n := \sum_j l_j ,$$

which is equal to the sum of all $\tilde{l}_j$ according to $(l - \tilde{l}) \perp a$, the vectors $l, \tilde{l}$ define two classes of states such that each state in one class is more likely than each state in the other class although the latter states have less energy.

Let $p$ have entries zero. Assume that there is some non-zero probability for a level which is not the ground state. Then there are 3 levels $0, 1, 2$ with $E_2, E_1 > E_0$ such that $p_2 = 0$, $p_1 \neq 0$. Consider a state with label $l$ in $O^{\otimes n}$ with $l_2 = 1, l_0 = n - 1$ and $l_j = 0$ for all the other $j$. Consider furthermore a state with label $\tilde{l}$ where $\tilde{l}_1 = n$ and $\tilde{l}_j = 0$ for all the other indices $j$. Clearly there is an $n$

such that $\bar{l}$ has more energy than $l$ even though the former has non-zero probability and the latter probability zero. □

In agreement with thermodynamic intuition, elementary calculation shows that the composition $\rho_A \otimes \rho_B$ of two equilibrium states $\rho_A$, $\rho_B$ with the same temperature is the unique equilibrium state of the composed system. This shows that the $n$ fold copy of an equilibrium state still allows no work extraction. We will clearly expect that if a state $\rho$ is *close to* an equilibrium state for some $T$ one will require a *large number* of copies of $\rho$ to extract energy. We will later see that this fact implies that two reservoirs consisting of hot and cold two-level systems, respectively, require many-qubit operations whenever the temperature difference between the two reservoirs is small. We give now a precise definition for *heat engines* and *optimal heat engines*:

*Definition 3.* (Unitary Heat Engine). A heat engine is a unitary transformation $U$ on a bipartite system with Hamiltonian $H := H_A \otimes \mathbf{1} + \mathbf{1} \otimes H_B$. It is initially in the state $\rho = \rho_A \otimes \rho_B$ where $\rho_A$, $\rho_B$ are equilibrium states with different temperatures $T_A$, $T_B$, respectively and $U$ extracts energy in the sense of Definition 1. A unitary $U$ is an optimal heat engine if it maximizes $E_{\text{gain}}$.

In order to run such a heat engine again one has to ensure that system $A$ and $B$ interact with heat baths with temperatures $T_A$ and $T_B$, respectively.

## 3. SWAP AS THE MOST ELEMENTARY HEAT ENGINE

Classical thermodynamics states that one can in principle use any two systems with different temperature to extract work in a Carnot cycle [19]. For two quantum systems this is no longer true if we demand unitary heat engines as in Definition 1. As also noted in [7–10] there are additional constraints because unitaries do not only conserve entropy but also the whole spectrum of a density operator.

If the systems $A$ and $B$ in Definition 3 are two-level systems with equal energy gap $E$ but different temperatures $T_A$, $T_B$ one checks easily that the 4 states 00, 01, 10, 11 of the bipartite system already satisfy $p_{00} > p_{10}$, $p_{01} > p_{11}$. Therefore no work extraction is possible since this order coincides with ordering the states according to their energy: $E_{00} < E_{01} = E_{10} < E_{11}$. However, we can construct a heat engine if the energy gaps $E_A$ and $E_B$ of system $A$ and $B$ satisfy

$$\frac{T_A}{E_A} > \frac{T_B}{E_B}\,. \tag{2}$$

One observes easily that the state 10 has more energy than 01 even though the latter is more likely due to

$$\frac{p_{10}}{p_{01}} = e^{-E_A/T_A} e^{E_B/T_B} = e^{(E_B/T_B - E_A/T_A)}\,.$$

That the latter term should be greater than 1 leads directly to Eq. (2). Then we can gain energy by implementation of the SWAP-gate, i.e., the permutation $10 \leftrightarrow 01$. The condition (2) is specific to our molecular heat engine and seems not to be directly related with the second law; such additional constraints become less relevant in larger systems.

It is easy to see that the SWAP gate is the only possible unitary operation that extracts an *maximal* amount of energy since it is clear that the states 00 and 11 must remain unchanged as they already have both extremal energy and probability. Only for the two states 10 and 01 the order corresponding to increasing energy is not consistent with the order corresponding to decreasing probability and we must exchange the states.

One could easily think of transformations $U$ which are close to the unique optimal one. It is intuitively obvious that one could find some trade-off relations between *efficiency* of the heat engine $U$ and its *reliability* as a SWAP gate. This trade-off relation would also hold if convex sums of unitaries (a "random unitary heat engine") were applied.

## 4. APPROXIMATE COMPUTATION OF ROOTS AND POWERS WITH OSCILLATOR MODES

To show that heat engines may involve quite complex transformations we have to consider larger systems. A very natural system in physics is a quantum harmonic oscillator. Its Hilbert space $l^2(\mathbb{N}_0)$ is spanned by the number states $|0\rangle, |1\rangle, |2\rangle, \ldots$ with $0, 1, 2, \ldots$ quanta. Such a system can be a quantum optical mode or a mechanical oscillator. A state with $j$ quanta of frequency $\omega$ has the energy $E(j) = j\hbar\omega$ and the system Hamiltonian is therefore

$$H := \hbar\omega \sum_{j=0}^{\infty} j\,|j\rangle\langle j|\,.$$

The bipartite system on which our heat engine will be defined consists of two modes with different frequencies $\omega_A$ and $\omega_B$. In studying optimal heat engines on such a bipartite system a problem specific to infinite systems will arise: we have usually constructed the optimal heat engine $U$ by forming two lists, one containing the basis states ordered by decreasing probability and the other by increasing energy. Then $U$ is given by the map $|a\rangle \mapsto |b\rangle$ for each corresponding pair $(a, b)$. Unfortunately the first list may be incomplete even though the other is complete. Then $U$ is not defined on all states. This situation occurs if one oscillator is initially in its ground state. For every bijection on the basis states there is always a bijection extracting more energy. Below we will ignore this problem because one can easily check that the maps described there can be approximated by unitary heat engines in an appropriate way.

First we assume $\omega_A = \omega_B = \omega$ and $T_A \neq T_B = 0$. Then the only states with non-vanishing probability are of the form

$$|n, 0\rangle \quad n \in \mathbb{N}_0 .$$

To construct the image of the state $|n, 0\rangle$ with respect to an optimal heat engine we recall that the eigenspace of the joint Hamiltonian

$$H \otimes \mathbf{1} + \mathbf{1} \otimes H$$

is degenerate. Since $\omega$ is irrelevant in the following we assume $\hbar\omega = 1$ such that we obtain $\mathbb{N}_0$ as the spectrum. The eigenspace $\mathcal{H}_k$ corresponding to eigenvalue $k \in \mathbb{N}_0$ has dimension $k + 1$. The optimal heat engine $U$ has to map the state $|n, 0\rangle$ into an eigenspace $\mathcal{H}_k$ where $k$ is uniquely specified by the following conditions:

$$\dim(\oplus_{l<k}\mathcal{H}_l) < n + 1 ,$$

and

$$\dim(\oplus_{l\leq k}\mathcal{H}_l) \geq n + 1.$$

By calculating the dimensions we obtain

$$n + 1 > \sum_{l=0}^{k-1}(l + 1) = \sum_{l=1}^{k} l = \frac{k^2 + k}{2} ,$$

and

$$n + 1 \leq \sum_{l=0}^{k}(l + 1) = \frac{k^2 + 3k + 2}{2} .$$

The conditions are equivalent to

$$(k^2 + k)/2 < n + 1 \leq (k^2 + 3k + 2)/2 .$$

For large $n$ we have $k \approx \sqrt{n}$. Hence we have a calculator which reduces the approximative computation of $\sqrt{n}$ to an addition of numbers by the following procedure: apply the heat engine to the state $|n, 0\rangle$ and measure $\tilde{n}, \tilde{m}$ of the resulting state. Then $\tilde{n} + \tilde{m}$ is an estimation for $\sqrt{n}$.

Two modes can also be used for the calculation of squares. Let $\omega_B < c\omega_A$ with some real $c \gg 1$. Then choose the temperatures such that $T_A = cT_B$. This implies that all states $|n, m\rangle$, $|n', m'\rangle$ with $n + m = n' + m'$ have equal probability. The optimal heat engine on these two oscillators can compute approximately $(n + m)^2$ for the input $n, m$ whenever the result is sufficiently smaller than $c$. This is seen as follows: for a given pair $n, m$ with $n + m = k$ there is a $(k^2 + k)/2$-dimensional space for which the eigenvalue of the joint density matrix is greater than the eigenvalue corresponding to the state $|n, m\rangle$. This space must be mapped into the

span of all states $|0, \tilde{m}'\rangle$ with $\tilde{m}' \leq (k^2 + k)/2$. The subspace

$$\oplus_{l \leq k} \mathcal{H}_l$$

has to be mapped on the span of all $|0, \tilde{m}'\rangle$ with $\tilde{m}' \leq (k^2 + 3k + 2)/2$. When we initialize the heat engine to a state $|n, m\rangle$ and measure the right quantum number we obtain therefore some $\tilde{m}$ with

$$\frac{k^2 + 3k + 2}{2} \geq m \geq \frac{k^2 + k}{2}.$$

Hence we obtain $\tilde{m} \approx k^2/2$.

The schemes above generalize in a straightforward way to the computation of higher powers and higher roots when more than two oscillators are used. To calculate $k$th roots we start with 1 hot and $k - 1$ zero-temperature oscillators and to calculate the $k$th power we start with $k$ hot and 1 cold modes where the hot modes have $c$ times larger energy gap and the temperatures $T_A = cT_B$ are also chosen such that the probability for a state $|n_1, n_2, \ldots, n_k\rangle$ is only determined by $N := \sum_j n_j$. Then the optimal heat engine maps all states with $N < c$ onto a state $|0, 0, \ldots, \overline{N}\rangle$ where $\overline{N}$ is an approximation for $\sqrt{k}N$.

Now we assume that the ratio $e := \omega_A/\omega_B$ is irrational. This ensures that the Hamiltonian of the composite system is non-degenerate. Up to irrelevant constants, the energy of a state with $n_A$ quanta in mode $A$ and $n_B$ quanta in mode $B$ is

$$E(n_A, n_B) = en_A + n_B$$

with $e \in \mathbb{R} \setminus \mathbb{Q}$. We define a bijective function $k : \mathbb{N}_0^2 \to \mathbb{N}_0$ such that $k(n_A, n_B)$ indicates the number of the pair $(n_A, n_B)$ when all pairs are put into an increasing order with respect to $E(n_A, n_B)$. Now we choose the temperatures $0 \neq T_A \neq T_B \neq 0$ such that

$$q := \frac{E_A/T_A}{E_B/T_B}$$

is also irrational which holds for instance when $T_A/T_B$ is rational. It follows that the density operator $\rho_A \otimes \rho_B$ is also non-degenerate. Up to an additive constant and a negative factor, the logarithm of the probability for a state $|n_A\rangle \otimes |n_B\rangle$ is given by

$$Q(n_A, n_B) := qn_A + n_B.$$

A larger value $Q(n_A, n_B)$ indicates that the state is less likely. In analogy to the map $k$ we define a bijective function $l : \mathbb{N}_0^2 \to N_0$ indicating the order of the pairs $(n_A, n_B)$ with respect to their values $Q(n_A, n_B)$. Define a permutation $\pi$ on $\mathbb{N}_0^2$ by

$$\pi := k \circ l^{-1}.$$

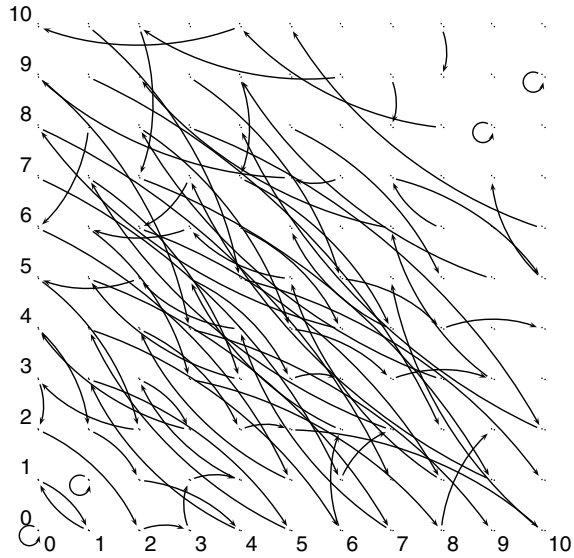



**Fig. 1.** Optimal heat engine of two harmonic oscillators with frequency ratio $\omega_A/\omega_B = \sqrt{2}$ and temperature ratio $T_B/T_A = \omega_B/(\sqrt{3}\omega_A)$. A point in row $n$ and column $m$ is a basis state with $n$ quanta in mode $A$ and $m$ in mode $B$. An arrow $(n, m) \to (\tilde{n}, \tilde{m})$ indicates that a state with $n$ quanta in mode A and $m$ in mode B has to be converted into a state with $\tilde{n}, \tilde{m}$ quanta, respectively. Points which have their image or pre-image outside the depicted area obtain no arrow.

This permutation of basis states $|n_A, n_B\rangle$ defines a unitary $U_\pi$ by linear extension.[4] The density operator of the whole system after having implemented the heat engine $U_\pi$ is

$$U_\pi(\rho_A \otimes \rho_B)U_\pi^\dagger .$$

The heat engine permutes the eigenvalues such that they are reordered according to the corresponding energy values. We have computed the corresponding reordering of states for the values $e = \sqrt{2}$ and $q = 1/\sqrt{3}$. The mapping is depicted in Fig. 1, showing that the heat engine defines a quite *complex* flow in the discrete two-dimensional plane. Here complexity is understood in a rather intuitive sense. We will come to more precise versions of complexity in Sections 6, 7, and 8.

Another interesting case is when one temperature is zero. For $T_A = 0$ only states $|0, n_B\rangle$ have non-zero probability. Here the number $n_B$ indicates already the ordering of all states which have non-zero probability. The optimal heat engine would have to map $(0, n_B)$ onto the state $(\tilde{n}_A, \tilde{n}_B)$ with $k(\tilde{n}_A, \tilde{n}_B) = n_B$. Hence the heat engine solves the computation problem of *inverting* $k$.

[4] Note that the ordering of pairs given by $E$ or $Q$ is a term order in the sense of [20] .

## 5. CONVERTING BETWEEN DIFFERENT NUMBER SYSTEMS WITH $N$-LEVEL SYSTEMS

The heat engines above could only be used for approximate calculations. Here we present an example with some finite dimensional systems which perform an exact computation. Consider two $N_A$-level systems with temperature $T_A$ and two $N_B$-level systems with temperature $T_B = 0$. Let all 4 systems have equidistant energy levels where the first system of type $A$ has energy gaps $E_A$ and the second $N_A E_A$. For the $N_B$-level systems we have energy gaps $E_B$ and $N_B E_B$ and assume furthermore $N_B E_B < E_A$. Then the $N_B^2$ states with least energy are given by

$$|0,0\rangle \otimes |\tilde{n},\tilde{m}\rangle\,,$$

where the rightmost vector denotes the states of the two $N_B$-level systems. The energy is increasing according to an increase of $\tilde{n}N_A + \tilde{m}$. The $N_A^2$ most likely states are given by

$$|n,m\rangle \otimes |0,0\rangle\,,$$

and their probability is decreasing with increasing $nN_A + m$. It is easy to check that the optimal heat engine for this level spacing and this temperature configuration can convert natural numbers from the $N_A$-ary representation to the $N_B$-ary representation: Initialize the system to the state

$$|n,m\rangle \otimes |0,0\rangle\,,$$

such that $nN_A + m < N_B^2 - 1$. Then we obtain a state

$$|0,0\rangle \otimes |\tilde{n},\tilde{m}\rangle$$

such that $\tilde{n}N_B + \tilde{m} = nN_A + m$, i.e. the representation of the input number in the $N_B$-system. The scheme generalizes canonically to numbers with more than 2 digits but since the energy gaps grow exponentially this would not be useful to transform numbers with many digits. Nevertheless the example shows that optimal heat engines could perform some useful calculations.

## 6. COMPUTER SCIENTIST'S HEAT ENGINE

Note that a system with two oscillator modes can never be an *efficient* computer even though it may perform some computations since the energy resource requirements for representing an $n$ bit input increases exponentially with $n$ instead of increasing only polynomially. Therefore $n$ qubits are more natural for studying whether the implementation of heat engines is close to computing. The heat engine with two 2-level systems studied in Section 3 requires different energy gaps. One can easily conclude from Theorem 1 that heat engines are also possible with two-level systems with equal energy gap if one has a few of them: the composition

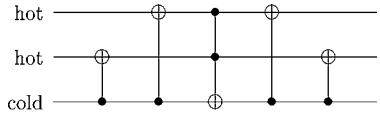



**Fig. 2.** Heat engine with 3 two-level systems with equal energy gap.

of 2 two-level systems with temperatures $T_A \neq T_B$

$$\rho := \gamma_{T_A} \otimes \gamma_{T_B}, \text{ where } \gamma_{T_A} \text{ and } \gamma_{T_B} \text{ are equilibrium states,}$$

is not an equilibrium state for any temperature. Therefore, there is an $n$ such that $\rho^{\otimes n}$ allows a unitary heat engine. If the temperatures differ sufficiently this is already true for $n = 2$. One can even implement an heat engine with 2 hot and 1 cold system. Assume $T_A > 2T_B$. One checks easily that the state 110 is more likely than 001 even though its energy is twice as much. Hence the process $110 \leftrightarrow 001$ extracts some energy. Figure 2 shows a quantum circuit implementing this heat engine.

The required number of systems which are necessary in order to make a heat engine possible at all increases whenever the temperature quotient gets closer to 1:

**Theorem 2.** *(Complexity of Using Small Temperature Gaps) A heat engine on $n_A$ hot and $n_B$ cold qubits with temperatures $T_A$ and $T_B$, respectively, and equal energy gaps, is possible if and only if*

1. *(for $n_A \leq n_B$)*

$$\frac{T_A}{T_B} > \frac{n_A}{n_A - 1}$$

2. *(for $n_A > n_B$)*

$$\frac{T_A}{T_B} > \frac{n_B + 1}{n_B}$$

*Furthermore, every heat engine acting on an infinite reservoir of hot and cold qubit level systems must use operations which connect at least $n_A$ hot and $n_B$ cold systems such that the above conditions hold.*

**Proof:** We note that a heat engine can work if and only if a pair of states exist such that the first has more energy even though it is more likely. Let $(l_A, l_B)$ denote the Hamming weights (i.e. the number of symbols 1) of a basis state in the $n_A + n_B$ qubit system. The pair $(l_A, l_B)$ and $(k_A, k_B)$ satisfies this condition if

$$(l_A - k_A) - (l_B - k_B) > 0$$

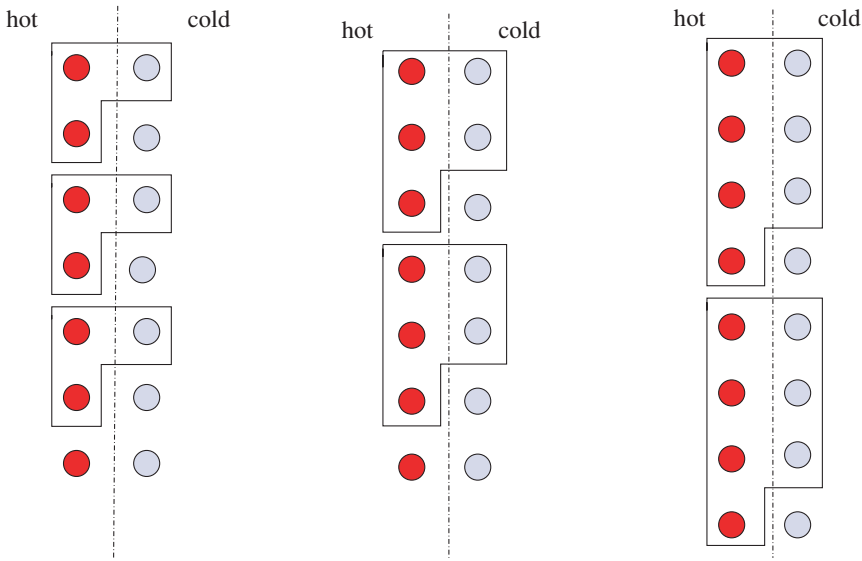



**Fig. 3.** Heat engines with $T_A/T_B > 2$ can be implemented with joint operations on 2 hot and 1 cold qubit (left). For $2 \geq T_A/T_B > 3/2$ operations on 3 hot and 2 cold qubits are needed (middle), and heat engines for $3/2 \geq T_A/T_B > 4/3$ must involve 4 hot and 3 cold qubits (right). Color online

and

$$(l_A - k_A)T_A - (l_B - k_B)T_B < 0.$$

Elementary computation shows that this implies

$$\frac{T_A}{T_B} > \frac{l_A - k_A}{l_B - k_B} > 1\,.$$

Clearly the modulus of the numerator and the denominator are at most $n_A$ and $n_B$, respectively. The smallest possible quotient which is still greater than 1 is therefore $n_A/(n_A - 1)$ or $(n_B + 1)/n_B$, respectively. This shows that the conditions (1), respectively (2) are necessary in order to make a heat engine possible.

For the converse we observe that in case (1) a permutation of the states $(n_A, 0)$ and $(0, n_A - 1)$ extracts some amount of energy. In case (2) one extracts energy by permuting $(n_B + 1, 0)$ and $(0, n_B)$. □

Figure 3 illustrates how the complexity of heat engines on two-level systems with equal energy gap increases when the temperature gaps decrease in the sense that more qubits have to be involved. Note that Fig. 3 furthermore suggests a simple method to obtain *suboptimal* heat engines on many particles by independently applying few-qubit heat engines.

We would like to know whether the increase of complexity with decreasing temperature difference occurs also with respect to the *number of required gates* in a circuit consisting of simple elementary gates. Therefore we have checked which heat engines are possible when only a few number gates are allowed and restricted the attention to TOFFOLI gates [21] since (1) they permute only basis states and can therefore easily be treated with computer algebra (CA) systems (2) they are universal for classical computation and they seem therefore sufficiently powerful to generate good heat engines.[5] The restriction to one type of gate simplifies the complete search for all circuits that can be obtained with $k$ gates. In CA experiments the energy release of the heat engines obtained by a small number of TOFFOLI gates was compared to the maximal release. The latter can easily be computed by reordering the energy levels according to their probabilities.

In the first experiment we consider 3 hot and 2 cold qubits with temperatures $T_A = E/\ln 2$ and $T_B = 0$. The probabilities for the upper state is hence for a hot qubit given by $1/3$. CA calculations have shown that 3 gates are necessary in order to have positive energy gain. The circuit Fig. 4, left, acts on only $3 + 1$ qubits and does not make use of the second available cold qubit. With this circuit we have $E_{\text{gain}} = 1/27$ which is considerably less than the optimal heat engine on $3 + 2$ qubits having $E_{\text{gain}} = 5/27$. If we increase the temperature of the cold system such that $T_B = E/\ln 5$ the circuits with 3 gates do not decrease the average energy any more and at least 4 gates are needed for a heat engine. One possibility with 4 gates is shown in Fig. 4, right, with $E_{\text{gain}} = 1/72$. For temperature $T_B = E/\ln 4$ there is even no heat engine with 5 TOFFOLI gates. Note that in this situation a heat engine is still possible by Theorem 2 because $T_A/T_B = \ln 4/\ln 2 = 2 > 3/2$; therefore the state exchange $|111\rangle \otimes |00\rangle \leftrightarrow |000\rangle \otimes |11\rangle$ extracts energy. CA calculations show furthermore that there is indeed a circuit with 31 Toffoli gates which implements the state exchange above such that all the other states are mapped onto basis states with the same Hamming weight[6]. There are probably much simpler circuits but the exhaustive search has shown that at least 6 are required.

## 7. MAJORITY GATE ON 2N+1 QUBITS

Here we present an example where the complexity of the optimal heat engine can be compared to the complexity of a circuit computing a well-known boolean function. Consider $2n$ two-level systems with temperature $T_A = \infty$ and 1 system with $T_B = 0$. The basis states of the system are binary words of length $2n + 1$.

[5] Note, however, that TOFFOLI gates do not generate the full group $S_N$ of permutations on $N = 2^n$ basis states of $n$ qubits (see Section 7)

[6] Recall that the Hamming weight of a binary word is defined as the number of symbols '1'.

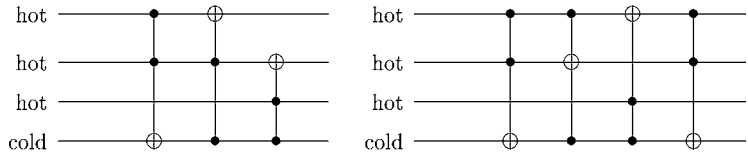



**Fig. 4.** (left:) The simplest possible heat engine which uses only Toffoli gates. (right:) A heat engine with 4 gates can extract work from reservoirs with smaller temperature gaps.

The joint Hamiltonian of the system is given by

$$H := E \sum_b wgt(b)|b\rangle\langle b| \,,$$

where $E$ is the energy gap of each two-level system and $wgt(b)$ denotes the Hamming weight of the binary word $b$. Let the suffix of each of this binary words indicate the state of system $B$. Then all binary words with suffix 0 have probability $1/2^n$ and words with suffix 1 never occur. Every optimal heat engine $U$ has to map the subspace spanned by the former $2^n$ words onto the subspace corresponding to the $2^n$ smallest eigenvalues of $H$. It is the space spanned by all words with Hamming weight at most $n$. Therefore the inverse of the heat engine, i.e., $U^{-1}$ computes the boolean function MAJORITY in the sense that the rightmost qubit in the state

$$U^{-1}|b\rangle$$

is 1 if and only if $wgt(b) > n$, i.e., the majority of the qubits are in the 1 state. We would like to estimate the gate complexity of $U$ when it is implemented by elementary gates. If the set of elementary gates contains with every gate also its inverse the complexity of $U$ and $U^{-1}$ coincide. To obtain a lower bound on the circuit complexity we could therefore use bounds on the circuit complexity of MAJORITY. In [22] one can find bounds for classical circuits with bounded depth consisting of AND and OR with arbitrary fan-in. We can give a lower bound on the circuit depth which holds for arbitrary $k$-qubit gates. The observable which measures whether the suffix of a binary word is 1 or 0 is $A := \mathbf{1}^{\otimes 2n} \otimes \sigma_z$. This is obviously a 1-qubit observable since $A$ acts only on the rightmost qubit non-trivially. The observable $UAU^\dagger$ which measures whether the majority of qubits are 1 is a proper $2n+1$-qubit observable because the logical states of all qubits are relevant. In [23] we have argued that a circuit of depth $l$ can convert a 1-qubit observable at most into a $k^l$-qubit observable. Therefore we otain

$$l \geq \log_k(2n+1)$$

as lower bound on the depth. This shows after all that the depth must necessarily increase with $n$ even though logarithmic growth would be quite slow. We summarize:

**Theorem 3.** *(Lower Bound on the Depth) Let $U$ be an optimal heat engine on $2n$ two-level systems with temperature $T_A \neq 0$ and one two-level system with $T_B = 0$ where all $2n + 1$ systems have the same energy gap. Then the implementation of $U$ with $k$-qubit gates requires at least a circuit of depth $\log_k(2n + 1)$.*

We would like to know which set of gates would be sufficient to implement $U$. First we observe that no ciruit which consists only of NOT and CNOT can implement $U$. The action of CNOT permutes the basis states of two qubits according to

$$|a_1\rangle \otimes |a_2\rangle \mapsto |a_1\rangle \otimes |a_1 \oplus a_2\rangle,$$

where $\oplus$ denotes the exclusive or. If one identifies the pair $(a_1, a_2)$ with a vector in a two-dimensional space over $F_2$, CNOT is a $F_2$-linear map. By embedding the action of CNOT into a $2n + 1$-dimensional space over $F_2$ it remains linear. The action of NOT on qubit $j$ corresponds to adding the vector $0 \ldots 010 \ldots 0$ with 1 at position $j$. Therefore every circuit $V$ with CNOT and NOT gates acts as

$$V|b\rangle = |Ab + c\rangle\,,$$

where $A$ is a $2n + 1 \times 2n + 1$-matrix over $F_2$ and $c$ a vector in $F_2^{2n+1}$. If the majority function would be affine it could up to an additive constant be written as an inner product over $F_2$, i.e., there existed a vector $v$ and a number $w \in F_2$ such that $(v|b) \oplus w$ is 1 whenever $wgt(b) > n$. This is certainly not the case. It is also easy to see that TOFFOLI gates alone cannot be sufficient to implement $U$ or $U^{-1}$. Otherwise $U$ and $U^{-1}$ would leave all binary words with Hamming weight at most 1 invariant. But the state $|0 \ldots 01\rangle$ has to be mapped into the space spanned by words with Hamming weight greater than $n$. This shows that too restricted sets of logical operations even though they may be quite powerful (like TOFFOLI gates) are not sufficient for optimal work extraction.

The insight that the inverse of $U$ would compute MAJORITY gave some hints on its complexity, however it does not show that the heat engine itself can be used for computing this boolean function. A thermodynamic machine which can directly be used as a MAJORITY gate is the reverse of the heat engine, namely a refrigerator. Assume we have given $2n + 1$ two-level systems with the same temperature $T \neq 0, \infty$. Then an optimal refrigerator for the rightmost qubit is a transformation $U$ which reduces the probability for its upper state as much as possible. This is certainly the case only when $U$ maps all states $|b\rangle$ with $wgt(b) > n$ to the subspace $S$ spanned by words with suffix 1 and all with $wgt(b) \leq n$ to the orthogonal complement of $S$. Hence the rightmost qubit is the output qubit of a MAJORITY computation.

We summarize:

**Theorem 4.** *(Relation to Complexity of MAJORITY) Let $U$ be an optimal heat engine on $2n$ two-level systems with temperature $T_A \neq 0$ and one two-level system*

*with $T_B = 0$ where all $2n + 1$ systems have the same energy gap. Let the set of elementary gates be closed under inversion. Then the implementation of $U$ requires at least as many elementary quantum gates as a computation of the function MAJORITY of the $2n + 1$-qubit input requires which uses no additional memory space.*

## 8. UNIVERSAL CLASSICAL COMPUTATION ON PAIRS OF 3-LEVEL SYSTEMS

It is clear that every optimal heat engine on 2 two-level systems leaves the states 00 and 11 invariant because these are the states with minimal and maximal energy and with maximal and minimal probability, respectively, at the same time. Therefore the only non-trivial logical operation is a SWAP-gate. To find more interesting logical gates in a heat engine on a bipartite system we will therefore consider two 3-level systems $A$ and $B$. We assume that system $A$ and $B$ have both equidistant levels $|0\rangle, |1\rangle, |2\rangle$ with energy gaps $E_A$ and $E_B$, respectively. Up to an irrelevant factor the energy of a state $|n, m\rangle$ with $n, m = \{0, 1, 2\}$ is given by

$$E(n, m) = en + m$$

with $e := E_A/E_B$. The inverse logarithm of the probabilities is, up to irrelevant additive and multiplicative constants, given by

$$Q(n, m) = qn + m$$

with $q := E_A T_B/(E_B T_A)$. When $e$ and $q$ are not in $\{1/2, 1, 2\}$ the Hamiltonian as well as the density matrix of the bipartite system are non-degenerate and the optimal heat engine implements a unique reordering of basis states. The following choice of values $e, q$ turns out to be useful: setting $1 < e < 2$ we induce an order on energy values of the pairs $n, m$ which is a refinement of the degenerate order induced by $n + m$ such that for pairs with equal $n + m$ preference is given to the pair with smaller $m$. Explicitly, this is the order 00, 10, 01, 20, 11, 02, 21, 12, 22. With $q > 2$ the probabilities are in the lexicographic order 00, 01, 02, 10, 11, 12, 20, 21, 22. By comparing these orders one checks easily that the optimal heat engine implements the map

$$\begin{aligned} 00 &\mapsto 00 \\ 01 &\mapsto 10 \\ 02 &\mapsto 01 \\ 10 &\mapsto 20 \\ 11 &\mapsto 11 \\ 12 &\mapsto 02 \end{aligned} \tag{3}$$

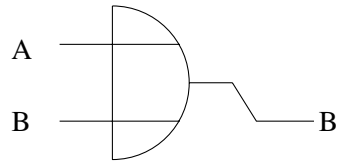
$$20 \mapsto 21$$

$$21 \mapsto 12$$

$$22 \mapsto 22\,.$$

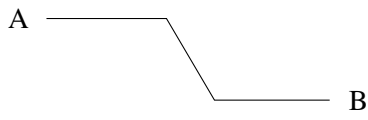
Assume we are given a collection of systems of type $A$ and type $B$. If we are able to implement the heat engine above on every pair of 3-level systems consisting of one system of type $A$ and one of type $B$ we can also implement classical computation on the collection of these 3-level systems. In order to show this, we chose the encoding such that the logical states 0, 1 are the states $|1\rangle$ and $|2\rangle$, respectively and obtain a universal set of logical operations as follows:

1. **OR from A, B to B :**



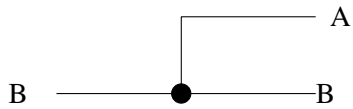

Apply $U$ once. One checks easily on tabular (3) that the second state is $|2\rangle$ if the input is one of the states $|12\rangle$, $|21\rangle$, $|22\rangle$ and $|1\rangle$ if the input is $|11\rangle$.

2. **WIRE from A to B :**




Use our OR gate by initializing B to $|1\rangle$, i.e., the logical 0 state.

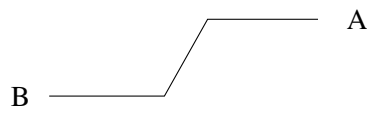
3. **FANOUT from B to A, B :**




Initialize system $B$ to $|1\rangle$. Apply $U$ 4 times. We get the mapping $12 \mapsto 20$ and $11 \mapsto 11$. The output on $A$ coincides already with the input on $B$. The output on $B$ is 1 or 0 according to whether the input on $B$ was 1 or 2. Hence the information has already been copied to $B$ but with the wrong

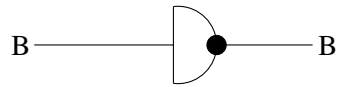
encoding. For the decoding we initialize an additional system $A'$ to the state $|1\rangle$ and apply $U^4$ to $A'$, $B$. We get $10 \mapsto 02$ and $11 \mapsto 11$. Hence $B$ agrees with the original input on $B$.

4. **WIRE from B to A :**




Use the FANOUT.

5. **NOT from B to B :**




Implement the first part of the FANOUT operation which changes the input state 2 to 0 and leaves 1 invariant. By Initializing an additional system $A'$ to $|2\rangle$ and apply $U$ once we decode and negate the information on $B$ simultaneously : $20 \mapsto 21$ and $21 \mapsto 12$.

These operations allow obviously universal computation since every boolean function can be computed from circuits which consist only of NOR gates. We summarize:

**Theorem 5.** *(Universal Computing with Heat Engines on 3-level Systems) Given two reservoirs of 3-level systems with temperature $T_A$ and $T_B$ and energy gap $E_A$ and $E_B$, respectively, such that*

$$2\frac{T_A}{E_A} < \frac{T_B}{E_B}$$

*and*

$$2 > \frac{E_A}{E_B} > 1,$$

*then the ability to implement the optimal heat engine on any chosen pair consisting of one system of type A and one of type B implies the ability to implement universal classical computation on the 3-level systems.*

## 9. OPTIMAL HEAT ENGINE AS NP-SOLVER

So far we have only shown some examples of heat engines which *perform* relatively 'simple' logical operations or computations and heat engines which are *generated by* some simple operations. Now we will consider an instance of a heat engine which had to solve a computationally hard problem in order to be optimal. Consider a collection of two-level systems with different energy gaps where one of them has temperature $T_A$ and all the others have temperature $T_B$. Then the optimal heat engine is a computer which solves an NP-complete problem. We recall that the following instance of KNAPSACK is NP-complete [24]:

*Definition 4.* (KNAPSACK) Given the natural numbers $E_1, \ldots, E_n, K, V$ with $K \leq V$. Is there a subset of the values $E_1, \ldots, E_n$ such that their sum $S$ satisfies $K \leq S \leq V$?

It is commonly believed in computer science that no algorithm can exist that computes the answer of this question such that the running time increases only polynomially in the number of bits specifying the input values $E_1, \ldots, E_n, K, V$ [25]. Therefore it is remarkable that the following instance of an optimal heat engine had to solve KNAPSACK. Consider $n$ two-level systems with temperature $T_A$ and energy gaps $E_1, \ldots, E_n$ and one hot two-level system with gap $E_A := V - 1$. Here the energy values can be given with respect to an arbitrary unit (therefore the physical energy gaps do not necessarily increase with increasing numbers of $E_j$ and $K$). Let the temperature of the hot two-level system be given by $T_B = (K-1)T_A/E_A$. Then we have:

**Theorem 6.** *(Optimal Heat Engine Solves NP) Let $E_A, E_1, E_2, \ldots, E_n$ be the energy gaps of $n+1$ two-level systems. Let $T_A$ be the temperature of the 0th system and $T$ of the remaining $n$. Let the values be such that there is no $b \in \{0,1\}^n$ such that*

$$\sum_{j=1}^{n} b_j E_j = \frac{E_A T_B}{T_A}\,.$$

*Let $U$ acting on $\mathbb{C}^2 \otimes (\mathbb{C}^2)^{\otimes n}$ be an optimal unitary heat engine for this system. Let $b \in \{0,1\}^n$ be a possible result obtained by reading out the $n$ rightmost qubits being in the state*

$$U(|1\rangle \otimes 0 \ldots 0\rangle)\,.$$

*Then $b$ satisfies*

$$E_A > \sum_j b_j E_j > E_A \frac{T_B}{T_A} \tag{4}$$

*if and only if such a binary word $b$ exists.*

**Proof:** We only have to show that if there is a string $b$ satisfying (4) it will always show up as a measured result. Write $(b|E)$ for $\sum_{j=1}^{n} b_j E_j$. Intuitively, inequality (4) implies that the state $|0\rangle \otimes |b\rangle$ has less energy than $|1\rangle \otimes |0\rangle$ but is less likely. The assumption that there is no $b \in \{0, 1\}^n$ such that

$$(b|E) = \frac{E_A T_B}{T_A}$$

means that $|1\rangle \otimes |0\rangle$ is an eigenvector in a non-degenerate subspace. This uniqueness of the eigenvalue ensures that the optimal heat engine does not have 'too much choice' on which states the state $|1\rangle \otimes |0\rangle$ has to be mapped to.

First consider the subspace $\mathcal{H}_1$ spanned by all vectors $|0\rangle \otimes |c\rangle$ with $(E|c) < E_A T_B / T_A$. The restriction of the joint density operator $\rho$ to this subspace (note that this is indeed an invariant subspace of $\rho$) is left invariant by every optimal $U$ since the ordering of eigenvalues of $\rho$ and of $H$ coincide here. All these states are more likely than $|1\rangle \otimes |0\rangle$ and have less energy.

Binary words $c$ with $(E|c) = E_A T_B / T_A$ do not exist by assumption. Now consider the subspace $\mathcal{H}_2$ spanned by all $|0\rangle \otimes |c\rangle$ with $E_A > \langle E|c\rangle > E_A T_B / T_A$. They have less energy than $|1\rangle \otimes |0\rangle$ but they are also less likely, i.e., all eigenvalues of $\rho$ on this subspace are smaller than the eigenvalue $p$ of $\rho$ for the eigenvector $|1\rangle \otimes |0\rangle$. Note that $\mathcal{H}_1$ and $\mathcal{H}_2$ are spectral subspaces of the total Hamiltonian, i.e., the only states with energy in the specified intervals are states $|0\rangle \otimes |c\rangle$ with $c$ satisfying the considered inequalities. Hence every optimal $U$ has to map $|1\rangle \otimes |0\rangle$ into $\mathcal{H}_2$ since its eigenvalue $p$ is the largest one except from the eigenvalues which have already filled the lower spectral subspace $\mathcal{H}_1$. □

Clearly it is essential for the proof that the heat engine is optimal. Efficient algorithms for suboptimal heat engines are possible. Note that it is is a well-known phenomenon in the theory of NP-complete optimization problems that a slightly relaxed demand on the optimality may already allow efficient approximations [(26)]. To implement a suboptimal heat engine one can implement the few-qubit heat engines considered in Section 6 involving only some of the qubits in the reservoir $B$.

For macroscopic numbers of two-level systems the above complexity theoretic limitations will probably become irrelevant because the amount of energy which is wasted by an efficient suboptimal engine will be negligible compared to the total energy release. The remarks above should only suggest that there is in principle a trade-off between complexity and efficiency of heat engines on a mesoscopic scale even though suboptimal engines with low complexity may be only be a little bit worse.

## 10. CONCLUSIONS

Using several examples of toy heat engines we have shown that there is, on the molecular scale, a strong coincidence between the task of *computation* and the task of *energy extraction* from heat reservoirs. The ability to extract a *maximal* amount of work even requires operations for some systems even solve hard computational problems. Even though suboptimal heat engines may in general not require computationally hard operations we have argued that work extraction from two-level systems with *almost* equal temperatures require *many-qubit* operations. We conclude that heat engines which extract work from reservoirs with similar temperature require relative complex physical processes.

Clearly, we do not expect that future heat engines on the molecular scale will be implemented by the type of gates we have considered. However, the 'Strong Church Turing Thesis' [27,28] states that *any physical device can be simulated by a Turing machine in a number of steps polynomial in the resources used by the computing device*. The quantum version of this replaces the classical Turing machine with a *quantum* Turing machine [29]. Believing in this principle, one should expect that every process implementing a heat engine which solves an NP-complete problem has an efficient simulation on a quantum computer. Provided that one does not believe in efficient quantum algorithms for NP-hard problems, our results indicate therefore that there are complexity-theoretic limitations to the efficiency of heat engines on the molecular scale.

## APPENDIX: INCLUDING THE TARGET SYSTEM

So far we have considered systems which are informationally closed in the sense that only unitary operations are available. At the same time they are not energetically closed since it was exactly our goal to extract energy from the system. Our above justification for such a model was that we do not want to allow the energy sink to *absorb entropy* because this could trivialize the whole problem. The following paradox arises from this justification: the energy extraction in the above unitary heat engines is only a probabilistic phenomenon since they decrease only the *average* energy of the system. Some energy eigenstates of the system are mapped onto states with higher energy and some onto lower energy states. This implies that the energy of the target system is decreased or increased, depending on the state of the system. Such a probabilistic change of the energy of the target increases necessarily its entropy even though this was exactly what we wanted to avoid. Now we show that there are natural situations where this entropy increase is negligible. Let for simplicity the eigenvalues of the system Hamiltonian $H_s$ be some integers and the energy spectrum of the target be $\mathbb{Z}$, i.e., its Hamiltonian $H_t$ on $l^2(\mathbb{Z})$ be given by

$$H_t|j\rangle = j|j\rangle$$

for all $j \in \mathbb{Z}$. Let $U$ be some unitary heat engine permuting energy eigenstates of $H_s$ and $(P_j)$ be a complete set of orthogonal projections on the energy eigenstates of $H_s$. Let $\Delta(j)$ be the energy difference between the eigenvalues corresponding to $P_j$ and to $UP_jU^\dagger$ and $S^k$ be the shift of $l^2(\mathbb{Z})$ defined by

$$S^k|j\rangle = |k+j\rangle\,.$$

Then we define a unitary operation $V$ on the joint Hilbert space

$$\mathcal{H}_s \otimes l^2(\mathbb{Z})\,,$$

of $s$ and $t$ by

$$V := (U \otimes \mathbf{1}) \sum_j P_j \otimes S^{\Delta(j)}\,.$$

One checks easily that $V$ commutes with the joint Hamiltonian

$$H := H_s \otimes \mathbf{1} + \mathbf{1} \otimes H_t\,.$$

Furthermore, we choose an initial state vector $|\psi\rangle \in l^2(\mathbb{Z})$ of the energy sink such that $\langle\psi|S^{\Delta(j)}\psi\rangle \approx 1$ for all possible energy differences $\Delta(j)$. Then the completely positive positive map $G$ given by the partial trace (over the target $t$)

$$G(\rho) := tr_t(V(\rho \otimes |\psi\rangle\langle\psi|)V^\dagger)$$

coincides almost with the unitary operation $\rho \mapsto U\rho U^\dagger$. The reason is that a superposition of all the eigenstates in a large interval of energy values is insensitive to energy increase or decrease and obtains therefore almost no information about the energy gain. An upper bound on the entropy increase of the target system is given as follows. The final target state is a mixture of shifted states $S^{\Delta(j)}|\psi\rangle\langle\psi|S^{-\Delta(j)}$ over all possible energy differences $\Delta(j)$. Given that for this finite set of values $\Delta(j)$ we have

$$\|S^{\Delta(j)}|\psi\rangle\langle\psi|S^{-\Delta(j)} - |\psi\rangle\langle\psi|\,\| \leq \delta\,,$$

the entropy of the mixture is smaller than some $\epsilon(\delta)$ which converges to zero for $\delta \to 0$ because the von-Neumann entropy is continuous in finite dimensions.

These remarks show that the restriction of the energy conserving unitary $V$ to $s$ can indeed approximately be the unitary $U$, when the initial state of the energy sink is a pure state with large energy spread. If the Hilbert space of the energy sink is replaced with $l^2(\mathbb{N}_0)$ the construction of unitaries and initial vectors which yield, by restriction, approximately the unitary $U$ is technically a bit more difficult. A coherent state in quantum optics which has large photon number expectation would be a physical example for a state with large energy spread. We conclude that the unitary heat engine appears as a limit with macroscopic control fields and is therefore a consistent model.

The statement that $V$ does not increase the entropy of $t$ by an considerable amount holds also when the initial state of $t$ is a mixture of energy eigenstates over a large interval of energy values. One checks easily that the restriction of $V$ to $s$ is no longer close to a unitary operation. Instead, it destroys superpositions between all those energy eigenstates with different $\Delta(j)$. Nevertheless it permutes the basis states in the same way as the unitary heat engine $U$ does which implies that it implements the same classical computation steps as the unitary model would do.

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