Rapid Communications

Energy bounds for entangled states

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(Received 4 April 2019; accepted 6 May 2020; published 11 June 2020)

We find the minimum and the maximum value for the local energy of an arbitrary finite bipartite system for any given amount of entanglement, also identifying families of states reaching these bounds and sharing formal analogies with thermal states. Then, we numerically study the probability of randomly generating pure states close to these energy bounds finding, in all the considered configurations, that it is extremely low except for the two-qubit and highly degenerate cases. These results can be important in quantum technologies to design energetically more efficient protocols.

DOI: 10.1103/PhysRevResearch.2.022057

Introduction. Energy and entanglement are two fundamental quantities in physics. The concept of energy has been of great importance in the development of physics [1] while entanglement is one of the most, if not the most, exotic feature of quantum mechanics [2]. Therefore, it has been extensively studied since its conception both from the theoretical and the experimental points of view [3], also in connection with nonlocality [4–7] and measurements [8,9], even nondemolitive ones [10]. Entanglement also plays a fundamental role in the development of quantum technologies [11] and is considered as a resource in several contexts such as quantum teleportation [12–14], quantum cryptography [15–17], quantum communication [18], quantum computation [11], quantum energy teleportation [19], and in protocols exploiting repeated measurements [20–24]. As a result, the quest for entanglement generation protocols has been one of the most flourishing fields in recent physics literature [25–29].

Although quantum algorithms typically make use of two-level systems (qubits) [11], it has been shown that d-level systems (qudits) may be more powerful for information processing [30,31]. Indeed, the higher dimensionality allows for information coding with increased density, leading to a simplification of the design of circuits [32], since the number of logic gates is reduced. The realization of high-dimensional systems and their control has thus attracted much attention [33,34].

Understanding how energy and entanglement are connected can be crucial in order to design quantum technologies in a more efficient manner [35]. In this context, some works investigated the energy cost of generating or extracting entanglement [36,37]. In particular, some entanglement extraction protocols can be optimized by finding a minimum energy pure state with an assigned entanglement [37]. However, this has been done for interacting systems and the explicit solution has been found only for a specific toy model.

In this Rapid Communication, we investigate, for an arbitrary finite bipartite system, the connection between local energy and entanglement in the case of discrete local Hamiltonians. In particular, for any given amount of entanglement, we look for the range of possible values for the local energy and search for quantum states that reach, respectively, the lower and the upper bounds on the local energy. Moreover, we numerically study the probability of randomly generating pure states close to these energy bounds. This analysis can be helpful to design energetically efficient entanglement generation protocols. Since the dimensions of the bipartite system are arbitrary, our analysis naturally applies to protocols exploiting qudits.

Definition of the problem. We consider a bipartite system A-B composed of two arbitrary quantum systems A and B, with local Hamiltonian $H = H_A + H_B$, where N_A and N_B are the dimensions of, respectively, H_A and H_B, being $N_A \leqslant N_B$. H_A and H_B can be written as

$$H_X = \sum_{n=0}^{N_X-1} X_n |X_n\rangle\langle X_n|, \quad X = A, B, \tag{1}$$

where $X_0 \leqslant X_1 \leqslant \cdots \leqslant X_{N_X-1}$.

The above local Hamiltonian H suitably describes systems at the start and at the end of most quantum protocols, in which the possible interaction between the subsystems takes place only during the protocol.

We will first consider the case of pure states. In order to quantify the degree of entanglement of a pure state $|\psi\rangle$ of system A-B, we use the entropy of entanglement, which is regarded as the standard entanglement measure for pure states [38,39] and is equal to the Von Neumann entropy of one of the reduced states, i.e., $\mathcal{E}(|\psi\rangle) = S(\mathrm{Tr}_{A(B)}\{|\psi\rangle\langle\psi|\})$, where $S(\rho) = -\mathrm{Tr}\{\rho \ln \rho\}$.

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Every pure state of system A-B can be rewritten according to its Schmidt decomposition as [11]:

$$|\psi\rangle = \sum_{i=0}^{N_A-1} \sqrt{\lambda_i}|a_i b_i\rangle, \tag{2}$$

where $\langle a_i|a_j\rangle = \langle b_i|b_j\rangle = \delta_{ij}$, $\sum_{i=0}^{N_A-1}\lambda_i = 1$, and $0 \leqslant \sqrt{\lambda_{N_A-1}} \leqslant \cdots \leqslant \sqrt{\lambda_1} \leqslant \sqrt{\lambda_0} \leqslant 1$. Accordingly, $\mathcal{E}(|\psi\rangle) = -\sum_i \lambda_i \ln \lambda_i$.

Minimum energy and corresponding states. For each value of entanglement, $\mathcal{E}$, multiple sets of squared Schmidt coefficients such that the correct amount of entanglement is attained can be found. Therefore, let us concentrate on one of these sets, $\vec{\lambda} \equiv \{\lambda_i\}_{i=0}^{N_A-1}$. In Sec. I of the Supplemental Material (SM) [40], we prove Theorem 1, showing that no pure state with the corresponding Schmidt coefficients can have less energy than the state

$$|\psi_{\vec{\lambda}}\rangle = \sum_{i=0}^{N_A-1} \sqrt{\lambda_i}|A_i B_i\rangle, \tag{3}$$

having energy

$$E_{\vec{\lambda}} \equiv \langle\psi_{\vec{\lambda}}|H|\psi_{\vec{\lambda}}\rangle = \sum_{i=0}^{N_A-1} \lambda_i E_i, \quad E_i = A_i + B_i. \tag{4}$$

To minimize $E_{\vec{\lambda}}$ by varying $\vec{\lambda}$, we use the following bijection (valid up to phase factors on the kets $|A_i B_i\rangle$):

$$|\psi_{\vec{\lambda}}\rangle = \sum_{i=0}^{N_A-1} \sqrt{\lambda_i}|A_i B_i\rangle \leftrightarrow \tilde{\rho}_{\vec{\lambda}} = \sum_{i=0}^{N_A-1} \lambda_i |A_i B_i\rangle\langle A_i B_i|, \tag{5}$$

from which we get $\mathcal{E}(|\psi_{\vec{\lambda}}\rangle) = S(\tilde{\rho}_{\vec{\lambda}})$. Moreover, after introducing

$$\tilde{H} = \sum_{i=0}^{N_A-1} E_i |A_i B_i\rangle\langle A_i B_i|, \tag{6}$$

we can express the average energy in terms of the density operator $\tilde{\rho}_{\vec{\lambda}}$ because $\langle\psi_{\vec{\lambda}}|H|\psi_{\vec{\lambda}}\rangle = \mathrm{Tr}\{\tilde{H}\tilde{\rho}_{\vec{\lambda}}\}$. Thus, the problem of minimizing $E_{\vec{\lambda}}$ with respect to $\vec{\lambda}$ for a given degree of entanglement $\mathcal{E}$ is equivalent to finding the diagonal density matrix $\tilde{\rho}_g$ that minimizes energy when its entropy $S = \mathcal{E}$ is fixed. In Sec. II of the SM [40], we show that, if $\mathcal{E} > \ln d_g$ where $d_g \geqslant 1$ is the number of $\tilde{H}$ eigenstates with lowest energy ($E_{d_g-1} = \cdots = E_1 = E_0$), the density matrix we search is the thermal state

$$\tilde{\rho}_g = \frac{e^{-\beta_g \tilde{H}}}{Z_g}, \quad Z_g = \mathrm{Tr}\{e^{-\beta_g \tilde{H}}\}, \tag{7}$$

with respect to the fictitious Hamiltonian $\tilde{H}$ and inverse temperature β_g obtained as the positive solution of

$$\left(-\beta_g \frac{\partial}{\partial \beta_g} + 1\right) \ln Z_g = \mathcal{E}. \tag{8}$$

In view of Eq. (5), this density operator corresponds (up to phase factors) to a minimum energy state given by

$$|\psi_g\rangle = \frac{1}{\sqrt{Z_g}} \sum_{i=0}^{N_A-1} e^{-\frac{\beta_g}{2}(A_i+B_i)}|A_i B_i\rangle. \tag{9}$$

Its energy can be easily calculated as $E_g = -\partial_{\beta_g} \ln Z_g$. We stress that Eq. (8) can be solved numerically in a straightforward way and that, in the two-qubit case, analytical expressions can be found.

We observe that the state of Eq. (9) is not the unique state with minimal energy. Every other state that can be reached from it through the application of local and energy-conserving unitary operators fulfills this request (see Sec. II of the SM [40] for more details).

To conclude our analysis we consider the case $\mathcal{E} \leqslant \ln d_g$. In such a situation, the minimum energy is E_0 and a minimum energy pure state can be searched in the ground-energy eigenspace so that the problem is trivial.

It is worth stressing that our treatment is valid for every finite N_A and N_B, even immensely large. Therefore, on a physical ground, we conjecture that our analysis holds good even for discrete Hilbert spaces of infinite dimensions, as in the case of two harmonic oscillators.

Maximum energy and corresponding states. The result can be easily obtained by searching for the minimum energy state when considering the Hamiltonians $\bar{H}_{A(B)} = -H_{A(B)}$. Hence, if $\mathcal{E} > \ln d_e$, where d_e is the lowest of the degeneracies of the maximum eigenvalues of H_A and H_B, a maximum energy state is given by

$$|\psi_e\rangle = \frac{1}{\sqrt{Z_e}} \sum_{i=0}^{N_A-1} e^{\frac{\beta_e}{2}(A_i+B_{i+\Delta})}|A_i B_{i+\Delta}\rangle, \tag{10}$$

where $\Delta = N_B - N_A$, $Z_e = \sum_{i=0}^{N_A-1} e^{\beta_e(A_i+B_{i+\Delta})}$, and β_e is the positive solution of the equation $(-\beta_e\partial_{\beta_e} + 1)\ln Z_e = \mathcal{E}$. Similarly to the minimum energy case, the energy of $|\psi_e\rangle$ can be easily calculated as $E_e = \partial_{\beta_e} \ln Z_e$.

The same considerations made for the minimum energy case about the uniqueness of the state hold good here. If $\mathcal{E} \leqslant \ln d_e$, then the maximum energy is $A_{N_A-1} + B_{N_B-1}$ and a maximum energy pure state can be searched in the eigenspace of the highest possible energy.

We finally observe that the minimization (maximization) process we have developed can be easily extended to any other couple of local observables. Indeed, whatever is the local operator $O = O_A + O_B$ we want to minimize (maximize) for an assigned value of entanglement, we can simply assume that $H_X = O_X$.

Energy-entanglement distribution. It is worth commenting at this point about the energy distribution of the states corresponding to the same amount of entanglement. We have made several numerical simulations finding, in all the studied configurations, that the density of states in the proximity of the bounding curves is extremely low, except for the two-qubit case and highly degenerate cases. In fact, the main part of the states occupy the intermediate region, and the discrepancy between the peripheral and central densities becomes higher and higher as the dimensionality of the systems increases. We report here, as an example, the density of states corresponding to two local Hamiltonians having spectra given by $\sigma(H_A) = \{0, 2, 4\}$ and $\sigma(H_B) = \{0, 1, 6, 9\}$ in arbitrary units. In particular, in Fig. 1 we show the two curves defining the energy bounds for assigned entanglement and the distribution of a large number of randomly generated pure states [41] (the behavior of β_g and β_e is shown in Sec. II of the SM

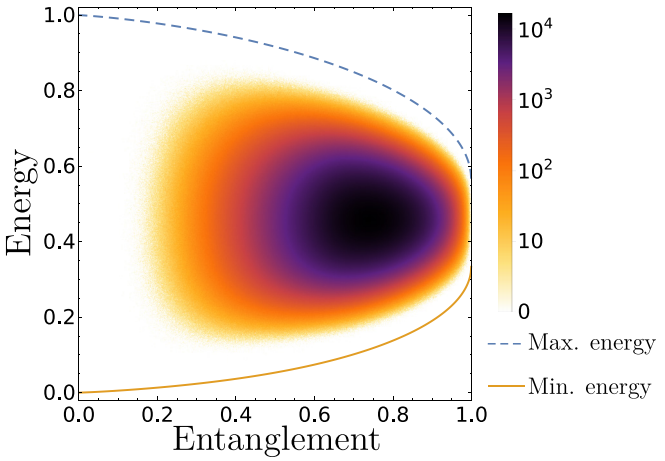

FIG. 1. Distribution of 10^9 randomly generated pure states with respect to the entropy of entanglement and the local energy in a 1000×1000 grid. The Hamiltonians have spectra: $\sigma(H_A) = \{0, 2, 4\}$ and $\sigma(H_B) = \{0, 1, 6, 9\}$ in arbitrary units. Both the entanglement and the energy are normalized with respect to their maxima.

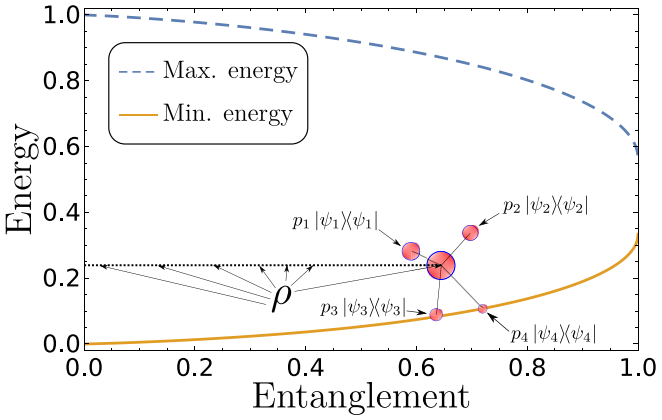

FIG. 2. Representation of the energy-entanglement relation for a mixed state obtained as a convex sum of four pure states. The assigned energy value (obtained as the average of the energies of the pure states) and the possible values of entanglement (from zero to the average of the entanglement values of the single pure states) identify a segment. This segment always lies between the curves of minimum and maximum energy because of their monotonicity and convexity properties.

[40]). It is well visible that the majority of the states lies in the central zone, while none of the generated states is very close to the bounding curves. This circumstance allows one to better appreciate the relevance of our results since, for example, in an entanglement generation process, one could choose to generate the state $|\psi_g\rangle$ having the lowest energy for the desired amount of entanglement, instead of any of all the other states which require more energy. We finally observe that the randomly generated states numerically satisfy the known theoretical expected averages both in entanglement and energy [42–44].

Two-qubit system. Now we apply our general results to the case of two qubits, i.e., to the case $N_A = N_B = 2$. By using the purity P [where $P(\rho) = \mathrm{Tr}\{\rho^2\}$] of one of the reduced states instead of the entropy of entanglement $\mathcal{E}$ as entanglement quantifier, it is possible to obtain through straightforward calculations closed analytical expressions both for the minimum and maximum energy states and for the energy bounds using Eqs. (9) and (10). This is possible thanks to the fact that for a two-qubit system the Von Neumann entropy and the purity can be bijectively connected. Starting from $|\psi_g\rangle = \sqrt{\lambda}|A_0B_0\rangle + \sqrt{1-\lambda}|A_1B_1\rangle$ and imposing $(1-\lambda)/\lambda = \exp[-\beta_g(E_1 - E_0)]$, one can easily obtain $\beta_g = -(E_1 - E_0)^{-1}\ln[(1-\lambda)/\lambda]$, where $\lambda = (1 + \sqrt{2P-1})/2$. Analogously, one can find $\beta_e = \beta_g$. Moreover, we can express the energy bounds as $E_g = \lambda E_0 + (1-\lambda)E_1$ and $E_e = (1-\lambda)E_0 + \lambda E_1$.

Mixed states. We now show that the bounds derived above are still valid even when we extend the analysis to mixed states. Contrarily to the pure state case, a standard entanglement quantifier does not exist [3]. However, it is in general required that the convexity property is satisfied [38,39], i.e., for any arbitrary quantifier $\mathcal{E}_m$

$$\rho = \sum_i p_i \rho_i \Rightarrow \mathcal{E}_m(\rho) \leqslant \sum_i p_i \mathcal{E}_m(\rho_i), \tag{11}$$

where $p_i \geqslant 0\ \forall i$ and $\sum_i p_i = 1$. In addition, we make the standard assumption that $\mathcal{E}_m$ applied to pure states is equal to the entropy of entanglement [39]. In Sec. III of the SM [40], we show that this assumption can be relaxed.

Every mixed state can be written as a combination of pure states, $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. Thus, every mixed state has energy equal to $\mathrm{Tr}\{H\rho\} = \sum_i p_i \langle\psi_i|H|\psi_i\rangle$ and entanglement $\mathcal{E}_m(\rho) \leqslant \sum_i p_i \mathcal{E}_i$, where $\mathcal{E}_i = \mathcal{E}_m(|\psi_i\rangle)$. Since one can prove (see Sec. III of the SM [40]) that the curves $E_g(\mathcal{E})$ and $E_e(\mathcal{E})$ are, respectively, the former increasing and convex, and the latter decreasing and concave, the following chain of relations holds:

$$\mathrm{Tr}\{H\rho\} \geqslant \sum_i p_i E_g(\mathcal{E}_i) \geqslant E_g\left(\sum_i p_i \mathcal{E}_i\right) \geqslant E_g(\mathcal{E}_m(\rho)). \tag{12}$$

Analogously, it holds that $\mathrm{Tr}\{H\rho\} \leqslant E_e(\mathcal{E}_m(\rho))$.

It follows that, in an energy-entanglement graph, every mixed state can be found on a segment that is entirely between the minimum and maximum energy curves. In Fig. 2 an example of this situation is clearly shown.

Connections with thermodynamics, entanglement Hamiltonian, and LOCC. The minimum and maximum energy states are characterized by coefficients that can be directly linked to the Boltzmann factors of a fictitious thermal state and, as a consequence, their energy can be calculated through their fictitious partition function. This is worth mentioning because entanglement and thermodynamics are believed to be conceptually connected in the context of typicality [44,45] and they have various formal analogies when treated within resource theories such as local operations and classical communication (LOCC) and thermodynamic resource theory (TRT) [3,46,47]. In fact, a connection with thermodynamics has been also found in the study conducted in Ref. [48]. There, the authors dealt with the problem of creating the maximum amount of correlations (quantified by mutual information) by employing a limited amount of energy, through the application of

a unitary operator. They considered noninteracting bipartite systems starting from thermal product states. In the zero-temperature limit, since the mutual information is twice the entropy of entanglement, their problem coincides with our search for the minimum energy states for a given amount of entanglement. Indeed, they have found that to maximize the correlations one has to generate states of the form of Eq. (9) [49]. Their proof relies on the concept of passive states (states the energy of which cannot be lowered by unitary operations), thus providing an additional link between our results and the field of thermodynamics.

It is also interesting to consider the limit case of Eq. (9) when $B_{N_A-1} = B_{N_A-2} = \cdots = B_0$. In this case, the reduced state of A, $\rho_g^A \equiv \mathrm{Tr}_B\{|\psi_g\rangle\langle\psi_g|\}$, is equal to

$$\rho_g^A = \frac{1}{Z_g}\sum_{i=0}^{N_A-1} e^{-\beta_g A_i}|A_i\rangle\langle A_i|, \quad Z_g = \sum_{i=0}^{N_A-1} e^{-\beta_g A_i}, \tag{13}$$

which is a thermal state with respect to H_A at temperature $T = 1/(k_B\beta_g)$, where k_B is the Boltzmann constant. This result can be easily obtained without using Eq. (9) since in this limit the problem reduces to find the minimum energy state for a fixed entropy of subsystem A.

Our results also present connections with some studies based on the entanglement Hamiltonian formalism. Indeed, when $N_A = N_B$, the reduced states of $|\psi_g\rangle$ are ($\rho_g^B \equiv \mathrm{Tr}_A\{|\psi_g\rangle\langle\psi_g|\}$)

$$\rho_g^{A(B)} = \frac{1}{Z_g} e^{-\beta_g \mathrm{Tr}_{B(A)}\{\tilde{H}\}}. \tag{14}$$

Thus, the reduced states have been easily written in the entanglement Hamiltonian formalism (this can be done for ρ_g^A even when $N_A < N_B$), which has been proved to be useful to get various insights into solid-state physics research [50–54]. In Sec. IV of the SM [40], we show that some many-body systems of interest are characterized, under appropriate approximations [52], by ground states belonging to the family of minimal energy states for a given entanglement.

Lastly, we point out that minimum or maximum energy states with respect to the same local Hamiltonians are connected through one-shot LOCC (see Sec. V of the SM [40] for the proof). This has two direct implications. The first one is that, given any pure state $|\psi\rangle$, one can immediately write down a family of states that are LOCC connected to it (see Sec. V of the SM [40]). The second one is that if two distant parties share a minimum energy state having more entanglement than needed, they can recover, with certainty, the maximum amount of local energy compatible with the needed entanglement.

Connections to quantum technologies. Our results are particularly relevant in protocols exploiting partially entangled qudits. Although maximally entangled states are requested in many applications, nonmaximally entangled states have been proven useful in quantum technologies, for example in processes involving two-mode squeezed states [55,56], in quantum telecloning of qudits [57,58], and in probabilistic quantum teleportation [59]. In the last two cases, our results allow one to implement the procedure by exploiting less expensive entangled states, through the direct utilization of minimum energy states or of Theorem 1 (see Sec. VI of the SM [40]).

More in general, in the LOCC asymptotic limit, n copies of a state $|\phi\rangle$ can be converted to m copies of a state $|\phi'\rangle$ if and only if $n\mathcal{E}(|\phi\rangle) \geqslant m\mathcal{E}(|\phi'\rangle)$, with $n, m \to \infty$, thus making the entropy of entanglement the quantifier of the resource entanglement [11]. For example, Bell states can always be obtained by entanglement distillation [11]. In this framework, given a certain amount of energy, it is then particularly relevant that it is possible to generate more entanglement overall by producing many copies of our minimum energy states with nonmaximal entanglement (see Sec. VII of the SM [40]).

Our results also permit one to identify bounds in the production of pure entangled states within the framework of the TRT, which has recently drawn a lot of attention [47,60]. Its goal is to study what states are reachable through thermal operations given an arbitrary starting state ρ and the environmental temperature T. Since the energy amount of reachable states from the state ρ is bounded, when TRT is equipped with our results, it lets us individuate which are the reachable pure states with the maximum allowed degree of entanglement. Indeed, allowing the use of catalysts [60], the state we search is one of our minimum energy states with energy equal to $\mathrm{Tr}\{\rho(H_A + H_B)\} - k_B T S(\rho)$.

We have also proven, under the conjecture that our analysis is valid also in the case of discrete Hilbert spaces of infinite dimensions, that two-mode squeezed states are minimum energy states for a given amount of entanglement (see Sec. VIII of the SM [40]). Therefore, these states, extensively exploited in quantum optics laboratories [55,56,61,62], are the most energetically convenient states to generate. In general, a possible way to generate minimum energy states is to exploit dissipative processes leading to a unique steady state, such as simple zero-temperature thermalizations [63]. In this case, choosing a suitable interaction Hamiltonian leads the bipartite system to the desired state, i.e., the ground state. We give an example of this process for a two-qubit system and for a two-harmonic-oscillator system in Sec. IX of the SM [40]. Such kind of processes involving a simple thermalization have been studied, for example, in Ref. [64].

Conclusive remarks. In summary, we have found the minimum and maximum permitted local energy of an arbitrary finite bipartite system for a given quantity of entanglement, also reporting the explicit form of a family of minimum and maximum energy states. Then, we have numerically investigated the energy distribution of entangled pure states, finding, in all the studied configurations, that the probability of randomly generating states with a fixed entanglement close to the energy bounds is extremely low except for the two-qubit case and highly degenerate cases.

Our results can be important in quantum technologies since, given the degree of entanglement necessary for a certain application, our approach allows one to identify a class of states having this entanglement and whose generation requires the lowest energy cost. Such an identification appears even more important also in the light of our numerical simulations, showing that the energies of the majority of the states with a fixed entanglement typically lie quite far from the energy bounds. Finally, we stress that Theorem 1 can bring by itself great practical advantages in optimization problems

depending exclusively on the Schmidt coefficients, given some energy constraints, as discussed in detail in Sec. VI of the SM [40].

Acknowledgments. N.P. thanks Mauro Paternostro, Andrea Smirne, Jan Sperling, and Alexander Streltsov for useful discussions about the results of this Rapid Communication.

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