Driven spin systems as quantum thermodynamic machines: Fundamental limits

Markus J. Henrich* and Günter Mahler
Institute of Theoretical Physics I, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Mathias Michel
Advanced Technology Institute, School of Electronics and Physical Sciences, University of Surrey, Guildford GU2 7XH, United Kingdom

(Received 7 April 2006; revised manuscript received 22 February 2007; published 24 May 2007)

We show that coupled two-level systems like qubits studied in quantum-information processing can be used as a thermodynamic machine. At least three qubits or spins are necessary and they must be arranged in a chain. The system is interfaced between two split baths and the working spin in the middle is externally driven. The machine performs Carnot-type cycles and is able to work as a heat pump or engine depending on the temperature difference of the baths, ΔT, and the energy difference in the spin system, ΔE. It can be shown that the efficiency is a function of ΔT and ΔE.

DOI: 10.1103/PhysRevE.75.051118 PACS number(s): 05.70.Ln, 03.65.−w

I. INTRODUCTION

One of the main goals of thermodynamics has been to study heat engines and thermodynamic processes, dating back to the now famous work of Carnot in 1824 [1]. With the advent of nanophysics and the control of quantum systems down to single atoms, a better understanding of thermodynamics on the basis of quantum mechanics is necessary.

Since the first attempts to analyze thermodynamic machines on the quantum level [2,3], considerable progress has been made in the last decades. Different kinds of models like machines built of harmonic oscillators, uncoupled spins, particles in a potential, or different three-level systems have been studied [4–8].

Also the question about the violation of the second law of thermodynamics in the quantum regime has come up now and then. For a heat engine this would lead to an efficiency larger than the Carnot efficiency. All attempts to do this have failed and could be resolved, e.g., with the help of Maxwell's demon [9].

Two level systems (TLS's) like spins or qubits are the essential ingredients for quantum computation [10]. Much effort has been directed toward control of small clusters and chains of qubits in quantum optical systems [11], nuclear magnetic resonance [12], and solid state systems [13]. A serious problem in any such realization is the interaction of the respective quantum network with its environment.

In the present work we study a model consisting of three TLS's arranged in a chain in contact with two baths of different temperatures as studied for transport scenarios, e.g., in [14–16]. Here, an energy gradient on the system and an incoherent driving of the TLS in the middle let this system act as a thermodynamic machine. For possible experiments the setup may require more TLS's.

Under special conditions the Carnot efficiency may be reached by a TLS heat engine but the efficiency can never go beyond: If the Carnot efficiency is reached the machine flips its function, e.g., from a heat pump to a heat engine.

We start with a discussion of the concepts of work and heat. This is done by considering the change of the energy expection value of a quantum system. With the help of the Gibbs relation, heat can be associated with a change of occupation numbers of a quantum system, whereas work is a change of the spectrum.

We then introduce our thermodynamic machine consisting of three TLS's [17]. Thermodynamic properties can be imparted to this system by an appropriate embedding into a larger quantum environment [18–20], without the need of any thermal bath. In the present context, though, it is much simpler to settle for the open system approach based on a quantum master equation (QME). In Sec. III B the QME used will be introduced.

Our numerical results are detailed in Sec. IV. In Sec. V we compare the numerical investigation with an ideal TLS machine where ideal process steps are assumed. The obtained result is rather general and valid for any kind of TLS machine.

II. THERMODYNAMIC VARIABLES

A. Work and heat

To describe thermodynamic processes and machines, one first has to define the pertinent variables, heat, work, temperature, and entropy, for the system under consideration. Starting from the energy expectation value

$$U = \langle E \rangle = \mathrm{Tr}\{\hat{H}\hat{\rho}\} \tag{1}$$

for a quantum system $\hat{H}$ with discrete spectrum ($\hat{\rho}$ is the density operator) and considering the temporal change of $\langle E \rangle$,

$$\frac{d}{dt}\langle E \rangle = \mathrm{Tr}\left\{\frac{d}{dt}\hat{H}\hat{\rho}\right\} + \mathrm{Tr}\left\{\hat{H}\frac{d}{dt}\hat{\rho}\right\}, \tag{2}$$

change of work W can be associated with the first term of (2) where only the spectrum changes,

*Electronic address: Markus.Henrich@itp1.uni-stuttgart.de

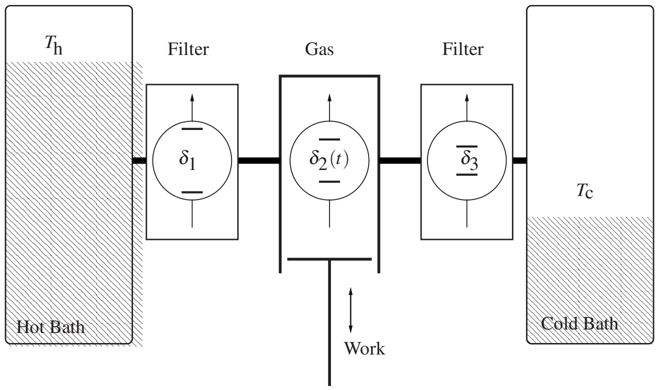

FIG. 1. Schematic representation of the system under investigation. An inhomogeneous three-spin chain is interfaced between two baths. Spin 1 (with energy splitting δ_1) and spin 3 (δ_3) act as filters whereas spin 2 [$\delta_2(t)$] is the working gas by deformation of its spectrum.

$$\frac{d}{dt}W = \mathrm{Tr}\left\{\frac{d}{dt}\hat{H}\hat{\rho}\right\} = \sum_i \dot{E}^i p^i. \tag{3}$$

$\dot{E}^i$ is the change per time of the ith eigenvalue and p^i is the corresponding occupation probability. The change of heat Q is then the second part of (2),

$$\frac{d}{dt}Q = \mathrm{Tr}\left\{\hat{H}\frac{d}{dt}\hat{\rho}\right\} = \sum_i \dot{p}^i E^i. \tag{4}$$

Equation (2) thus boils down to the famous Gibbs relation

$$\Delta U = \Delta W + \Delta Q, \tag{5}$$

where ΔU is the energy change of the system. For cyclic processes, the work ΔW and heat ΔQ can also be calculated with the help of the ST diagram. For a closed path, in the ST plane, $\Delta U=0$ and thus

$$\Delta W = -\Delta Q = -\oint T\, dS. \tag{6}$$

While connected with a bath $\alpha, \Delta Q_\alpha$ can alternatively be calculated from the corresponding heat current J_α over one cycle of duration τ,

$$\Delta Q_\alpha = \int_0^\tau J_\alpha dt. \tag{7}$$

Typically there are two baths $\alpha=h,c$ and thus two contributions (see Fig. 1)

$$\Delta Q = \Delta Q_h + \Delta Q_c. \tag{8}$$

B. Temperature and entropy

The temperature of a system can be defined if the state in the energy eigenbasis is canonical. For a TLS μ, the temperature is given by

$$T_\mu = -\frac{E_\mu^1 - E_\mu^0}{\ln p_\mu^1 - \ln p_\mu^0}, \tag{9}$$

with occupation probability p_μ^i of the energy level E_μ^i. Due to the fact that all coherences will be damped out by the bath, it is always possible to get a local temperature for a single TLS. The von Neumann entropy

$$S_\mu = -\mathrm{Tr}\{\hat{\rho}_\mu \ln \hat{\rho}_\mu\} = -\sum_i p_\mu^i \ln p_\mu^i \tag{10}$$

can then be taken as the thermodynamic entropy.

C. Efficiencies

The efficiency of a heat pump is defined by the ratio of the heat ΔQ_h pumped per cycle to the hot reservoir and the work applied,

$$\eta^p = -\Delta Q_h/\Delta W, \tag{11}$$

which reduces for the Carnot heat pump to

$$\eta^p_{\mathrm{Car}} = T_h/(T_h - T_c). \tag{12}$$

For the heat engine the efficiency is

$$\eta^e = -\Delta W/\Delta Q_h, \tag{13}$$

which in the Carnot case leads to

$$\eta^e_{\mathrm{Car}} = 1 - T_c/T_h. \tag{14}$$

III. DRIVEN SPIN SYSTEM

A. Hamilton model

The model under investigation is an inhomogeneous spin chain with nearest-neighbor coupling of Heisenberg type described by the Hamiltonian

$$\hat{H} = \sum_{\mu=1}^{3}\left\{\frac{\delta_\mu}{2}\hat{\sigma}_\mu^z + \lambda \sum_{i=x,y,z} \hat{\sigma}_\mu^i \otimes \hat{\sigma}_{\mu+1}^i\right\}. \tag{15}$$

The $\hat{\sigma}_\mu^i$'s are the Pauli operators of the μth spin. λ is the coupling strength, which is chosen to be small compared to the local Zeeman splitting δ_μ, $\lambda \ll \delta_\mu$. Because $\delta_\mu \neq \delta_{\mu+1}$, we call the spin chain inhomogeneous.

We will need at least three spins in order to have this system work as a thermodynamic pump or machine. The spin chain is brought into contact locally with two baths at different temperatures as depicted in Fig. 1. The detuning between spin 1 and spin 3 is $\delta_{13}=(\delta_1-\delta_3)/2>0$.

B. Quantum master equation

There are different ways to describe the thermal behavior of quantum systems coupled to environments. Examples are the path integral method [21], or schemes based on the complete Schrödinger dynamics of a small system embedded into a larger quantum environment [18–20]. Because it is much simpler for the present context, we settle for a master equation approach. Such an approach has been widely applied to describe system bath models [22,23].

To derive the master equation for our model, one usually starts from the Liouville–von Neumann equation for the total system (we set $\hbar$ and the Boltzmann constant k_B equal to 1),

$$\frac{d}{dt}\hat{\rho}(t) = -i[\hat{H},\hat{\rho}(t)]. \tag{16}$$

The Hamiltonian is composed of three terms,

$$\hat{H} = \hat{H}_{\mathrm{s}} + \hat{H}_{\mathrm{env}} + \kappa\hat{H}_{\mathrm{int}}, \tag{17}$$

with $\hat{H}_{\mathrm{s}}$ the Hamiltonian of the relevant system, $\hat{H}_{\mathrm{env}}$ the environment or bath Hamiltonian, and $\hat{H}_{\mathrm{int}}$ the interaction of coupling strength κ between system and bath. With the help of a projection operator technique up to second order in κ and with the use of the Born-Markov approximation, the dynamics of the reduced system density $\hat{\rho}_{\mathrm{s}}(t)$ reads

$$\frac{d}{dt}\hat{\rho}_{\mathrm{s}}(t) = -\kappa^2\int_{t_0}^{t} ds\,\mathrm{Tr}_{\mathrm{env}}\{[\hat{H}_{\mathrm{int}}(t),[\hat{H}_{\mathrm{int}}(t-s),\hat{\rho}_{\mathrm{s}}(t)\otimes\hat{\rho}_{\mathrm{env}}]]\}, \tag{18}$$

where $\hat{\rho}_{\mathrm{env}}$ is a fixed state of the environment and $\mathrm{Tr}_{\mathrm{env}}$ denotes the trace over all degrees of freedom of the environment (see [22]).

In general, the interaction Hamiltonian $\hat{H}_{\mathrm{int}}$ is defined as

$$\hat{H}_{\mathrm{int}} = \sum_i \hat{X}_i \otimes \hat{B}_i, \tag{19}$$

where $\hat{X}_i$ operates on the system and $\hat{B}_i$ on the environment. For the coupling with a single spin we take $\hat{X}=\hat{\sigma}^x$. By putting (19) into (18) and going to the Schrödinger picture, the following compact form can be obtained:

$$\frac{d}{dt}\hat{\rho}_{\mathrm{s}} = -i[\hat{H}_{\mathrm{s}},\hat{\rho}_{\mathrm{s}}] + \hat{\mathcal{D}}(\hat{\rho}_{\mathrm{s}}). \tag{20}$$

As in [16] we use the dissipator $\hat{D}(\hat{\rho}_{\mathrm{s}})$,

$$\hat{\mathcal{D}}(\hat{\rho}) = [\hat{X},\hat{R}\hat{\rho}] + [\hat{X},\hat{R}\hat{\rho}]^{\dagger} \tag{21}$$

with

$$\langle l|\hat{R}|m\rangle = \langle l|\hat{X}|m\rangle\Phi(E_l - E_m), \tag{22}$$

suppressing the system label "s" in the following. $\langle l|$ and $|m\rangle$ are system eigenstates with the corresponding energy eigenvalue $E_{l(m)}$. $\Phi(E_l-E_m)=\Phi(\omega_{lm})$ is the bath correlation tensor,

$$\Phi(\omega_{lm}) = \int_0^{\infty} e^{\omega_{lm}s}\langle\hat{B}(s)\hat{B}(0)\rangle ds, \tag{23}$$

containing the bath correlation function

$$\langle\hat{B}(s)\hat{B}(0)\rangle = \mathrm{Tr}_{\mathrm{env}}\{\hat{B}(s)\hat{B}(0)\hat{\rho}_{\mathrm{env}}\}. \tag{24}$$

Assuming that the state of the bath is a thermal one,

$$\hat{\rho}_{\mathrm{env}} = \frac{e^{-\beta\hat{H}_{\mathrm{env}}}}{Z_{\mathrm{env}}} \tag{25}$$

(Z_{env} being the partition function), and that the bath consists of uncoupled harmonic oscillators, $\Phi(\omega_{lm})$ takes the form

$$\Phi(\omega_{lm}) = \kappa\left(\frac{\theta(\omega_{lm})}{\mathrm{e}^{\omega_{lm}\beta_\alpha}-1} + \theta(\omega_{ml})\frac{\mathrm{e}^{\omega_{ml}\beta_\alpha}}{\mathrm{e}^{\omega_{ml}\beta_\alpha}-1}\right). \tag{26}$$

$\theta(\omega_{lm})$ is the step function and β_α the respective inverse bath temperature.

For a three-spin chain between two heat baths of different temperatures T_h and T_c and local coupling at the two chain boundaries with

$$\hat{X}_h = \hat{\sigma}_1^x \otimes \hat{1}_2 \otimes \hat{1}_3, \tag{27}$$

$$\hat{X}_c = \hat{1}_1 \otimes \hat{1}_2 \otimes \hat{\sigma}_3^x, \tag{28}$$

we get instead of (20) (cf. [16])

$$\frac{d}{dt}\hat{\rho} = -i[\hat{H},\hat{\rho}] + \hat{\mathcal{D}}_h(\hat{\rho}) + \hat{\mathcal{D}}_c(\hat{\rho}). \tag{29}$$

The stationary state of (20) for fixed δ_μ is easily shown to be canonical of the form $\hat{\rho}^{\mathrm{stat}}=e^{-\beta\hat{H}_{\mathrm{s}}}/\mathrm{Tr}\{e^{-\beta\hat{H}_{\mathrm{s}}}\}$. However, with both baths in place, the spin chain might be viewed as a molecular bridge generating a stationary leakage current $J_L=J_h=-J_c$. Here the heat current J_α between the three-spin system and the bath α can be defined by the energy dissipated via bath α (cf. [22])

$$J_\alpha = \mathrm{Tr}\{\hat{H}\hat{\mathcal{D}}_\alpha(\hat{\rho})\}. \tag{30}$$

In the following a current out of the bath α into the machine will be defined as positive.

IV. NUMERICAL RESULTS

A. Nonequilibrium stationary states of a spin chain

First we note that the heat current through a spin chain depends on the local Zeeman splittings within the system. To analyze the heat current we solve (29) and calculate the stationary state of the system $\hat{\rho}^{\mathrm{stat}}$. With this solution and with the help of (30) we can then calculate the currents J_α for each bath.

We consider a system with $\delta_1=\delta_3=1$. Both heat currents (30) as function of δ_2 are shown in Fig. 2. J_h is positive and the relation $J_h=-J_c$ is satisfied. If $\delta_2=\delta_1=\delta_3$ (the homogeneous case) the heat currents reach their maximum. By detuning the local energy splitting it is thus possible to uncouple the respective bath from the rest of the system. This resonance effect will now be used to build out of three spins a quantum thermodynamic machine.

B. Time-dependent behavior: Spin system as thermodynamic heat pump or machine

1. The heat current

The above situation changes when the energy splitting of spin 2 is chosen to be time dependent, i.e.,

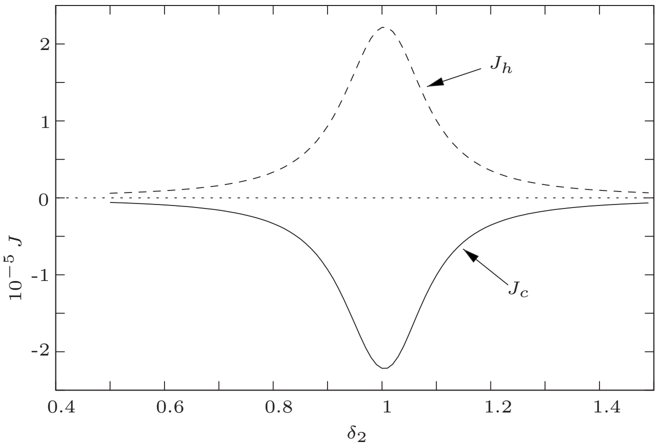

FIG. 2. Stationary heat current J_h [see (30)] (from hot bath) and J_c (to cold bath) as a function of the local energy splitting δ_2 of spin 2 with $\delta_1=\delta_3=1$, $T_h=2.63$, and $T_c=2.5$.

$$\delta_2(t) = \sin(\omega t)b + b_0. \tag{31}$$

Different energy splittings of the boundary spins, e.g., $\delta_1=2.25$ and $\delta_3=1.75$, are used to install left- and right-selective resonance effects. The parameters of (31) are chosen as $b_0=(\delta_1+\delta_3)/2$ and b is the detuning δ_{13}. To enable the bath to damp the system, $\omega \ll \delta_2$ must be satisfied.

For solving (29) we have used a four-step Runge-Kutta algorithm. At each time step the bath correlation function is calculated explicitly. We choose the following parameters for our numerical results: $\lambda=0.01$, $\kappa=0.001$, $\delta_1=2.25$, $\delta_3=1.75$, $\omega=1/128$, $T_c=2.5$, and T_h is varied, unless stated otherwise. Both coupling parameters λ and κ are chosen to stay in the weak coupling limit.

Now when spin 2 is driven periodically as in (31), we can distinguish four different steps.

(1) Spin 2 (the "working gas") is in resonance with spin 3 [$\delta_2(t)\approx\delta_3$] and thus couples with bath c at temperature T_c. Because of this energy resonance, the current J_c via spin 3 will be large, whereas the current J_h via spin 2 will be negligible. The occupation probabilities of spins 2 and 3 approach each other, and so do the respective local temperatures.

(2) A quasiadiabatic step: Spin 2 is out of resonance with spin 3 [$\delta_1>\delta_2(t)>\delta_3$]; now J_c is suppressed while J_h stays nearly unchanged. The occupation probability of spin 2 does not change significantly and there is almost no change in the entropy S_2.

(3) Spin 2 is in resonance with spin 1 [$\delta_2(t)\approx\delta_1$] and by that in contact with bath h at temperature T_h. J_h is large whereas J_c is very small. The local temperatures of spin 1 and 2 nearly equal each other.

(4) A quasiadiabatic step, as in step 2.

Figure 3 shows the heat currents J_α of both baths over one period with the bath temperatures $T_h=2.63$ and $T_c=2.5$. As can be seen, the resonance effect decouples spin 2 from the bath if its energy splitting is different from the boundary or filter spins. This decoupling is never perfect, though. As a consequence there is a leakage current J_L which will be discussed in more detail later on.

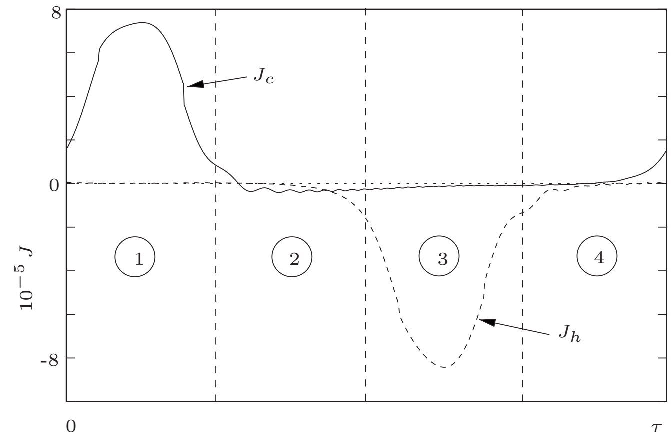

FIG. 3. Heat currents $J_\alpha(t)$ for the heat pump over one cycle with duration $\tau=2\pi/\omega=804.25$ for $T_h=2.63$ and $T_c=2.5$. The peaks are a result of the resonance effect.

2. Heat, work, and efficiencies

That the studied system indeed works as a heat pump can be seen from the S_2T_2 diagram of spin 2 in Fig. 4. The local entropy S_2 of spin 2 is given by (10) and the local temperature T_2 by (9). The four different steps as explained in Sec. IV B 1 are shown, as well as the direction of circulation.

To determine the efficiency of this heat pump one needs to know the quantity of heat ΔQ_h pumped to the hot bath and the used work ΔW. ΔQ_h can be calculated by integrating the heat current J_h over one period [cf. (7)].

The exchanged work ΔW is given by the area enclosed in the S_2T_2 plane according to (6). We find that indeed $\Delta W+\Delta Q_c+\Delta Q_h=0$ in all cases, and by that confirm the use of T_2 and S_2 as effective thermodynamic variables.

In contrast to the Carnot model, our machine is working in finite time. If driven too fast the bath is not able to damp the system, and if driven too slowly (quasistationary) the system reaches its momentary steady state transport configuration (i.e., $\omega \ll \kappa$). The S_2T_2 area then vanishes as depicted in Fig. 5. This is caused by the leakage current.

Figure 6 shows the Carnot efficiency for the heat pump η^p_{Car} and the machine η^e_{Car} and the respective efficiencies for

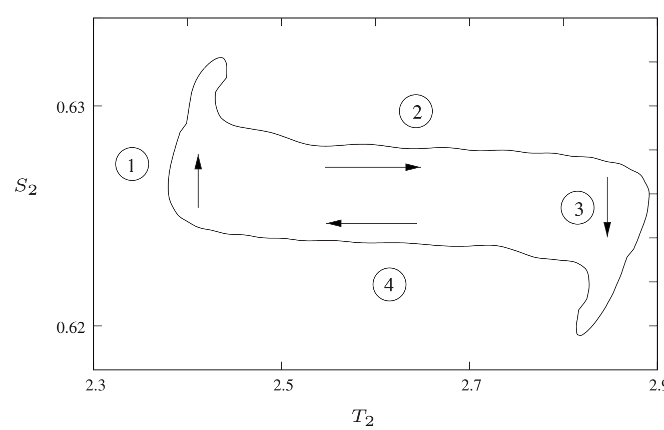

FIG. 4. S_2T_2 diagram for the quantum heat pump for $T_h=2.63$, $T_c=2.5$ ($\Delta T=0.13$), and $\tau=2\pi/\omega=804.25$. The arrows indicate the direction of circulation.

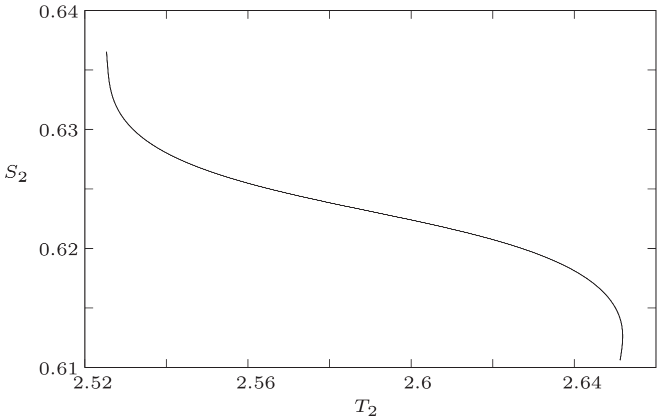

FIG. 5. S_2T_2 diagram for the quasistatically driven quantum heat pump (with parameters as in Fig. 4). Because of the leakage current the enclosed S_2T_2 area vanishes and no work is exchanged.

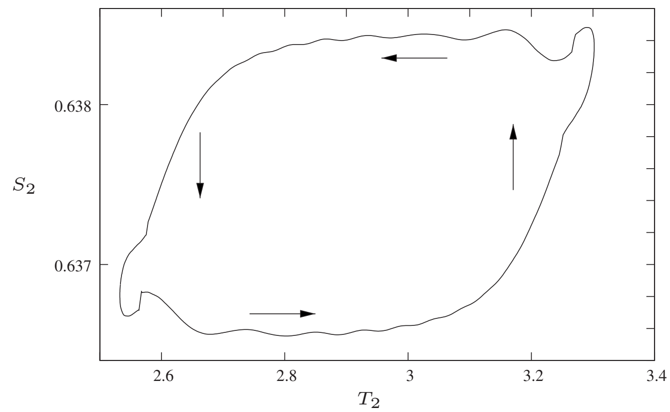

FIG. 7. S_2T_2 diagram for the quantum heat engine ($\Delta T=0.83>\Delta T_{\max}$ with $T_h=3.33$, $T_c=2.5$, and $\tau=2\pi/\omega=804.25$). The arrows indicate the direction of circulation.

our quantum heat pump η^p_{qm} [according to (11)] and machine η^e_{qm} [according to (13)] as a function of the temperature difference $\Delta T=T_h-T_c$. We point out the following interesting findings.

(1) The efficiency curve of the quantum heat pump or machine is always below the respective Carnot efficiency. As expected, the second law is never violated.

(2) For $\Delta T=0$, η^p_{qm} neither diverges nor goes to zero. This means that the machine can start out of equilibrium and begin to cool a reservoir.

(3) At a specific temperature difference ΔT, here $\Delta T_{\max}\approx 0.6$, the heat pump switches to operate as a heat engine. To illustrate this fact Fig. 7 shows the area in the S_2T_2 plane for $\Delta T=3.33>\Delta T_{\max}$. As depicted, the direction of circulation has reversed.

To make the last point more plausible Fig. 8 shows the work ΔW and the heat Q_h and Q_c as functions of ΔT. While ΔT is increasing, ΔQ_h and ΔQ_c are decreasing, as well as ΔW, until first ΔQ_c changes its sign, then Q_h, and last ΔW. At the point where $\Delta W=0$ (for $\Delta T=\Delta T_{\max}$) only the leakage current J_L is flowing from the hot bath to the cold one. Beyond this $\Delta T_{\max}$ the system starts to work as an engine.

V. ANALYTICAL RESULTS

A. Ideal quantum machine

To understand the above numerical results we compare them to the maximal reachable heat and work that could be pumped or extracted by a TLS quantum machine. All process steps will be taken to be ideal steps. By "ideal" we mean that we have total control of each process step. Then no leakage current will disturb the system and the heat exchange at bath contact will be without loss.

In addition, we assume a machine that only works during the adiabatic steps. Heat will be exchanged only if the machine is in contact with a bath. This can be compared with the Otto cycle [6,24].

We start with spin 2 in contact with spin 3 and thus with cold bath. The state of spin 2 after this contact is a canonical one of the form

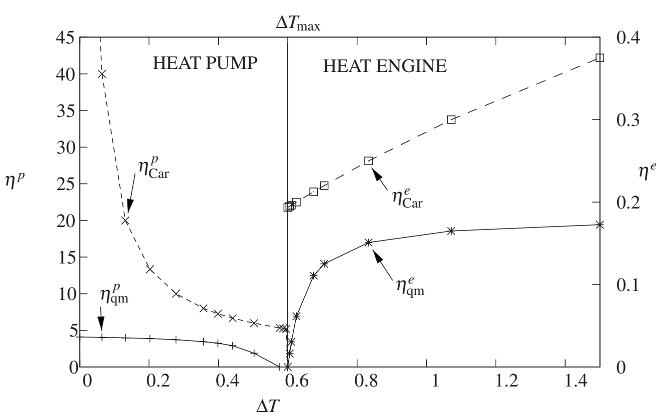

FIG. 6. Carnot efficiency η^p_{Car} and efficiency η^p_{qm} of the quantum heat pump ($\Delta T<\Delta T_{\max}$) and η^e_{Car} and η^e_{qm} of the heat engine ($\Delta T>\Delta T_{\max}$) as functions of the temperature difference ΔT. The following parameters are chosen: $T_c=2.5$, $\delta_1=2.25$, $\delta_3=1.75$, and $\tau=2\pi/\omega=804.25$.

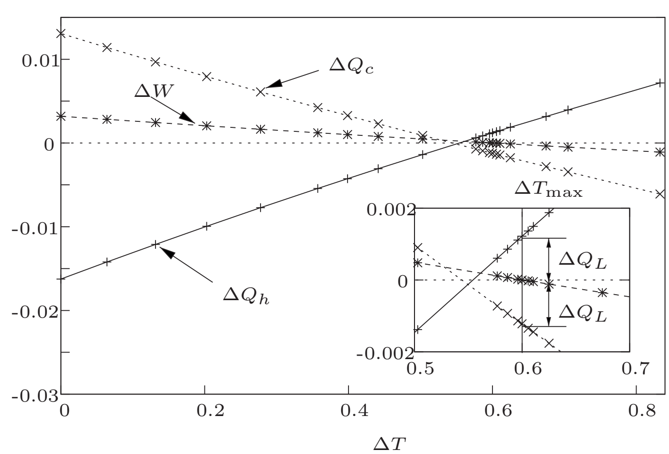

FIG. 8. Heat ΔQ_c and ΔQ_h and work ΔW performed over one cycle as function of the temperature difference ΔT (same parameters as in Fig. 6). The inset shows these functions around the point $\Delta T=\Delta T_{\max}$ in more detail. ΔQ_L is the leakage heat per cycle.

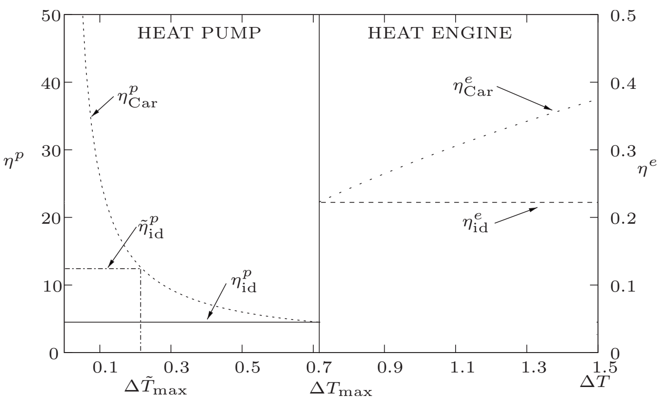

FIG. 9. Carnot efficiency $\eta^p_{\rm Car}$ for the heat pump and engine $\eta^e_{\rm Car}$ as functions of temperature difference ΔT while $T_c=2.5$, $\delta_1=2.25$, and $\delta_3=1.75$ as in Fig. 6. $\eta^p_{\rm qm}$ and $\eta^e_{\rm qm}$ are the efficiencies of the ideal pump and engine [see (39) and (40)]. $\tilde{\eta}^p_{\rm id}=12.36$ and $\Delta\tilde{T}_{\rm max}=0.22$ can be realized for $\delta_1=1.904$, $\delta_3=1.75$, and $T_c=2.5$.

$$\hat{\rho}_{\rm s}=\frac{1}{Z}\begin{pmatrix} e^{\delta_3/(2T_c)} & 0 \\ 0 & e^{-\delta_3/(2T_c)} \end{pmatrix}. \tag{32}$$

Z is the partition function and we have assumed that the energy of the ground state is $E_2^0=E_3^0=-\delta_3/2$ and of the excited state $E_2^1=E_3^1=\delta_3/2$, because both spins are in resonance.

After this equilibration with the cold bath at T_c, the spin 2 is driven until its local energy splitting is equal to that of spin 1 ($E_2^0=E_1^0=-\delta_1/2$ and $E_2^1=E_1^1=\delta_1/2$). The work for this step can be calculated with (3). This step is adiabatic as $\hat{\rho}_2$ does not change. The work $W_{3\to 1}$ is then given by the energy difference before and after reaching the splitting of spin 1,

$$W_{3\to 1}=\frac{1}{2}(\delta_3-\delta_1)\tanh\left(\frac{\delta_3}{2T_c}\right). \tag{33}$$

In contact with spin 1, spin 2 exchanges heat $\Delta Q_h^{\rm id}$ with the hot bath at T_h. No work will be done and only the occupation probabilities of spin 2 will change to a thermal state with $T_2=T_h$. The exchanged heat can be calculated by the energy difference before and after thermalization,

$$\Delta Q_h^{\rm id}=-\frac{1}{2}\delta_1\left[\tanh\left(\frac{\delta_1}{2T_h}\right)-\tanh\left(\frac{\delta_3}{2T_c}\right)\right]. \tag{34}$$

Then spin 2 is driven back to the energy splitting of spin 3 ($E_2^0=E_3^0=\delta_3/2$ and $E_2^1=E_3^1=\delta_3/2$). The work $W_{1\to 3}$ for this step is given by

$$W_{1\to 3}=\frac{1}{2}(\delta_1-\delta_3)\tanh\left(\frac{\delta_1}{2T_h}\right). \tag{35}$$

Finally, the heat $Q_c^{\rm id}$

$$\Delta Q_c^{\rm id}=-\frac{1}{2}\delta_3\left[\tanh\left(\frac{\delta_3}{2T_c}\right)-\tanh\left(\frac{\delta_1}{2T_h}\right)\right] \tag{36}$$

will be exchanged with the cold bath via spin 3. The total work $\Delta W_{\rm tot}$ is given by

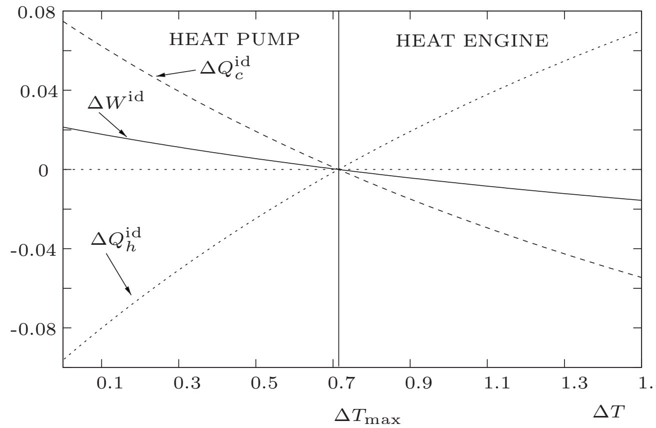

FIG. 10. Work $\Delta W^{\rm id}$ and heat $\Delta Q_h^{\rm id}$ from (to) the hot bath and heat $\Delta Q_c^{\rm id}$ from (to) the cold bath for the ideal machine as functions of temperature difference ΔT, while $T_c=2.5$, $\delta_1=2.25$, and $\delta_3=1.75$ as in Fig. 8. At $\Delta T=\Delta T_{\rm max}$ $\eta^p_{\rm id}=\eta^{p(e)}_{\rm Car}$ and therefore $\Delta W^{\rm id}=0$, $\Delta Q_h^{\rm id}=0$, and $\Delta Q_c^{\rm id}=0$.

$$\Delta W_{\rm tot}=W_{3\to 1}+W_{1\to 3}. \tag{37}$$

The Gibbs relation

$$\Delta W_{\rm tot}+\Delta Q_h^{\rm id}+\Delta Q_c^{\rm id}=0 \tag{38}$$

can easily be verified.

With the help of (33)–(37) it is now possible to calculated the efficiency of this ideal machine. For the heat pump we get

$$\eta^p_{\rm id}=-\frac{\Delta Q_h^{\rm id}}{\Delta W_{\rm tot}}=\frac{\delta_1}{\delta_1-\delta_3}, \tag{39}$$

and for the machine

$$\eta^e_{\rm id}=-\frac{\Delta W_{\rm tot}}{\Delta Q_h^{\rm id}}=\frac{\delta_1-\delta_3}{\delta_1}. \tag{40}$$

This result is similar to that obtained by Kieu [9,25] and is the maximum a TLS can reach. Here we want to compare the efficiencies of the ideal pump $\eta^p_{\rm id}$ and engine $\eta^e_{\rm id}$ with the respective Carnot efficiencies for the parameters used for our numerical results.

Figure 9 shows the Carnot efficiencies as well as the one from (39) and (40). $\eta^{p(e)}_{\rm id}$ is always below $\eta^{p(e)}_{\rm Car}$ until it reaches a maximal temperature difference $\Delta T_{\rm max}$ (with $T_c=2.5$, $\delta_1=2.25$, and $\delta_3=1.75$, we get $\Delta T_{\rm max}=0.714$). At this temperature the heat pump is working losslessly and no heat can be pumped. Just like the quasistationary Carnot heat pump, this pump has zero power. Only in this particular case does $\eta^p_{\rm id}=\eta^p_{\rm Car}$. By further increasing the temperature T_h the heat pump starts working as a heat engine.

Figure 10 illustrates this behavior where $\Delta W^{\rm id}$, $\Delta Q_h^{\rm id}$, and $\Delta Q_c^{\rm id}$ are depicted as functions of ΔT. At $\Delta T_{\rm max}$ no heat $\Delta Q_h^{\rm id}$ is pumped and therefore no work used or heat exhausted to do work.

This is qualitatively the same behavior as our model shows in Figs. 6 and 8. Two differences can be seen. First, the critical temperature in our numerical result deviates from

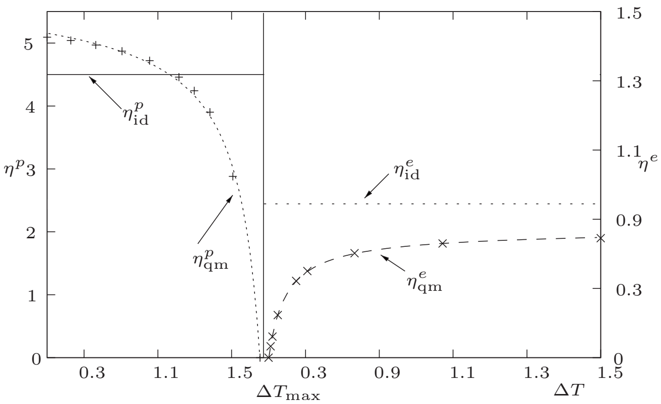

FIG. 11. Fitted efficiency $\eta^p_{\rm qm}$ for the quantum heat pump and quantum engine $\eta^e_{\rm qm}$ as a function of temperature difference ΔT while $T_c=2.5$, $\delta_1=2.25$, and $\delta_3=1.75$ as in Fig. 6. $\eta^p_{\rm id}$ and $\eta^e_{\rm id}$ are the efficiencies of the ideal pump and engine [see (39) and (40)].

the theoretically expected one. From the numerics we get $\Delta T_{\rm max}\approx 0.6$. Second, the inset in Fig. 8 shows that ΔQ_c changes its sign before ΔQ_h does. The reason for both effects is the leakage current as will be explained below.

For a given bath temperature (like, in our example, $T_c=2.5$) it is possible by changing the energy splittings of δ_1 and/or δ_3 to influence $\Delta T_{\rm max}$. In Fig. 9 also a different efficiency $\tilde{\eta}^p_{\rm id}$ is depicted. $\tilde{\eta}^p_{\rm id}$ can be realized by increasing δ_1 so that $\Delta T_{\rm max}$ will be decreased to $\Delta\tilde{T}_{\rm max}$.

B. Quantum machine with leakage current

The efficiency of an ideal two-level quantum machine is independent of ΔT except at $\Delta T=\Delta T_{\rm max}$, where it jumps between its heat pump and its heat engine value. The efficiency obtained from the numerical simulation deviates somewhat from this expected behavior. For the heat pump the efficiency of our model is even larger than the ideal one (see Fig. 11). To understand this effect we analyze the leakage current from a phenomenological point of view.

First, we assume that the leakage current causes the gas spin 2 to approach a thermal state that is not in accordance with the bath temperature. In this case ΔQ_h and ΔQ_c will be decreased. This effect is responsible for the vanishing of $\eta^{p(m)}_{\rm qm}$ before reaching $\Delta T_{\rm max}$. But it cannot explain why the efficiency $\eta^p_{\rm qm}$ is sometimes larger than $\eta^p_{\rm id}$.

Taking into account that also less work is performed due to the leakage current, it is possible to find a larger efficiency. This can be interpreted in that the gas spin 2 does not "see" the full energy splitting δ_1. As shown in Fig. 11 our phenomenological model fits the numerical data quite well.

For the efficiency of the heat engine, $\eta^e_{\rm qm}$, it can be seen from Fig. 11 that it is always worse than that of the ideal engine, $\eta^p_{\rm id}<\eta^e_{\rm qm}$.

VI. CONCLUSION

We have studied a driven three-spin system coupled to two split heat baths. We have shown that such small quantum networks may be used not only as quantum-information processors but also as quantum thermodynamic machines. For the latter proposal we would primarily exploit the (time-dependent) deformation of discrete spectra and associated resonance transfer.

While interesting functionality appears already for $N=3$ spins, larger spin networks subject to such very limited control could also be envisaged without losing inherent stability: eventually this stability is dictated by the increase of entropy, i.e., by the second law of thermodynamics.

For a thermodynamic TLS machine working with ideal heat transport and adiabatic steps, we have derived an ideal efficiency. This efficiency is independent of the bath temperatures. By tuning the energy splitting of the TLS, the quantum thermodynamic machine can be used as a heat pump or heat engine. The Carnot efficiency will be reached only when a TLS machine is working losslessly.

Taking dissipation into account, it is possible to understand the leakage current present in our numerics from a phenomenological point of view. Surprisingly, a leakage current could even increase the efficiency of a heat pump, whereas for a heat engine it only decreases the efficiency.

There are a number of different options for implementations [26,27] and also various possibilities for introducing time-dependent control. For simplicity we have restricted ourselves here to external driving; alternatively, one might look for autonomous system designs [28], e.g., by using a mechanical oscillator (cantilever) [29]. Artificial autonomous nanomotors powered by visible light have recently been demonstrated experimentally [30].

From a fundamental point of view several interesting questions remain. What is the status of thermodynamic variables for such quantum systems? To what extent are these measurable in the nanodomain, without being operators? And, if measured, how would the measurement result fluctuate [31]?

As noted already, a two-level system diagonal in its local energy basis can always be described as canonical with some temperature T, i.e., there is conceptually no space for nonequilibrium here. It is remarkable that for periodic operation work can then be associated with the area defined by the closed path in the effective entropy-temperature plane for the driven spin, as in macroscopic models.

This may challenge the subjective-ignorance interpretation of nonpure states as classical mixtures, i.e., assuming the individual spin to be either up or down at any time. If the thermal state was taken to result from quantum entanglement with the environment [18], this classical picture would no longer be needed; those concepts from quantum information seem to be more appropriate here.

ACKNOWLEDGMENTS

We thank J. Gemmer, F. Rempp, G. Reuther, H. Schmidt, H. Schröder, J. Teifel, P. Vidal, and H. Weimer for fruitful discussions. We thank the Deutsche Forschungsgemeinschaft for financial support.

[1] S. Carnot, *Refléctions sur la Puissance Motrice du Feu et sur les Machines Propres à Développer Cette Puissance* (Bachlier, Paris, 1824).
[2] E. Geusic, E. Schultz-Duboi, and H. Scovil, Phys. Rev. **156**, 262 (1967).
[3] H. Scovil and E. Schultz-Dubois, Phys. Rev. Lett. **2**, 262 (1959).
[4] A. E. Allahverdyan, R. S. Gracia, and T. M. Nieuwenhuizen, Phys. Rev. E **71**, 046106 (2005).
[5] C. M. Bender, D. C. Brody, and B. K. Meister, J. Phys. A **33**, 4427 (2000).
[6] T. Feldmann and R. Kosloff, Phys. Rev. E **68**, 016101 (2003).
[7] J. P. Palao, R. Kosloff, and J. M. Gordon, Phys. Rev. E **64**, 056130 (2001).
[8] D. Segal and A. Nitzan, Phys. Rev. E **73**, 026109 (2006).
[9] T. D. Kieu, Eur. Phys. J. D **39**, 115 (2006).
[10] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).
[11] J. I. Cirac and P. Zoller, Nature (London) **404**, 579 (2000).
[12] N. A. Gershenfeld and I. L. Chuang, Science **275**, 350 (1997).
[13] Y. Makhlin and G. Schön, Nature (London) **398**, 305 (1999).
[14] M. Michel, J. Gemmer, and G. Mahler, Eur. Phys. J. B **42**, 555 (2004).
[15] M. Michel, M. Hartmann, J. Gemmer, and G. Mahler, Eur. Phys. J. B **34**, 325 (2003).
[16] K. Saito, S. Takesue, and S. Miyashita, Phys. Rev. E **61**, 2397 (2000).
[17] M. J. Henrich, M. Michel, and G. Mahler, Europhys. Lett. **76**, 1057 (2006).
[18] J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamcis—Emergence of Thermodynamic Behavior within Composite Quantum Systems*, Lecture Notes in Physics Vol. 657 (Springer, Berlin, 2005).
[19] M. J. Henrich, M. Michel, M. Hartmann, G. Mahler, and J. Gemmer, Phys. Rev. E **72**, 026104 (2005).
[20] M. Michel, G. Mahler, and J. Gemmer, Phys. Rev. Lett. **95**, 180602 (2005).
[21] U. Weiss, *Quantum Dissipative Systems*, 2nd ed. (World Scientific, Singapore, 1999).
[22] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
[23] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II* (Springer, Berlin, 1985).
[24] T. Feldmann and R. Kosloff, Phys. Rev. E **70**, 046110 (2004).
[25] T. D. Kieu, Phys. Rev. Lett. **93**, 140403 (2004).
[26] H. Häfner *et al.*, Nature (London) **438**, 643 (2005).
[27] Y. Maklin, G. Schön, and A. Shnirman, Rev. Mod. Phys. **73**, 357 (2001).
[28] F. Tonner and G. Mahler, Phys. Rev. E **72**, 066118 (2005).
[29] K. C. Schwab and M. L. Roukes, Phys. Today **58**(7), 36 (2005).
[30] V. Balzani *et al.*, Proc. Natl. Acad. Sci. U.S.A. **103**, 1178 (2006).
[31] M. Esposito and S. Mukamel, Phys. Rev. E **73**, 046129 (2006).