Entanglement boost for extractable work from ensembles of quantum batteries

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Motivated by the recent interest in thermodynamics of micro- and mesoscopic quantum systems we study the maximal amount of work that can be reversibly extracted from a quantum system used to temporarily store energy. Guided by the notion of passivity of a quantum state we show that entangling unitary controls extract in general more work than independent ones. In the limit of a large number of copies one can reach the thermodynamical bound given by the variational principle for the free energy.

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I. MOTIVATION

The recent interest in models of quantum engines and refrigerators stimulates theoretical efforts to precisely formulate fundamental thermodynamical principles and bounds valid on the micro- and nanoscale. In principle these can differ from the standard ones and converge to them only in the limit of macroscopic systems. A sample of references, including both general considerations and particular models, is given in Ref. [1].

This paper is about the amount of work that can be extracted from a small quantum mechanical system that is used to temporarily store energy to transfer it from a production to a consumption center. To do so we are not coupling such a quantum battery to external thermal baths in order to drive thermodynamical engines (see, for example, [2]) but we address it by controlling its dynamics by external time-dependent fields. The battery comes with its initial state ρ and own internal Hamiltonian H. The idealized process of reversible energy extraction is then governed by the system dynamics plus some fields that are only turned on during a certain interval $[0,\tau]$ of time. This leads to a time-dependent unitary dynamics of the battery. We now wonder about the maximal amount of work that can be extracted by such a process.

It has been known for a long time that some states cannot deliver work in this way. Such states are called passive [3,4]. The maximal amount of work extractable from a battery is then the surplus energy of the initial state with respect to the passive state σ_ρ with the same eigenvalues as ρ.

Because we are dealing with small quantum systems we may wonder whether using processes that entangle two identical copies of a given battery can yield a higher energy extraction. More generally, what happens to a large number of copies?

We numerically demonstrate that the efficiency of energy extraction grows with the number of copies. Next we show rigorously that the maximal amount of extractable energy per battery asymptotically equals the energy difference between the initial state ρ of the battery and the energy of the Gibbs state $\omega_{\overline{\beta}}$ with the same entropy as ρ. We indicate how to construct in principle a unitary that achieves this optimal bound.

II. GENERAL CONTEXT

The Hilbert space $\mathcal{H}$ of wave functions of the battery is for simplicity chosen to be d dimensional and we pick as standard basis for $\mathcal{H}$ the eigenvectors of the system Hamiltonian

$$H = \sum_{j=1}^{d} \epsilon_j \, |j\rangle\langle j| \quad \text{with} \quad \epsilon_{j+1} > \epsilon_j. \tag{1}$$

We assume here that the energy levels are nondegenerate, which holds for a generic Hamiltonian.

The time-dependent fields that will be used to extract energy from the battery are described by $V(t) = V^\dagger(t)$ where $V(t)$ is possibly only different from zero for $0 \leqslant t \leqslant \tau$. The initial state of the battery is described by a density matrix ρ and the time evolution of ρ is obtained from the Liouville-von Neumann equation

$$\frac{d}{dt}\,\rho(t) = -i[H + V(t), \rho(t)], \quad \rho(0) = \rho. \tag{2}$$

The work extracted by this procedure is then

$$W = \mathrm{Tr}(\rho H) - \mathrm{Tr}[\rho(\tau) H], \tag{3}$$

where the state at time τ is related to the initial state ρ by a unitary transformation

$$\rho(\tau) = U(\tau)\,\rho\,U^\dagger(\tau), \tag{4}$$

with $U(t)$ the time-ordered exponential of the total Hamiltonian $H + V(t)$:

$$U(\tau) = \mathrm{Texp}\left(-i \int_0^\tau ds\, [H + V(s)] \right). \tag{5}$$

Note that by a proper choice of controlling term V any unitary U can be obtained for $U(\tau)$. Therefore the maximal amount of extractable work (called *ergotropy* in [5]) can be defined as

$$W_{\max} := \mathrm{Tr}(\rho H) - \min \mathrm{Tr}(U\,\rho\,U^\dagger H), \tag{6}$$

where the minimum is taken over all unitary transformations of $\mathcal{H}$.

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Following Pusz and Woronowicz [3] and Lenard [4], we call a state σ passive if no work can be extracted from σ, i.e., if for all unitaries U

$$\mathrm{Tr}(\sigma H) \leqslant \mathrm{Tr}(U\,\sigma\,U^{\dagger}H).$$

The following theorem then holds:

Theorem 1 [3,4]. σ is passive if and only if

$$\sigma = \sum_{j=1}^{d} s_j\,|j\rangle\langle j| \quad \text{with} \quad s_{j+1} \leqslant s_j. \tag{7}$$

In other words, σ is passive if and only if it commutes with the system Hamiltonian and its eigenvalues are nonincreasing with the energy. Given ρ there is a unique passive state σ_ρ minimizing $\mathrm{Tr}(U\,\rho\,U^{\dagger}H)$. This state is obtained by a unitary rotation of ρ denoted by U_ρ and has the form

$$\sigma_\rho = U_\rho\,\rho\,U_\rho^{\dagger} = \sum_{j=1}^{d} r_j\,|j\rangle\langle j|, \tag{8}$$

where $\{r_j\}$ are the eigenvalues of ρ arranged in nonincreasing order: $r_{j+1} \leqslant r_j$. The corresponding minimal energy is $\sum_{j=1}^{d} r_j\epsilon_j$ and the maximal amount of extractable work is given by

$$W_{\max} := \mathrm{Tr}(\rho H) - \mathrm{Tr}(\sigma_\rho\,H). \tag{9}$$

III. A GENERAL BOUND ON AVAILABLE WORK

We obtain here a bound on $W_{\max}$ by comparing the energies of the passive state σ_ρ and of the canonical Gibbs state $\omega_{\overline{\beta}}$ with the same entropy as ρ. Recall that the canonical Gibbs state at inverse temperature β is given by

$$\omega_\beta = \frac{\exp(-\beta H)}{\mathcal{Z}}, \tag{10}$$

and that its von Neumann entropy is strictly monotonically decreasing in β with range $[0, \ln d]$. The von Neumann entropy $S(\rho)$ of a density matrix ρ is

$$S(\rho) = -\mathrm{Tr}\rho\log\rho. \tag{11}$$

For any given density matrix ρ on $\mathcal{H}$ there exists therefore a unique inverse temperature $\overline{\beta}$ such that $S(\rho) = S(\omega_{\overline{\beta}})$. The relation between ρ and $\overline{\beta}$ is, of course, highly nonlinear.

We now use the variational principle of statistical mechanics that asserts that the Gibbs canonical density matrix is that which minimizes the free energy:

$$\mathrm{Tr}(\rho H) - \overline{\beta}^{-1}\,S(\rho) \geqslant \mathrm{Tr}(\omega_{\overline{\beta}}\,H) - \overline{\beta}^{-1}\,S(\omega_{\overline{\beta}}). \tag{12}$$

With our choice of $\overline{\beta}$ we obtain that

$$\mathrm{Tr}(\rho H) \geqslant \mathrm{Tr}(\sigma_\rho H) \geqslant \mathrm{Tr}(\omega_{\overline{\beta}}\,H), \tag{13}$$

and hence the thermodynamical bound on the available work is

$$W_{\max} \leqslant \mathrm{Tr}(\rho\,H) - \mathrm{Tr}(\omega_{\overline{\beta}}\,H). \tag{14}$$

Generally, $\omega_{\overline{\beta}}$ is different from σ_ρ because $\omega_{\overline{\beta}}$ and σ_ρ or ρ have different eigenvalues. Note, however, that the two-dimensional case is exceptional because there is a one-to-one correspondence between the entropy of a qubit state and its ordered eigenvalues. Generally it is not true that a product of two independent copies of a passive state still is passive. It is therefore possible, for several copies of a system, to extract more work per copy than the amount given in Eq. (9). In other words, by using entangling unitaries, one can in principle beat Eq. (9).

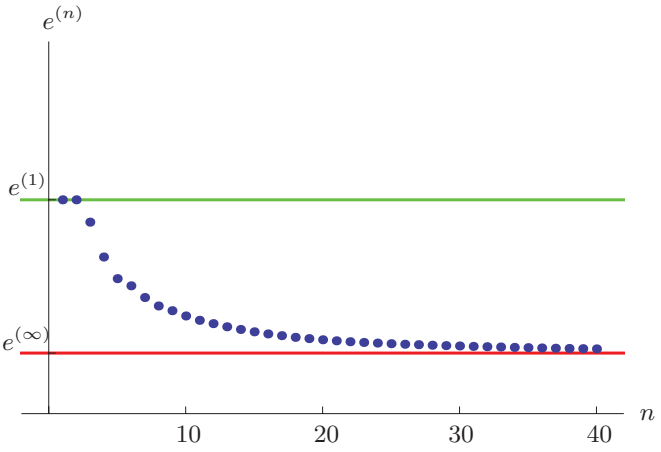

FIG. 1. (Color online) Energy per copy of passive state $\sigma_{\otimes^n\rho}$ associated with $\otimes^n\rho$.

In Fig. 1 the energies $e^{(n)}$ per copy of the passive state $\sigma_{\otimes^n\rho}$ obtained from a product state $\otimes^n\rho$ are plotted as dots for $n = 1,2,\ldots,40$. The lower line shows the asymptotic value of $e^{(n)}$. The system is a three-level battery with energy levels $\{0,0.579,1\}$, and the passive state corresponding to the initial density matrix has eigenvalues $\{0.538,0.237,0.224\}$. The values $e^{(n)}$ have been obtained by rearranging the eigenvalues of $\otimes^n\rho$ and the n-copy Hamiltonian $H^{(n)}$, see Eq. (15). The maximal additional work that can be extracted on top of the single copy extractable work using entangling unitaries is the difference between $e^{(1)}$ and $e^{(\infty)}$. We will compute this value in the next section.

IV. ENTANGLING BATTERIES

A state σ is called completely passive if $\otimes^n\sigma$ is passive for all $n = 1,2,\ldots$ with respect to the sum Hamiltonian

$$H^{(n)} = \sum_{j=1}^{n} H_j, \tag{15}$$

where H_j is the jth independent copy of H. Thermodynamic equilibrium is equivalent to complete passivity:

Theorem 2 [3,4]. σ is completely passive if and only if it is a Gibbs state.

We now consider n independent copies of our battery and apply the general bound (14) to estimate the maximal amount of available work per battery:

$$\begin{aligned} w_{\max}^{n} &:= \frac{1}{n}\left\{\mathrm{Tr}[(\otimes^n\rho)\,H^{(n)}] - \mathrm{Tr}(\sigma_{\otimes^n\rho}\,H^{(n)})\right\} \\ &\leqslant \mathrm{Tr}(\rho H) - \mathrm{Tr}(\omega_{\overline{\beta}}\,H). \end{aligned} \tag{16}$$

It is our aim to show that this bound is actually asymptotically achievable:

Theorem 3.

$$\lim_{n\to\infty} w^n_{\max} = \mathrm{Tr}(\rho H) - \mathrm{Tr}(\omega_{\overline{\beta}} H). \tag{17}$$

Proof. The proof is based on the idea of typical configurations: for shift-invariant many-particle states with good clustering properties one can show that the reduced n-particle density matrices are almost entirely supported by a subspace of dimension $\exp(n\sigma)$ where σ is the average entropy of the state [6]. Here, we need an elementary version of this result as we consider only perfectly clustering states for which the n-particle reduced density matrices are just products of n independent copies of a given single-particle density matrix ρ. For such states $\sigma = S(\rho)$.

We first diagonalize ρ and obtain its eigenvalues $\{r_i\}$ in nonincreasing order with corresponding eigenvectors $|i\rangle$. To each configuration $\mathbf{i} = (i_1, i_2, \ldots, i_n)$ of length n we then associate the eigenvector $|\mathbf{i}\rangle := |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle$ of $\otimes^n \rho$ with corresponding eigenvalue $r_{\mathbf{i}} := r_{i_1} r_{i_2} \cdots r_{i_n}$. The eigenvalues of the reduced density matrix are highly degenerated with multinomial multiplicities. This leads, for large n, to a sharply peaked eigenvalue distribution which can be controlled by using Stirling's formula.

Let us denote by n_j the multiplicity of the index j in a configuration $\mathbf{i}$ and by $I(n,\epsilon)$ the set of configurations $\mathbf{i}$ for which $n(r_j - \epsilon) \leqslant n_j \leqslant n(r_j + \epsilon)$. Here ϵ is a fixed error bar that can be taken arbitrarily small. By Stirling's formula we obtain

$$e^{n[S(\rho)-\delta]} \leqslant [I(n,\epsilon)] \leqslant e^{n(S(\rho)+\delta)}, \text{ and} \tag{18}$$

$$\sum_{\mathbf{i}\in I(n,\epsilon)} r_{\mathbf{i}} \geqslant 1 - \delta. \tag{19}$$

Here δ can be chosen arbitrarily small provided n is sufficiently large. The subspace spanned by the eigenvectors $|\mathbf{i}\rangle$ with $\mathbf{i} \in I(n,\epsilon)$ is a typical subspace of $\otimes^n \rho$.

Now we repeat the same construction for the product of n copies of the Gibbs state $\omega_{\overline{\beta}}$. As $S(\omega_{\overline{\beta}}) = S(\rho)$, the typical subspaces of $\otimes^n \rho$ and $\otimes^n \omega_{\overline{\beta}}$ have approximately the same dimension. Moreover, for both product states the probability of finding a system outside the typical subspaces is $\mathrm{o}(\epsilon)$. We can now find a unitary $U^{(\epsilon)}$ on $\otimes^n \mathcal{H}$ that maps one subspace into the other. This unitary is highly non-unique, and generally differs from the optimal reordering given by $U_{\otimes^n \rho}$ but nevertheless produces a state with energy close to the optimal one, i.e.,

$$|\mathrm{Tr}[U^{(\epsilon)}(\otimes^n \rho)\, U^{(\epsilon)\dagger}\, H^{(n)}] - \mathrm{Tr}[(\otimes^n \omega_{\overline{\beta}})\, H^{(n)}]| \leqslant n\, \mathrm{o}(\epsilon). \tag{20}$$

Using Eq. (13) we obtain

$$\begin{aligned} \mathrm{Tr}(\otimes^n \omega_{\overline{\beta}}\, H^{(n)}) &\leqslant \mathrm{Tr}(\sigma_{\otimes^n \rho}\, H^{(n)}) \\ &\leqslant \mathrm{Tr}[U^{(\epsilon)}(\otimes^n \rho)\, U^{(\epsilon)\dagger}\, H^{(n)}], \end{aligned} \tag{21}$$

which combined with Eq. (20) yields the final estimation

$$\begin{aligned} \mathrm{Tr}(\rho H) - \mathrm{Tr}(\omega_{\overline{\beta}} H) &\geqslant w^n_{\max} \\ &\geqslant \mathrm{Tr}(\rho H) - \mathrm{Tr}(\omega_{\overline{\beta}} H) - \mathrm{o}(\epsilon). \end{aligned} \tag{22}$$

■

Note that the proof of Theorem 3 does not provide an efficient construction of the unitary dynamics transforming $\otimes^n \rho$ into a state close to the optimal state $\otimes^n \omega_{\overline{\beta}}$ but only ensures its existence. To design a practical scheme one can use the following observations:

(1) The unitary dynamics must be "entangling," i.e., cannot be executed by a time-dependent Hamiltonian which is a sum of single-system Hamiltonians. This is the meaning of "entanglement" in the title.

(2) The unitary dynamics cannot be driven by a Hamiltonian invariant with respect to permutations of the systems.

(3) The optimal procedure of work extraction should be globally invariant with respect to permutations of the systems.

Obviously, item (1) follows from the fact that by local unitaries we can at best reach the product of passive states $\otimes^n \sigma_\rho$ while item (3) is a consequence of permutation invariance of the initial state $\otimes^n \rho$ and the optimal product state $\otimes^n \omega_{\overline{\beta}}$. Item (2) is a consequence of the theorem proved in [7] which states that the support of the product state $\otimes^n \rho$ is concentrated on the subspaces of $\otimes^n \mathcal{H}$ characterized by Young tableaux with rows of the lengths $\{l_j \simeq n r_j\}$. The Hamiltonian invariant with respect to permutations leaves such symmetric subspaces invariant and hence cannot move the support of the state to a new one concentrated on subspaces characterized by Young tableaux with rows of the lengths $\{l_j \simeq n e^{-\bar{\beta}\epsilon_j}/\mathcal{Z}\}$.

The following algorithm complies with the observations (1)–(3) and provides a possible design of optimal work extraction procedure:

(a) Choose randomly a pair of subsystems $\{k,l\}$.

(b) Choose randomly the interaction Hamiltonian $H_{k,l}$ from a preselected, large enough set of two-system interactions.

(c) Apply the unitary $e^{-i H_{k,l}}$ to the state $\Omega^{(n)}(N)$ of n systems and compute the change of mean energy δE.

(d) If $\delta E < 0$ accept this unitary, if $\delta E \geqslant 0$ go to (b).

(e) The accepted unitary applied to $\Omega^{(n)}(N)$ defines a new state $\Omega^{(n)}(N+1)$ [initial state $\Omega^{(n)}(0) = \otimes^n \rho$].

(f) Continue the iteration until the mean energy stabilizes within a given accuracy.

The product of the accepted unitaries defines the reversible work extraction procedure.

V. CONCLUSION

The notion of maximal reversibly extractable work for a quantum battery motivated by the concept of passivity is discussed. It is applicable to full quantum models of micro- or mesoscopic machines where work is supplied by or extracted from a quantum system (a quantum battery, or work reservoir) by means of a time-dependent perturbation of the Hamiltonian. A proper definition of work is important to develop a consistent thermodynamics of small quantum systems which is relevant in nanotechnology and biophysics. Generally, the extractable work is smaller than the thermodynamical bound computed using the variational principle for the free energy. Using entangling unitaries one can in general extract more work per battery from several independent copies of a battery and asymptotically reach the thermodynamical bound. However,

the optimal procedures of work extraction are generally difficult to implement by realistic control Hamiltonians. An interesting problem for future investigation is to find efficiency bounds when practical restrictions are imposed on the available control mechanisms.

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