Optimal local work extraction from bipartite quantum systems in the presence of Hamiltonian couplings

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We investigate the problem of finding the local analog of the ergotropy, which is the maximum work that can be extracted from a system if we can only apply local unitary transformation acting on a given subsystem. In particular, we provide a closed formula for the local ergotropy in the special case in which the local system has only two levels, and we give analytic lower bounds and semidefinite programming upper bounds for the general case. As nontrivial examples of application, we compute the local ergotropy for an atom in an electromagnetic cavity with Jaynes-Cummings coupling and the local ergotropy for a spin site in an XXZ Heisenberg chain, showing that the amount of work that can be extracted with a unitary operation on the coupled system can be greater than the work obtainable by quenching off the coupling with the environment before the unitary transformation.

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I. INTRODUCTION

As quantum technologies are expected to be highly sensitive to the interaction with the environment, it is often useful to explicitly include the environment in the modeling of a quantum process. One way of representing open quantum systems is to extend the Hilbert space of the quantum system of interest, regarding it as a subspace of a larger Hilbert space which includes the "environment" of the system.

The problem of work extraction from quantum systems embedded in an environment was first studied in Ref. [1], which introduced the concept of strong local passivity, or *CP-local passivity*. A quantum state is CP-local passive with respect to a given subsystem if its energy cannot be decreased with any completely positive map on the subsystem. As the energy extractable with a local completely positive and trace preserving (CPTP) map can be found with a "semidefinite program" optimization, Ref. [2] provided an algorithm for computing it and characterized the necessary and sufficient conditons for CP-local passivity.

As CPTP maps constitute the most general evolution that a quantum system can undergo, the extractable energy studied in Refs. [1,2] represents an ultimate upper bound on the energy that can be drained from a system using only local operations on a given subsystem. However, just like in the global case [3], it makes sense to consider the energy extractable under a more limited set of allowed operations.

In Ref. [4] the maximum energy extractable from a composite system has been found, if all the subsystems are coupled with heat baths at inverse temperature β. This is the local analog of the nonequilibrium free energy [5]. In this work we consider instead the local analog of the ergotropy [6], which is the energy that we can extract from an isolated system using only local unitary transformations.

The restriction to unitary operations is a commonly accepted model for the extraction of work in fully quantized heat engines, as they describe the dynamics of a quantum system under Hamiltonian interactions [7–11]. In the same spirit, local unitary transformations are the class of transformation that we can perform on the system if one is allowed to perform a Hamiltonian driving on only one subsystem of the global quantum system.

In analogy with the notion of (globally) passive states [12,13], one can define the concept of *locally passive* states [14], i.e., states whose energy cannot be decreased by arbitrary local unitary transformations. In Ref. [14] it was found a set of necessary and sufficient conditions for the local passivity, but only in the case in which the Hamiltonian of the system is a sum of local Hamiltonians. We can define the *local ergotropy* with respect to a subsystem S as the energy extractable using local unitary operations [15] on S. Since the problem of finding local ergotropy cannot be expressed as a semidefinite programming optimization (as the unitarity constraint $UU^\dagger = I$ is not linear), it has been considerably less studied. In general, any correlated system exhibits an *ergotropic gap* [4,16], meaning that the local ergotropy is strictly smaller than the global ergotropy or that correlations with the environment are detrimental for work extraction [17–22]. On the contrary, the role of initial correlations among the various subsystems can be beneficial when extracting work via global unitary operations [23–25].

It is important to stress that in all the works mentioned above concerning the extraction of work with local unitary transformations, the global Hamiltonian of the systems is always assumed to be interaction-free. Exceptions to this general trend can be found in Refs. [26–30] where, studying energy exchanges not directly related with ergotropy

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calculations, the presence of couplings among the various subsystems is taken into consideration by adding to the energy bill the cost associated with the abrupt switching off and switching on of such terms. Apart from these works, it seems, however, that no general study of the local ergotropy has been presented when the model explicitly exhibits coupling among the various subsystems. The aim of this paper is to fill this gap. In the case in which the local system of interest is a two-level system, we present a simple method to exactly compute the maximal amount of work one can extract locally from a correlated many-body quantum system for Hamiltonian models which explicitly exhibit coupling terms among the various subsystems. In the case in which the system has a bigger dimension, we present some general bounds for its local ergotropy.

The material is organized as follows. In Sec. II we formalize the notion of local ergoropy and draw some connection with previous literature. In Sec. III we describe a general optimization method to compute the local ergotropy which takes a considerably simpler form in the case in which the system S is a qubit. In Sec. IV we apply our technique to compute the local ergotropy of two simple systems: an atom in an optical cavity with Jaynes-Cummings coupling and a site in an anisotropic (XXZ) Heisenberg spin chain. In both systems, we find regimes in which the local ergotropy is bigger than the work that can be extracted by decoupling the system from its environment (i.e., of the ergotropy of the decoupled local system, minus the energetic cost of isolating the system). Conclusions and outlooks are finally presented in Sec. V.

II. LOCAL ERGOTROPY

Consider a bipartite quantum system SE initialized in the possibly correlated quantum state $\hat{\rho}_{SE}$ and characterized by the joint Hamiltonian

$$\hat{H}_{SE} := \hat{H}_S \otimes \hat{I}_E + \hat{I}_S \otimes \hat{H}_E + \hat{V}_{SE}, \tag{1}$$

with $\hat{H}_S$ and $\hat{H}_E$ being the local energy terms and with $\hat{V}_{SE}$ being the interaction contribution which we assume to have zero partial trace on the S side, i.e., $\mathrm{Tr}_S[\hat{V}_{SE}] = 0$. The (global) *ergotropy* [6] of the state $\hat{\rho}_{SE}$ with respect to the Hamiltonian $\hat{H}_{SE}$ is the maximum amount of energy that can be extracted from $\hat{\rho}_{SE}$ by means of unitary transformation acting on the bipartite system SE; in formula it is expressed by the positive-semidefinite functional

$$\begin{aligned}\mathcal{E}(\hat{\rho}_{SE}, \hat{H}_{SE}) &:= \max_{\hat{U}_{SE}\in\mathbf{U}(d_S d_E)} \{\mathrm{Tr}[\hat{H}_{SE}(\hat{\rho}_{SE} - \hat{U}_{SE}\hat{\rho}_{SE}\hat{U}_{SE}^\dagger)]\} \\ &= \mathrm{Tr}[\hat{\rho}_{SE}\hat{H}_{SE}] - \min_{\hat{U}_{SE}\in\mathbf{U}(d_S d_E)} \mathrm{Tr}[\hat{U}_{SE}\hat{\rho}_{SE}\hat{U}_{SE}^\dagger \hat{H}_{SE}]. \end{aligned} \tag{2}$$

To gain insight into the problem (2), it is useful to consider the following classical analog. Let S_{cl} be a classical system which may be in one of the d states $\{s_1, \dots s_d\}$, having energies $\{\epsilon_1, \dots \epsilon_d\}$. A *state* of this classical system is specified by a probability distribution $\vec{p} = \{p_1, \dots p_d\}$ over the d states. The expected value of the energy of the system in the state $\vec{p}$ is $\langle E\rangle = \sum_{i=1}^d p_i\epsilon_i$. We can act on the classical system by applying an arbitrary permutation $\pi \in S_d$ on the states, so that $\vec{p} \to \pi(\vec{p}) = \{p_{\pi(1)}, \dots p_{\pi(d)}\}$. Then the classical analog of the ergotropy problem is to find the permutation which maximizes the expected value of the energy decrement, that is,

$$\mathcal{E}_{\mathrm{cl}}(\vec{p}, \vec{\epsilon}) = \sum_{i=1}^d p_i\epsilon_i - \min_{\pi\in S_d} \sum_{i=1}^d p_{\pi(i)}\epsilon_i. \tag{3}$$

The classical problem (3) can be immediately solved using the *rearrangement inequality* [31], which states that

$$\min_{\pi\in S_d} \sum_{i=1}^d p_{\pi(i)}\epsilon_i = \sum_{i=1}^d p_i^{\downarrow}\epsilon_i^{\uparrow}, \tag{4}$$

where $p_i^{\downarrow}$ denote the components of the vector $\vec{p}$ arranged in decreasing order (that is, $p_1^{\downarrow} \geqslant \cdots \geqslant p_d^{\downarrow}$), and similarly $\epsilon_i^{\uparrow}$ are the energies arranged in increasing order. The quantum ergotropy problem (2) can be solved in a completely analogous way, invoking the Hermitian-matrices analog of the rearrangement inequality, i.e., Von Neumann's trace inequality [32]:

$$\min_{\hat{U}_{SE}\in\mathbf{U}(d_S d_E)} \mathrm{Tr}[\hat{U}_{SE}\hat{\rho}_{SE}\hat{U}_{SE}^\dagger \hat{H}_{SE}] = \sum_{i=1}^d p_i^{\downarrow}\epsilon_i^{\uparrow}, \tag{5}$$

where this time $p_i^{\downarrow}$ are the eigenvalues of the density matrix $\hat{\rho}_{SE}$ arranged in decreasing order, and $\epsilon_i^{\uparrow}$ are the eigenvalues (energy levels) of the Hamiltonian $\hat{H}_{SE}$ arranged in increasing order. Writing $\hat{\rho}_{SE} = \sum_{i=1}^d p_i^{\downarrow} |i\rangle_{SE}\langle i|$ and $\hat{H}_{SE} = \sum_{i=1}^d \epsilon_i^{\uparrow} |\epsilon_i\rangle_{SE}\langle\epsilon_i|$, the optimal unitary transformation which achieves the minimum is given by $\hat{U}_{SE}^{(\mathrm{opt})} := \sum_{i=1}^d |\epsilon_i\rangle_{SE}\langle i|$.

The *S-local ergotropy* of the model is now defined as the maximum amount of work one can extract from SE by means of local unitary operations that act locally on S while not affecting E, i.e.,

$$\begin{aligned}&\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) \\ &:= \max_{\hat{U}_S\in\mathbf{U}(d_S)} \mathrm{Tr}\{\hat{H}_{SE}(\hat{\rho}_{SE} - [\hat{U}_S \otimes \hat{I}_E)\hat{\rho}_{SE}(\hat{U}_S^\dagger \otimes \hat{I}_E)]\},\end{aligned} \tag{6}$$

where the maximization is performed over the set $\mathbf{U}(d_S)$ of the unitary transformations on the d_S-dimensional Hilbert space associated with S. This is a non-negative quantity which by construction is upper-bounded by $\mathcal{E}(\hat{\rho}_{SE}, \hat{H}_{SE})$. Simple algebra reveals that $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ bares no functional dependence upon the local Hamiltonian of H_E of the subsystem E and that it is convex with respect to $\hat{\rho}_{SE}$ and $\hat{H}_{SE}$. We observe that in the absence of interactions (i.e., for $\hat{V}_{SE} = 0$), the S-local ergotropy reduces to the ergotropy $\mathcal{E}(\hat{\rho}_S, \hat{H}_S) := \max_{\hat{U}_S\in\mathbf{U}(d_S)} \mathrm{Tr}[\hat{H}_S(\hat{\rho}_S - \hat{U}_S\hat{\rho}_S\hat{U}_S^\dagger)]$ of the reduced state $\hat{\rho}_S := \mathrm{Tr}_E[\hat{\rho}_{SE}]$ associated with the local Hamiltonian $\hat{H}_S$, i.e.,

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})|_{\hat{V}_{SE}=0} = \mathcal{E}(\hat{\rho}_S, \hat{H}_S), \tag{7}$$

which in the case where $\hat{V}_{SE} \neq 0$ is sufficiently regular can be replaced by the inequality

$$|\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) - \mathcal{E}(\hat{\rho}_S, \hat{H}_S)| \leqslant 2\|\hat{\rho}_{SE}\|_2\|\hat{V}_{SE}\|_2, \tag{8}$$

with $\|\hat{\Theta}\|_2 = \sqrt{\mathrm{Tr}[\hat{\Theta}^\dagger\hat{\Theta}]}$ representing the Hilbert-Schmidt norm of the operator $\hat{\Theta}$ (see Appendix A). Notice also that when the input state of the system factorizes $\hat{\rho}_{SE} = \hat{\rho}_S \otimes \hat{\rho}_E$, $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ reduces to the erogotropy of the density $\hat{\rho}_S$ evaluated for the effective free local Hamiltonian

$\hat{H}_S^{(\mathrm{eff})} := \hat{H}_S + \mathrm{Tr}_E[\hat{V}_{SE}\hat{\rho}_E]$ obtained by adding to $\hat{H}_S$ the interaction term contracted on the state of E, i.e.,

$$\mathcal{E}_S(\hat{\rho}_S \otimes \hat{\rho}_E, \hat{H}_{SE}) = \mathcal{E}\big(\hat{\rho}_S, \hat{H}_S^{(\mathrm{eff})}\big). \tag{9}$$

Besides Eq. (8) no universal ordering can be drawn between $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ and $\mathcal{E}(\hat{\rho}_S, \hat{H}_S)$. Similar considerations also apply if we compare $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ with the work $\mathcal{E}_S^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{H}_{SE})$ one can get in a two-stage procedure where first the coupling term $\hat{V}_{SE}$ is abruptly switched-off, as in Refs. [26–30], and then local operations are applied to the resulting interaction-free Hamiltonian model. As discussed in Appendix B, by neglecting Lamb-shift corrections this quantity can be estimated as

$$\mathcal{E}_S^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{H}_{SE}) := \mathcal{E}(\hat{\rho}_S, \hat{H}_S) - \Delta^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{V}_{SE}), \tag{10}$$

with

$$\Delta^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{V}_{SE}) := -\mathrm{Tr}[\hat{\rho}_{SE}\hat{V}_{SE}] \tag{11}$$

being the energy cost associated with the switching-off event. In this case, Eq. (8) gets replaced by the inequality

$$\big|\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) - \mathcal{E}_S^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{H}_{SE})\big| \leqslant \|\hat{\rho}_{SE}\|_2 \|\hat{V}_{SE}\|_2, \tag{12}$$

which while bounding the distance between $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ and $\mathcal{E}_S^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{H}_{SE})$ cannot be used to establish a general ordering among them.

III. GENERAL FORMULAS AND BOUNDS

The study of the local ergotropy functional (6) is considerably more complex than the study of the global one (2). To appreciate this fact, consider the local analog of the classical rearrangement problem (3),

$$\mathcal{E}_{S,\mathrm{cl}}(\vec{p}, \vec{\epsilon}) = \sum_{i,j} p_{i,j}\epsilon_{i,j} - \min_{\pi} \sum_{i,j} p_{\pi(i),j}\epsilon_{i,j}, \tag{13}$$

obtained by considering the case in which given a probability distribution $p_{i,j}$ on a set of bipartite classical states $\{s_{i,j}\}$ specified by two indices i and j, and characterized by energies $\epsilon_{i,j}$, one is asked to improve the mean energy of the model by permuting only one of two indices (i.e., sending $p_{i,j} \to p_{\pi(i),j}$). The minimization in Eq. (13) is an instance of the ubiquitous and widely studied *assignment problem* [33,34]. It can be efficiently solved with several algorithms [35–37], but the solution cannot be written with a closed formula in terms of $\{p_{i,j}\}$ and $\{\epsilon_{i,j}\}$. Since the quantum problem (6) includes as a special case the classical problem (13) (which can be seen as the case in which $\hat{\rho}_{SE}$ and $\hat{H}_{SE}$ are both diagonal in a tensor product basis), this implies that no general closed solution can exist for $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$. Even the set of states $\hat{\rho}$ for which $\mathcal{E}_S(\hat{\rho}, \hat{H}) = 0$ does not admit an easy characterization, and it is not, in general, a convex set, in contrast with the sets of states such that $\mathcal{E}(\hat{\rho}, \hat{H}) = 0$, which is a simplex in the space of density matrices [38]. As we see in the forthcoming subsections, an explicit formula can, however, be derived in the special case where the quantum system S has only two levels. Furthermore a bound for $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ can be obtained in terms of the maximum energy decrement under local unital transformation, which can be calculated with a semidefinite programming (SDP) optimization (see Sec. III B).

A. A closed formula for a single qubit

To get a closed expression for the S-local ergotropy we find it useful to adopt the generalized Pauli operator (GOP) expansion formalism reviewed in Appendix C. In the case where S is a finite-dimensional system, this allows us to represent the density matrix $\hat{\rho}_{SE}$ as

$$\hat{\rho}_{SE} = \frac{\hat{I}_S}{d_S} \otimes \hat{\rho}_E + \frac{1}{2}\sum_{i=1}^{d_S^2-1} \hat{\sigma}_S^{(i)} \otimes \hat{\rho}_E^{(i)}, \tag{14}$$

with $\hat{\rho}_E := \mathrm{Tr}_S[\hat{\rho}_{SE}]$ being the reduced state of E, $\hat{\rho}_E^{(i)} := \mathrm{Tr}_S[\hat{\sigma}_S^{(i)}\hat{\rho}_{SE}]$, and $\{\hat{\sigma}_S^{(i)}; i = 1, \ldots, d_S^2 - 1\}$ being the GPO set adopted for S. Similarly we can write the Hamiltonian terms $\hat{H}_S$ and $\hat{V}_{SE}$ as

$$\hat{H}_S = c\hat{I}_S + \sum_{i=1}^{d_S^2-1} h_i\, \hat{\sigma}_S^{(i)}, \tag{15}$$

$$\hat{V}_{SE} = \frac{1}{2}\sum_{i=1}^{d_S^2-1} \hat{\sigma}_S^{(i)} \otimes \hat{V}_E^{(i)}, \tag{16}$$

with $c := \mathrm{Tr}[\hat{H}_S]/d_S$, $h_i := \mathrm{Tr}[\hat{\sigma}_S^{(i)}\hat{H}_S]/2$, and $\hat{V}_E^{(i)} := \mathrm{Tr}_S[\hat{\sigma}_S^{(i)}\hat{V}_{SE}]$. Notice that in writing Eq. (16) we assumed that $\hat{V}_{SE}$ contains no expansion term that is proportional to the identity: as a matter of fact, in case such a term exists we can drop it by properly redefining $\hat{H}_E$ [39]. Invoking now the orthonormal conditions of the GPO [see Eq. (C1)], we can express Eq. (D1) in the compact form

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) = \max_{\hat{U}_S \in \mathbf{U}(d_S)} \mathrm{Tr}[\mathcal{O}_U\mathcal{M} - \mathcal{M}], \tag{17}$$

with $\mathcal{O}_U \in \mathbf{O}(d_S^2 - 1)$ being the orthogonal matrix which corresponds to the unitary $\hat{U}_S$ in the selected GOP representation and with $\mathcal{M}$ being the $(d_S^2 - 1) \times (d_S^2 - 1)$ real matrix of elements

$$\mathcal{M}_{ik} := -\big(r_i h_k + \tfrac{1}{2}\mathrm{Tr}_E\big[\hat{\rho}_E^{(i)}\, \hat{V}_E^{(k)}\big]\big), \tag{18}$$

with $r_i := \mathrm{Tr}[\hat{\sigma}_S^{(i)}\hat{\rho}_S]$ being the components of the generalized Bloch vector of the reduced density matrix $\hat{\rho}_S$. The solution which maximizes the right-hand side of Eq. (17) has, in general, no closed formula expression; but it can be solved with a convex optimization algorithm (e.g., steepest descent). An exception to this is provided by the special case where S is a qubit, i.e., for $d_S = 2$ [40]. Under these circumstances, in fact, one has that $\{\mathcal{O}_U \mid \hat{U}_S \in U(2)\}$ exactly coincides with the subgroup SO(3) of the orthogonal group O(3). If the matrix $\mathcal{M}$ has an even number of negative eigenvalues—that is, if $\det[\mathcal{M}] \geqslant 0$—we can find by polar decomposition a matrix in SO(3) which turns $\mathcal{M}$ into $|\mathcal{M}|$. If instead $\mathcal{M}$ has an odd number of negative eigenvalues ($\det[\mathcal{M}] < 0$), no special orthogonal matrix can transform it into $|\mathcal{M}|$, and the best that one can do is to transform $\mathcal{M}$ into a matrix whose smallest eigenvalue is negative. Therefore, we can write

$$\begin{aligned}\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})|_{\mathrm{qubit}} &= \max_{\mathcal{O}\in\mathrm{SO}(3)} \mathrm{Tr}[\mathcal{O}\mathcal{M} - \mathcal{M}] \\ &= \begin{cases} \mathrm{Tr}[|\mathcal{M}| - \mathcal{M}], & \text{for } \det[\mathcal{M}] \geqslant 0, \\ \mathrm{Tr}[|\mathcal{M}| - \mathcal{M}] - \frac{2}{\|\mathcal{M}^{-1}\|}, & \text{for } \det[\mathcal{M}] < 0, \end{cases}\end{aligned} \tag{19}$$

with $|\mathcal{M}| := \sqrt{\mathcal{M}^\dagger \mathcal{M}}$ and $\|\cdots\|$ representing the operator norm.

B. Bounds for $d_S \geqslant 3$

In this section we derive some bounds for the local ergotropy functional $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ in the case of $d_S > 2$.

a. Polar upper bound. To begin with let us observe that the set of orthogonal matrices $\{\mathcal{O}_U \mid \hat{U}_S \in U(d_S)\}$ is a proper subgroup in the subgroup $\mathrm{SO}(d_S^2 - 1)$; it follows that the formula in the right-hand side of Eq. (19) is always a proper upper bound for $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$, i.e.,

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) \leqslant \max_{\mathcal{O} \in \mathrm{SO}(d_S^2-1)} \mathrm{Tr}[\mathcal{O}\mathcal{M} - \mathcal{M}] = \begin{cases} \mathrm{Tr}[|\mathcal{M}| - \mathcal{M}], & \text{for } \det[\mathcal{M}] \geqslant 0, \\ \mathrm{Tr}[|\mathcal{M}| - \mathcal{M}] - \frac{2}{\|\mathcal{M}^{-1}\|}, & \text{for } \det[\mathcal{M}] < 0. \end{cases} \tag{20}$$

Saturation of the inequality (20) is unlikely unless the matrix $\mathcal{M}$ admits polar decomposition

$$\mathcal{M} = \mathcal{O}_* |\mathcal{M}|, \tag{21}$$

with the orthogonal matrix $\mathcal{O}_*$ being an element of $\{\mathcal{O}_U \mid \hat{U}_S \in U(d_S)\}$ (a fact that always occurs for $d_S = 2$).

b. SDP upper bound. An alternative bound for the local ergotropy (6) can be obtained by exploiting a convexity argument (see Appendix E) to write

$$\min_{\hat{U}_S \in \mathbf{U}(d_S)} \mathrm{Tr}[\hat{H}_{SE}(\hat{U}_S \otimes \hat{I}_E)\hat{\rho}_{SE}(\hat{U}_S^\dagger \otimes \hat{I}_E)] = \min_{\Phi_S \in \overline{\mathbf{U}}(d_S)} \mathrm{Tr}[\hat{H}_{SE}(\Phi_S \otimes \mathbb{I}_E)(\hat{\rho}_{SE})], \tag{22}$$

where $\mathbb{I}_E$ represents the identity map on E and where $\overline{\mathbf{U}}(d_S)$ denotes the set of all convex combinations of unitary channels, i.e., $\overline{\mathbf{U}}(d_S) := \{\Phi_S \mid \Phi_S(\hat{\rho}_S) = \sum p_k U_k \hat{\rho}_S U_k^\dagger, U_k \in \mathbf{U}(d_S), p_k > 0, \sum p_k = 1\}$. Following Ref. [2] we can now introduce the operator

$$\hat{C}_{SS'} := \mathrm{Tr}_E\big[\hat{\rho}_{SE}^{T_S}\, \hat{H}_{S'E}\big], \tag{23}$$

where $\hat{\rho}_{SE}^{T_S}$ is the partial transpose of $\hat{\rho}_{SE}$ and recall that for any quantum channel Φ_S on S it holds that

$$\mathrm{Tr}[\hat{H}_{SE}(\Phi_S \otimes \mathbb{I}_E)(\hat{\rho}_{SE})] = \mathrm{Tr}\big[\hat{C}_{SS'}\hat{E}_{SS'}^{(\Phi_S)}\big], \tag{24}$$

with $\hat{E}_{SS'}^{(\Phi_S)}$ being the Choi matrix [41,42] of the channel Φ_S. Accordingly we can express Eq. (6) as

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) = \mathrm{Tr}[\hat{H}_{SE}\hat{\rho}_{SE}] - \min_{\Phi_S \in \overline{\mathbf{U}}(d_S)} \mathrm{Tr}\big[\hat{C}_{SS'}\hat{E}_{SS'}^{(\Phi_S)}\big]. \tag{25}$$

A computable upper bound can extracted from this by relaxing the minimization to include all the Φ_S's belonging to the set of *unital* channels, $\mathfrak{U}(d_S) \supset \overline{\mathbf{U}}(d_S)$ [43], i.e., the quantum channels such that $\Phi_S(I_S) = I_S$. With this relaxation, we obtain a SDP bound for the local ergotropy:

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) \leqslant \mathrm{Tr}[\hat{H}_{SE}\hat{\rho}_{SE}] - \min_{\hat{E}_{SS'}} \mathrm{Tr}[\hat{C}_{SS'}\hat{E}_{SS'}], \tag{26}$$

where now the minimum is now performed over the whole set of operators fulfilling the conditions

$$\hat{E}_{SS'} \geqslant 0, \tag{27}$$

$$\mathrm{Tr}_S \hat{E}_{SS'} = \hat{I}_{S'}, \quad \mathrm{Tr}_{S'} \hat{E}_{SS'} = \hat{I}_S, \tag{28}$$

(the first ensuring complete positivity, the second ensuring trace preservation, and the last ensuring the unitality requirement). Notice that, in the case $d_S = 2$, we have $\mathfrak{U}(d_S) = \overline{\mathbf{U}}(d_S)$, and therefore the bound (26) coincides with the exact formula (19). When $d_S \geqslant 3$, however, the bound (26) will be, in general, larger than the local ergotropy of the system.

IV. EXAMPLES

The simplest, yet nontrivial, model of quantum optics is the Jaynes-Cummings model, which describes the interaction of a two-level atom S, with energy levels spaced by ω_S, with the electromagnetic radiation field of a high-Q cavity mode E of frequency ω_E [44,45]. Expressed in terms of the two-level atom Pauli operators its Hamiltonian is given by

$$\hat{H}_{SE}^{(\mathrm{JC})} := \omega_E\, \hat{a}^\dagger \hat{a} + \frac{\omega_S}{2}\hat{\sigma}_S^z + \frac{\Omega}{2}(\hat{a} \otimes \hat{\sigma}_S^+ + \hat{a}^\dagger \otimes \hat{\sigma}_S^-), \tag{29}$$

with Ω being the Rabi frequency, a and $a^\dagger$ being the annihilation and creation operators of the mode, and $\hat{\sigma}_S^+ := (\hat{\sigma}_S^x - i\hat{\sigma}_S^y)/2$ and $\hat{\sigma}_S^- := (\hat{\sigma}_S^x + i\hat{\sigma}_S^y)/2$ being the raising and lowering operators of the atom (hereafter $\hbar = 1$). The Hamiltonian $\hat{H}_{SE}^{(\mathrm{JC})}$ admits as energy eigenvectors the (dressed) states

$$|n, +\rangle := \cos\theta_n\, |1\rangle \otimes |n\rangle + \sin\theta_n\, |0\rangle \otimes |n+1\rangle\,, \tag{30}$$

$$|n, -\rangle := \sin\theta_n\, |1\rangle \otimes |n\rangle - \cos\theta_n\, |0\rangle \otimes |n+1\rangle\,, \tag{31}$$

with $|n\rangle$ being the nth Fock state of the cavity mode and

$$\theta_n := \frac{1}{2}\arctan\left(\frac{\Omega\sqrt{n+1}}{\omega_S - \omega_E}\right), \tag{32}$$

the corresponding eigenvalues being $E_{n,\pm} := \omega_E n \pm \frac{1}{2}\sqrt{(\omega_S - \omega_E)^2 + \Omega^2(n+1)}$. By direct application of Eqs. (11) and (18) we get

$$\Delta^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{V}_{SE}) := -\frac{\Omega}{2}\big(\langle\hat{\sigma}_S^x \otimes \hat{X}\rangle - \langle\hat{\sigma}_S^y \otimes \hat{Y}\rangle\big), \tag{33}$$

and

$$\mathcal{M} = -\frac{1}{2}\begin{bmatrix} \Omega\langle\hat{\sigma}_S^x \otimes \hat{X}\rangle & -\Omega\langle\hat{\sigma}_S^x \otimes \hat{Y}\rangle & \omega_S\langle\hat{\sigma}_S^x\rangle \\ \Omega\langle\hat{\sigma}_S^y \otimes \hat{X}\rangle & -\Omega\langle\hat{\sigma}_S^y \otimes \hat{Y}\rangle & \omega_S\langle\hat{\sigma}_S^y\rangle \\ \Omega\langle\hat{\sigma}_S^z \otimes \hat{X}\rangle & -\Omega\langle\hat{\sigma}_S^z \otimes \hat{Y}\rangle & \omega_S\langle\hat{\sigma}_S^z\rangle \end{bmatrix}, \tag{34}$$

with $\hat{X} := (\hat{a}^\dagger + \hat{a})/2$ and $\hat{Y} := i(\hat{a}^\dagger - \hat{a})/2$, and where we used $\langle\cdots\rangle$ to indicate the expectation value with respect to $\hat{\rho}_{SE}$. In what follows we focus on the special cases where the input state $\hat{\rho}_{SE}$ corresponds to one of the eigenvectors $|n, \pm\rangle$ of the model, showing that under such assumption the S-local ergotropy values of the model are never smaller than the corresponding switch-off ergotropy values (10). To see this, let us start by observing that Eq. (33) gives $\Delta^{\mathrm{off}}(|n, \pm\rangle; \hat{V}_{SE}) = 0$. Therefore, using the fact that for θ_n as in Eq. (32) one has $\cos^2\theta_n \geqslant \sin^2\theta_n$, we get

$$\mathcal{E}_S^{\mathrm{off}}\big(|n, +\rangle, \hat{H}_{SE}^{(\mathrm{JC})}\big) = \mathcal{E}_S\big(\hat{\rho}_S^{(n,+)}, \hat{H}_S\big) = \omega_S \cos 2\theta_n, \tag{35}$$

which by construction is always positive semidefinite, and

$$\mathcal{E}_S^{\mathrm{off}}\big(|n, -\rangle, \hat{H}_{SE}^{(\mathrm{JC})}\big) = \mathcal{E}_S\big(\hat{\rho}_S^{(n,-)}, \hat{H}_S\big) = 0, \tag{36}$$

(in the above expressions $\hat{\rho}_S^{(n,\pm)}$ stand for the reduced density matrices on S of $|n, \pm\rangle_{SE}$). Notice next that replacing $|n, +\rangle$

in Eq. (34) we get instead

$$\mathcal{M}_+ = \frac{1}{2}\begin{bmatrix} -\Omega\frac{\sqrt{n+1}}{2}\sin 2\theta_n & 0 & 0 \\ 0 & \Omega\frac{\sqrt{n+1}}{2}\sin 2\theta_n & 0 \\ 0 & 0 & -\omega_S\cos 2\theta_n \end{bmatrix},$$

which has a determinant that is always positive semidefinite due to the fact that Eq. (32) forces $|\theta_n| \leqslant \pi/4$. Therefore in this case Eq. (19) implies

$$\mathcal{E}_S\big(|n,+\rangle, \hat{H}_{SE}^{(\mathrm{JC})}\big) = \omega_S\cos 2\theta_n + \frac{\sqrt{n+1}}{2}|\Omega\sin 2\theta_n|, \quad (37)$$

which is clearly greater than or equal to the corresponding switch-off value (35)—the gap being an increasing function of the intensity of the coupling term and of the index level n. Similarly assuming as input state $|n,-\rangle$, we obtain a matrix $\mathcal{M}_- = -\mathcal{M}_+$, whose determinant is now always negative semidefinite. Therefore, from Eq. (19) we get

$$\mathcal{E}_S\big(|n,-\rangle, \hat{H}_{SE}^{(\mathrm{JC})}\big) = \frac{\sqrt{n+1}}{2}|\Omega\sin 2\theta_n| - \min\left\{\omega_S\cos 2\theta_n, \frac{\sqrt{n+1}}{2}|\Omega\sin 2\theta_n|\right\}, \quad (38)$$

which again is always greater than the corresponding (zero) switch-off value $\mathcal{E}_S^{\mathrm{off}}(|n,-\rangle, \hat{H}_{SE}^{(\mathrm{JC})})$ reported in Eq. (35)—the only exception being the weak-coupling regime ($\omega_S\cos 2\theta_n \geqslant \frac{\sqrt{n+1}}{2}|\Omega\sin 2\theta_n|$) where also $\mathcal{E}_S(|n,-\rangle, \hat{H}_{SE}^{(\mathrm{JC})})$ nullifies. Most notably, at resonance ($\omega_S = \omega_E \Rightarrow |\theta_n| = \pi/4$) the gap between the local and the switch-off ergotropy terms of $|n,-\rangle_{SE}$ match that recorded for $|n,+\rangle_{SE}$ as one has $\mathcal{E}_S^{\mathrm{off}}(|n,\pm\rangle, \hat{H}_{SE}^{(\mathrm{JC})})|_{\mathrm{res}} = 0$ and $\mathcal{E}_S(|n,\pm\rangle, \hat{H}_{SE}^{(\mathrm{JC})})|_{\mathrm{res}} = \frac{\sqrt{n+1}}{2}|\Omega|$. On the contrary, one notices that, in the off-resonant regime (i.e., for $|\omega_S - \omega_E| \gg |\Omega|\sqrt{n+1} \Rightarrow |\theta_n| \simeq 0$), for both $|n,+\rangle_{SE}$ and $|n,-\rangle_{SE}$ the gap between $\mathcal{E}_S$ and $\mathcal{E}_S^{\mathrm{off}}$ always tends to collapse to zero. It is also worth noticing that, at variance with the global ergotropy, the local ergotropy functional does, in general, change with the time evolution of the system. In Fig. 1 we plot, as an example, the local ergotropy of a superposition of the states $|n=10,+\rangle$ and $|n=10,-\rangle$. The system alternates between time intervals in which $\mathcal{E}_S = 0$ and intervals in which $\mathcal{E}_S > 0$, with a behavior reminiscent of the entanglement sudden death and revival [46,47].

As a second example assume the system S to be one element of an XXZ Heisenberg model of N spin-1/2 particles disposed on a ring [48]. In this case the Hamiltonian can be expressed as

$$\hat{H}_{SE}^{(XXZ)} := \epsilon\sum_{i=1}^{N}\hat{\sigma}_i^z - \sum_{i=1}^{N}\left[J\big(\hat{\sigma}_i^x\otimes\hat{\sigma}_{i\oplus1}^x + \hat{\sigma}_i^y\otimes\hat{\sigma}_{i\oplus1}^y\big) + J_z\hat{\sigma}_i^z\otimes\hat{\sigma}_{i\oplus1}^z\right], \quad (39)$$

with the positive constants ϵ, J, and J_z representing the local energy contribution and the coupling terms of the model, and

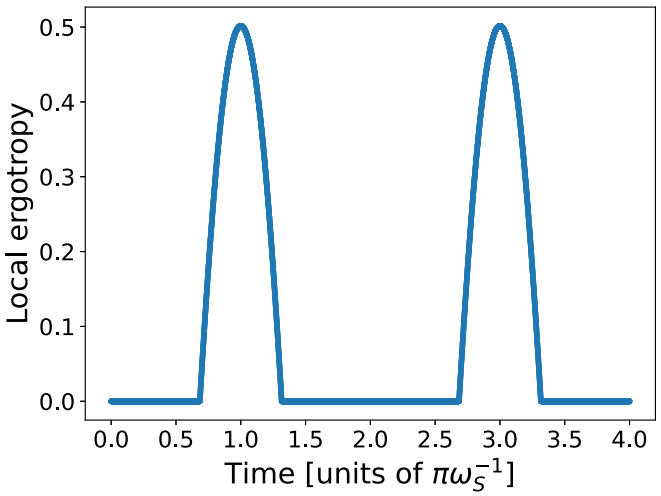

FIG. 1. Local ergotropy of the state $\cos\alpha\,|n,+\rangle + \sin\alpha\,|n,-\rangle\,e^{i\Omega t}$ as a function of the time t, for the choice of parameters $\omega_S = 1$, $\omega_E = 1.2$, $\Omega = 0.1$, $n = 10$, and $\alpha = 0.4\pi$.

where, to enforce periodic boundary conditions, $\oplus$ indicates the sum modulus N. We remind that as $\hat{H}_{SE}^{(XXZ)}$ admits the total magnetization $\hat{S}^z := \sum_{i=1}^N\hat{\sigma}_i^z$ as a conserved quantity ($[\hat{H}_{SE}^{(XXZ)}, S_z] = 0$), we can diagonalize it on subspaces of fixed values of $\hat{S}_z$. Specifically assuming J to be the subleading term with respect to ϵ and J_z, the ground state of the model is provided by $E_G := -N(\epsilon + J_z)$ corresponding to the all spin-down state $|\phi_G\rangle := \bigotimes_{i=1}^N|\downarrow\rangle_i$ (total magnetization sector with $\hat{S}^z = -N$). The next excited states $|\phi_k\rangle$ can instead be found on the $\hat{S}^z = -N+2$ sector spanned by superpositions of vectors $\hat{\sigma}_n^x|\phi_0\rangle := (\bigotimes_{i=1}^{n-1}|\downarrow\rangle_i)\otimes|\uparrow\rangle_n\otimes(\bigotimes_{i=n+1}^N|\downarrow\rangle_i)$, which have $n-1$ spin down and one spin up. Specifically, invoking the Bethe ansatz [49,50] the corresponding eigenvectors of $\hat{H}_{SE}^{(XXZ)}$ can be expressed as

$$|\phi_k\rangle := \frac{1}{\sqrt{N}}\sum_{n=1}^{N}e^{\frac{2\pi ki}{N}n}\hat{\sigma}_n^x|\phi_0\rangle, \quad (40)$$

with k being an integer term belonging to the interval $(-\lfloor N/2\rfloor, \lfloor N/2\rfloor]$, the associated eigenvalues being $E_k := -[(N-2)\epsilon + (N-4)J_z + 4J\cos(\frac{2k\pi}{N})]$. In what follows we compute the local ergotropy and the switch-off local ergotropy for these special states. To do so, we notice that, identifying the system S with the first site of the chain and identifying the environment E with the remaining ones, from Eqs. (11) and (18) we get

$$\Delta^{\mathrm{off}}(\hat{\rho}_{SE}, \hat{V}_{SE}) = J\langle\hat{\sigma}_S^x\otimes\hat{Y}_E\rangle + J\langle\hat{\sigma}_S^y\otimes\hat{X}_E\rangle + J_z\langle\hat{\sigma}_S^z\otimes\hat{Z}_E\rangle, \quad (41)$$

with $\hat{X}_E := \hat{\sigma}_N^x + \hat{\sigma}_2^x$, $\hat{Y}_E := \hat{\sigma}_N^y + \hat{\sigma}_2^y$, and $\hat{Z}_E := \hat{\sigma}_N^z + \hat{\sigma}_2^z$, and

$$\mathcal{M} = -\frac{1}{2}\begin{bmatrix} J\langle\hat{\sigma}_S^x\otimes\hat{X}_E\rangle & J\langle\hat{\sigma}_S^x\otimes\hat{Y}_E\rangle & \epsilon\langle\hat{\sigma}_S^x\rangle + J_z\langle\hat{\sigma}_S^x\otimes\hat{Z}_E\rangle \\ J\langle\hat{\sigma}_S^y\otimes\hat{X}_E\rangle & J\langle\hat{\sigma}_S^y\otimes\hat{Y}_E\rangle & \epsilon\langle\hat{\sigma}_S^y\rangle + J_z\langle\hat{\sigma}_S^y\otimes\hat{Z}_E\rangle \\ J\langle\hat{\sigma}_S^z\otimes\hat{X}_E\rangle & J\langle\hat{\sigma}_S^z\otimes\hat{Y}_E\rangle & \epsilon\langle\hat{\sigma}_S^z\rangle + J_z\langle\hat{\sigma}_S^z\otimes\hat{Z}_E\rangle \end{bmatrix}. \quad (42)$$

Taking hence as $\hat{\rho}_{SE}$ the pure state (40), this yields

$$\Delta^{\text{off}}(|\phi_k\rangle_{SE}, \hat{V}_{SE}) = \frac{8J}{N}\cos\left(\frac{2\pi k}{N}\right) + \frac{2N-8}{N}J_z \tag{43}$$

and

$$\mathcal{M}_k = \begin{bmatrix} \frac{2J}{N}\cos\left(\frac{2\pi k}{N}\right) & 0 & 0 \\ 0 & \frac{2J}{N}\cos\left(\frac{2\pi k}{N}\right) & 0 \\ 0 & 0 & \frac{N-1}{N}\epsilon + \frac{N-4}{N}J_z \end{bmatrix}.$$

Notice next that the reduced density matrix $\hat{\rho}_S$ of the first spin is given by $\hat{\rho}_S = \frac{N-1}{N}|0\rangle_S\langle 0| + \frac{1}{N}|1\rangle_S\langle 1|$, which is passive with respect to the local Hamiltonian $\hat{H}_S = \epsilon\hat{\sigma}_S^z$ of the model. Accordingly, from Eq. (10) we get

$$\mathcal{E}_S^{\text{off}}\left(|\phi_k\rangle_{SE}, \hat{H}_{SE}^{(XXZ)}\right) = -\frac{8J}{N}\cos\left(\frac{2\pi k}{N}\right) - \frac{2N-8}{N}J_z, \tag{44}$$

which can be positive for small N (i.e., $N \leqslant 4$) and $|k| \geqslant N/4$, while being always negative in the large N limit. Regarding the local ergotropy, we treat here explicitly the case where $\frac{N-1}{N}\epsilon + \frac{2N-8}{N}J_z \geqslant 0$, which from Eq. (19) allows us to write

$$\mathcal{E}_S\left(|\phi_k\rangle; \hat{H}_{SE}^{(XXZ)}\right) = \begin{cases} 0 & (|k| \leqslant N/4), \\ \frac{8J}{N}\left|\cos\left(\frac{2\pi k}{N}\right)\right| & (|k| > N/4). \end{cases} \tag{45}$$

We can hence recognize that, as long as $N \geqslant 4$, $\mathcal{E}_S(|\phi_k\rangle; \hat{H}_{SE}^{(XXZ)})$ is always greater or equal to the corresponding switch-off value. Exactly the opposite occurs instead for small ($N < 4$) rings as long as the ratio between J and J_z is small enough to ensure the applicability of Eq. (45): under these conditions, in fact, for $|k| \leqslant N/4$ we have $\mathcal{E}_S(|\phi_k\rangle, \hat{H}_{SE}^{(XXZ)}) = 0$, while $\mathcal{E}_S^{\text{off}}(|\phi_k\rangle_{SE}, \hat{H}_{SE}^{(XXZ)})$ becomes positive.

V. CONCLUSIONS

We derived an exact closed formula for the *local ergotropy* of a two-level system, or the maximum work that can be extracted with local unitary operations from said system interacting with a general environment. We have shown two examples in which the local ergotropy is strictly bigger than the amount of work that can be obtained by first isolating the system and then performing the unitary operation. This indicates that the environment may be a resource, and not only a nuisance, for work extraction.

The formula also gives a (loose) upper bound for the local ergotropy of a system of generic dimension d. The problem of finding the local ergotropy of a system of dimension d can be seen as a quantum generalization of the assignment problem; hence, we know that no general closed formula can exist for its solution. However, a more careful analysis may improve the bounds provided here.

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APPENDIX A: DERIVATION OF EQ. (8)

Indicating with $\hat{U}_S^{(\text{free})}$ the unitary transformation that enters in the computation of the local ergotropy in the non-interacting case (7), we can write

$$\begin{aligned} &\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) \\ &\quad\geqslant \text{Tr}\{\hat{H}_{SE}[\hat{\rho}_{SE} - (\hat{U}_S^{(\text{free})} \otimes \hat{I}_E)\hat{\rho}_{SE}(\hat{U}_S^{(\text{free})^\dagger} \otimes \hat{I}_E)]\} \\ &\quad= \mathcal{E}(\hat{\rho}_S, \hat{H}_S) + \text{Tr}[(\hat{\rho}_{SE} - \hat{U}^{(\text{free})}\hat{\rho}_{SE}\hat{U}^{(\text{free})\dagger})\hat{V}_{SE}] \\ &\quad\geqslant \mathcal{E}(\hat{\rho}_S, \hat{H}_S) - \|(\hat{\rho}_{SE} - \hat{U}^{(\text{free})}\hat{\rho}_{SE}\hat{U}^{(\text{free})\dagger})\|_2\|\hat{V}_{SE}\|_2 \\ &\quad\geqslant \mathcal{E}(\hat{\rho}_S, \hat{H}_S) - 2\|\hat{\rho}_{SE}\|_2\|\hat{V}_{SE}\|_2, \end{aligned} \tag{A1}$$

where in the third passage we applied the Cauchy-Schwarz inequality of the Hilbert-Smith scalar product. On the contrary by decomposing the maximization of Eq. (6) into two independent maximizations that involve the free and interaction terms of $\hat{H}_{SE}$, respectively, we can write maximization as

$$\begin{aligned} \mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) &\leqslant \mathcal{E}(\hat{\rho}_S, \hat{H}_S) + \mathcal{E}_S(\hat{\rho}_{SE}, \hat{V}_{SE}) \\ &\leqslant \mathcal{E}(\hat{\rho}_S, \hat{H}_S) + 2\|\hat{\rho}_{SE}\|_2\|\hat{V}_{SE}\|_2. \end{aligned} \tag{A2}$$

APPENDIX B: LOCAL ENERGY EXTRACTION FOR ABRUPT SWITCHING-OFF OF THE COUPLING TERMS

Here we present the derivation of Eq. (10) by estimating the maximum work we can extract from $\hat{\rho}_{SE}$ in the two-step scenario, where through a quench we first abruptly switch off the coupling between S and E and then use local unitaries $\hat{U}_S$. At the beginning of the process the mean energy contained in the model is given by the expectation value

$$\begin{aligned} E_0 &:= \text{Tr}[\hat{\rho}_{SE}\hat{H}_{SE}] \\ &= \text{Tr}[\hat{\rho}_S\hat{H}_S] + \text{Tr}[\hat{\rho}_E\hat{H}_E] + \text{Tr}[\hat{\rho}_{SE}\hat{V}_{SE}]. \end{aligned} \tag{B1}$$

The switch-off procedure transforms the initial Hamiltonian $\hat{H}_{SE}$ into an interaction-free term of the form

$$\hat{H}_{SE}^{\text{free}} = \hat{H}_S' \otimes \hat{I}_E + \hat{I}_S \otimes \hat{H}_E'. \tag{B2}$$

Notice that, in principle, due to the presence of Lamb-shift contributions, the new local terms $\hat{H}_S'$ and $\hat{H}_E'$ need not coincide with the corresponding values $\hat{H}_S$ and $\hat{H}_E$ appearing in Eq. (1). Determining the exact structure of $\hat{H}_S'$ and $\hat{H}_E'$ strongly depends on the specific physical model we are considering. Typically, however, one expects the discrepancies between $\hat{H}_S'$, $\hat{H}_E'$ and $\hat{H}_S$, $\hat{H}_E$ to be small, and for the sake of simplicity in our analysis we neglect them. Accordingly, we evaluate the energy of the system immediately after the quench as

$$\begin{aligned} E_1 &:= \text{Tr}[\hat{\rho}_{SE}\hat{H}_{SE}^{\text{free}}] = \text{Tr}[\hat{\rho}_S\hat{H}_S] + \text{Tr}[\hat{\rho}_E\hat{H}_E] \\ &= E_0 + \Delta^{\text{off}}(\hat{\rho}_{SE}, \hat{H}_{SE}), \end{aligned} \tag{B3}$$

where in the second line we invoke Eq. (11). When positive, the difference between E_1 and E_0 [i.e., the quantity $\Delta^{\text{off}}(\hat{\rho}_{SE}, \hat{H}_{SE})$] accounts for the energy we need to provide to the system SE in order to suppress the interactions between the subsystems. Such a term has hence to be subtracted from the maximal work we can extract from $\hat{\rho}_{SE}$ via local unitary on S in the second part of the protocol, i.e., the quantity

$$\begin{aligned}&\mathcal{E}_S\big(\hat{\rho}_{SE}, \hat{H}_{SE}^{\text{free}}\big)\\ &:= \max_{\hat{U}_S \in \mathbf{U}(d_S)} \text{Tr}\big\{\hat{H}_{SE}^{\text{free}}[\hat{\rho}_{SE} - (\hat{U}_S \otimes \hat{I}_E)\hat{\rho}_{SE}(\hat{U}_S^\dagger \otimes \hat{I}_E)]\big\}\\ &= \mathcal{E}(\hat{\rho}_S, \hat{H}_S). \end{aligned} \tag{B4}$$

Equation (10) then simply follows by putting together these observations.

The derivation of Eq. (12) follows along the same lines that led us to Eqs. (A1) and (A2). Specifically, we can write

$$\begin{aligned}&\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})\\ &\geqslant \mathcal{E}_S^{\text{off}}(\hat{\rho}_{SE}, \hat{H}_{SE}) - \text{Tr}\big[\hat{U}_S^{(\text{free})}\hat{\rho}_{SE}\hat{U}_S^{(\text{free})^\dagger}\hat{V}_{SE}\big]\\ &\geqslant \mathcal{E}_S^{\text{off}}(\hat{\rho}_{SE}, \hat{H}_{SE}) - \|\hat{\rho}_{SE}\|_2\|\hat{V}_{SE}\|_2, \end{aligned} \tag{B5}$$

where $\hat{U}_S^{(\text{free})}$ is the optimal unitary associated with the free model scenario (7). Similarly, we can write

$$\begin{aligned}&\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})\\ &\leqslant \mathcal{E}_S^{\text{off}}(\hat{\rho}_{SE}, \hat{H}_{SE}) - \min_{\hat{U}_S \in \mathbf{U}(d_S)} \text{Tr}[\hat{U}_S\hat{\rho}_{SE}\hat{U}_S^\dagger\hat{V}_{SE}]\\ &\leqslant \mathcal{E}_S^{\text{off}}(\hat{\rho}_{SE}, \hat{H}_{SE}) + \|\hat{\rho}_{SE}\|_2\|\hat{V}_{SE}\|_2. \end{aligned} \tag{B6}$$

APPENDIX C: GENERALIZED BLOCH VECTORS

Assuming that the Hilbert space $\mathcal{H}_S$ of S has a finite dimension d_S, a GPO set is a collection $\{\hat{\sigma}_S^{(i)}; i = 1, \ldots, d^2 - 1\}$ of $(d^2 - 1)$ self-adjoint operators that fulfill the properties

$$\text{Tr}\big[\hat{\sigma}_S^{(i)}\big] = 0, \quad \text{Tr}\big[\hat{\sigma}_S^{(i)}\hat{\sigma}_S^{(j)}\big] = 2\delta_{ij}. \tag{C1}$$

Together with the identity operator $\hat{I}_S$, a GPO set forms a basis for the operators $\hat{\theta}_S$ on $\mathcal{H}_S$ which leads to the following expansion formula:

$$\hat{\theta}_S = \frac{\text{Tr}[\hat{\theta}]}{d_S}\,\hat{I}_S + \frac{1}{2}\sum_{i=1}^{d^2-1} q_i\theta_S)\,\hat{\sigma}_S^{(i)}, \tag{C2}$$

where for $i \in \{1, \ldots, d_S^2 - 1\}$ the coefficients

$$q_i(\hat{\theta}_S) := \text{Tr}\big[\hat{\theta}_S\hat{\sigma}_S^{(i)}\big] \tag{C3}$$

are the complex components of a $(d_S^2 - 1)$-dimensional vector $\vec{q}(\hat{\theta}_S)$ whose norm corresponds to the Hilbert-Schmidt norm of $\hat{\theta}_S$ up to a scaling factor of

$$|\vec{q}(\hat{\theta}_S)| = \|\hat{\theta}_S - \text{Tr}[\theta_S]\hat{I}_S\|_2/\sqrt{2}. \tag{C4}$$

Equation (15) is a direct application of (C2), while Eqs. (14) and (16) follow from a trivial generalization of such an identity to the case of a joint operator $\hat{\theta}_{SE}$ of S and E. We also recall that given $\{|j\rangle_S\}_{j=0,\ldots,d_S-1}$, an orthonormal basis of $\mathcal{H}_S$, a special example of GPOs is provided by the matrices

$$\begin{aligned}&\hat{\sigma}_{S,jj'}^x := |j\rangle_S\langle j'| + |j'\rangle_S\langle j|,\\ &\hat{\sigma}_{S,jj'}^y := i(|j'\rangle_S\langle j| - |j\rangle_S\langle j'|),\\ &\hat{\sigma}_{S,k}^z := \sqrt{\frac{2}{d_S(d_S-1)}}\left((1-d_S+k)|0\rangle_S\langle 0| + \sum_{j=1}^{d_S-k-1}|j\rangle_S\langle j|\right), \end{aligned} \tag{C5}$$

for $0 \leqslant j < j' \leqslant d_S - 1$ and $0 \leqslant k \leqslant d_S - 2$. In the case of a qubit (i.e., $d_S = 2$), this choice leads to the *Bloch vector* representation [51], which induces a one-to-one correspondence between the quantum states $\hat{\rho}_S$ and the unitary ball of $\mathbb{R}^3$ via the mapping

$$\vec{r}(\hat{\rho}_S) = \big(\text{Tr}\big[\hat{\rho}_S\hat{\sigma}_S^x\big], \text{Tr}\big[\hat{\rho}_S\hat{\sigma}_S^y\big], \text{Tr}\big[\hat{\rho}_S\hat{\sigma}_S^z\big]\big), \tag{C6}$$

with $\hat{\sigma}_S^x := \hat{\sigma}_{S,01}^x$, $\hat{\sigma}_S^y := \hat{\sigma}_{S,01}^y$, and $\hat{\sigma}_S^z := \hat{\sigma}_{S,0}^z$ being the standard Pauli operators. We can also associate (up to a phase factor) with any unitary matrix $\hat{U}_S \in \mathbf{U}(2)$ an orthogonal matrix $\mathcal{O}_U \in \mathbf{O}(3)$, such that for every state $\hat{\rho}_S$ we get

$$\vec{r}(\hat{U}_S\hat{\rho}_S\hat{U}_S^\dagger) = \mathcal{O}_U\vec{r}(\hat{\rho}_S). \tag{C7}$$

For dimension $d_S > 2$, we can still define a generalized Bloch vector [52], $\vec{r}(\hat{\rho}_S) \in \mathbb{R}^{d_S^2-1}$, with coordinates as in Eq. (C3), and it is still true that to any unitary transformation in the Hilbert space corresponds an orthogonal transformation in the Bloch space verifying Eq. (C7). In this case, however, it is no longer true that any vector in the unitary ball $|\vec{r}| \leqslant 1$ can be associated with a physical state [53], and similarly, not all the orthogonal matrices $O \in \mathbf{O}(d_S^2 - 1)$ are associated with unitary transformations $\hat{U}_S \in \mathbf{U}(d_S)$ via Eq. (C7). However, it is known that if

$$|\vec{r}| \leqslant 2/d_S, \tag{C8}$$

there exists surely a legitimate quantum state $\hat{\rho}_S$ associated with the vector $\vec{r}$ [54].

We finally observe that, if also the dimension d_E of the system E is finite, one can also adopt a GPO decomposition for its elements [52,53]. In this case, defining

$$r_i := \text{Tr}\big[\hat{\sigma}_S^{(i)}\hat{\rho}_S\big], \quad q_i := \text{Tr}\big[\hat{\sigma}_E^{(i)}\hat{\rho}_E\big], \tag{C9}$$

$$t_{ij} := \text{Tr}\big[\hat{\rho}_{SE}\big(\hat{\sigma}_S^{(i)} \otimes \hat{\sigma}_E^{(j)}\big)\big], \tag{C10}$$

$$v_{ij} := \text{Tr}\big[\hat{V}_{SE}\big(\hat{\sigma}_S^{(i)} \otimes \hat{\sigma}_E^{(j)}\big)\big]/4, \tag{C11}$$

we can write

$$\begin{aligned}\hat{\rho}_{SE} &= \frac{1}{d_Sd_E}\hat{I}_S \otimes \hat{I}_E + \frac{1}{4}\sum_{i=1}^{d_S^2-1}\sum_{j=1}^{d_E^2-1} t_{ij}\,\hat{\sigma}_S^{(i)} \otimes \hat{\sigma}_E^{(j)}\\ &\quad + \frac{1}{2}\sum_{i=1}^{d_S} r_i\,\hat{\sigma}_S^{(i)} \otimes \hat{I}_E + \frac{1}{2}\sum_{j=1}^{d_E^2-1} q_j\,\hat{I}_S \otimes \hat{\sigma}_E^{(j)},\\ \hat{V}_{SE} &= \sum_{i=1}^{d_S^2-1}\sum_{j=1}^{d_E^2-1} v_{ij}\,\hat{\sigma}_S^{(i)} \otimes \hat{\sigma}_E^{(j)}, \end{aligned} \tag{C12}$$

which leads to a rewriting of Eq. (18) as

$$\mathcal{M}_{ik} = -\left(r_i h_k + \sum_{j=1}^{d_E^2-1} t_{ij} v_{kj} \right). \tag{C13}$$

APPENDIX D: TWO-LEVEL HAMILTONIAN WITH PURE INPUT STATE

A lower bound for $\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE})$ can be established by rewriting Eq. (6) as

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) = \max_{\hat{U}_S \in \mathbf{U}(d_S)} (\mathrm{Tr}[\hat{H}_S(\hat{\rho}_S - \hat{U}_S \hat{\rho}_S \hat{U}_S^\dagger)] + \mathrm{Tr}\{\hat{V}_{SE}[\hat{\rho}_{SE} - (\hat{U}_S \otimes \hat{I}_E)\hat{\rho}_{SE}(\hat{U}_S^\dagger \otimes \hat{I}_E)]\}), \tag{D1}$$

which, thanks to the spectral decompositions $\hat{H}_S + \hat{V}_{SE} = \sum_{k=0}^{d_S d_E} \epsilon_k |\epsilon_k\rangle_{SE} \langle\epsilon_k|$ and $\hat{\rho}_{SE} = \sum_{j=0}^{d_S d_E} p_j |j\rangle_{SE} \langle j|$, can be casted in the form

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) = \mathrm{Tr}[\hat{\rho}_{SE}(\hat{H}_S + \hat{V}_{SE})] + \max_{\hat{U}_S \in \mathbf{U}(d_S)} \sum_{k,j=1}^{d_S d_E} -p_j \epsilon_k \left| \mathrm{Tr}\left[\hat{U}_S \hat{N}_S^{(k,j)}\right] \right|^2, \tag{D2}$$

with $\hat{N}_S^{(k,j)} := \mathrm{Tr}_E[|\epsilon_k\rangle_{SE} \langle j|]$. Next we can notice that, thanks to the unitarity of $\hat{U}_S$, we have

$$\max_{\hat{U}_S \in \mathbf{U}(d_S)} \left| \mathrm{Tr}\left[\hat{U}_S \hat{N}_S^{(k,j)}\right] \right|^2 = \left\| \hat{N}_S^{(k,j)} \right\|_1^2, \tag{D3}$$

with $\| \cdots \|_1$ being the trace norm symbol. Up to a shift in the operator $\hat{H}_S + \hat{V}_{SE}$, we can always assume that $-\epsilon_k \geqslant 0$ for every k. Then, using Eq. (D3) in Eq. (D2), we immediately have the bound

$$\mathcal{E}_S(\hat{\rho}_{SE}, \hat{H}_{SE}) \geqslant \mathrm{Tr}[\hat{\rho}_{SE}(\hat{H}_S + \hat{V}_{SE})] - \sum_{k,j=1}^{d_S d_E} p_j \epsilon_k \left\| \hat{N}_S^{(k,j)} \right\|_1^2. \tag{D4}$$

Furthermore, we know that for every k and j there exists a unitary matrix $\hat{U}_{S*}^{(k,j)}$ which saturates the inequality (D3). Therefore, in the special case in which the state $\hat{\rho}_{SE} = |\Psi\rangle_{SE} \langle\Psi|$ is a pure state, and in which the Hamiltonian $\hat{H}_S + \hat{V}_{SE}$ has only two levels and a nondegenerate ground state (so that we can assume, without loss of generality, $\epsilon_1 = -E$ and $\epsilon_2 = 0$), the bound (D4) becomes an exact equality, and we have

$$\mathcal{E}_S\left(|\Psi\rangle_{SE}, \hat{H}_{SE}^{(\text{two-levels})} \right) = \mathrm{Tr}[\hat{\rho}_{SE}(\hat{H}_S + \hat{V}_{SE})] - E \left\| \hat{N}_S^{(1,1)} \right\|_1^2. \tag{D5}$$

APPENDIX E: DERIVATION OF EQ. (22)

In this section we prove the equality (22), which follows from the general fact that the maximum of a convex functional over a convex set must be on one of the vertices of the set.

Let $\Phi_S \in \overline{\mathbf{U}(d_S)}$ be a convex combination of local unitary maps on the subsystem S, i.e.,

$$(\Phi_S \otimes \mathbb{I}_E)(\hat{\rho}) = \sum_i p_i (\hat{U}_{S,i} \otimes \hat{I}_E) \hat{\rho}_{SE} (\hat{U}_{S,i}^\dagger \otimes \hat{I}_E). \tag{E1}$$

with $p_i \geqslant 0$ and $\sum_i p_i = 1$. By linearity of the trace functional we have

$$\begin{aligned} &\mathrm{Tr}[\hat{H}_{SE}(\Phi_S \otimes \mathbb{I}_E)(\hat{\rho}_{SE})] \\ &= \mathrm{Tr}\left\{ \hat{H}_{SE} \left[\sum_i p_i (\hat{U}_{S,i} \otimes \hat{I}_E) \hat{\rho}_{SE} (\hat{U}_{S,i}^\dagger \otimes \hat{I}_E) \right] \right\} \\ &= \sum_i p_i \mathrm{Tr}[\hat{H}_{SE}(\hat{U}_{S,i} \otimes \hat{I}_E) \hat{\rho}_{SE} (\hat{U}_{S,i}^\dagger \otimes \hat{I}_E)]. \end{aligned} \tag{E2}$$

Now let $U_S^\star \in \mathbf{U}(d_S)$ be a unitary transformation such that

$$\begin{aligned} &\mathrm{Tr}[\hat{H}_{SE}(U_S^\star \otimes \hat{I}_E) \hat{\rho}_{SE} (U_S^{\star\dagger} \otimes \hat{I}_E)] \\ &= \min_i \mathrm{Tr}[\hat{H}_{SE}(\hat{U}_{S,i} \otimes \hat{I}_E) \hat{\rho}_{SE} (\hat{U}_{S,i}^\dagger \otimes \hat{I}_E)]. \end{aligned} \tag{E3}$$

From Eq. (E2) it follows that

$$\begin{aligned} &\mathrm{Tr}[\hat{H}_{SE}(\Phi_S \otimes \mathbb{I}_E)(\hat{\rho}_{SE})] \\ &= \sum_i p_i \mathrm{Tr}[\hat{H}_{SE}(\hat{U}_{S,i} \otimes \hat{I}_E) \hat{\rho}_{SE} (\hat{U}_{S,i}^\dagger \otimes \hat{I}_E)] \\ &\geqslant \mathrm{Tr}[\hat{H}_{SE}(U_S^\star \otimes \hat{I}_E) \hat{\rho}_{SE} (U_S^{\star\dagger} \otimes \hat{I}_E)]. \end{aligned} \tag{E4}$$

Since this is valid for any possible map $\Phi_S \in \overline{\mathbf{U}(d_S)}$ (that is, for every convex combination of unitary transformation, we can always find a pure unitary which extracts more work), this implies the validity of Eq. (22).

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