# Frustration, interaction strength, and ground-state entanglement in complex quantum systems

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Entanglement in the ground state of a many-body quantum system may arise when the local terms in the system Hamiltonian fail to commute with the interaction terms in the Hamiltonian. We quantify this phenomenon, demonstrating an analogy between ground-state entanglement and the phenomenon of frustration in spin systems. In particular, we prove that the amount of ground-state entanglement is bounded above by a measure of the extent to which interactions *frustrate* the local terms in the Hamiltonian. As a corollary, we show that the amount of ground-state entanglement is bounded above by a ratio between parameters characterizing the strength of interactions in the system, and the local energy scale. Finally, we prove a qualitatively similar result for other energy eigenstates of the system.

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## I. INTRODUCTION

A central problem in physics is understanding the ground-state properties of a complex many-body Hamiltonian, especially the ground-state correlations. As an outgrowth of that interest, there has recently been considerable work on understanding the *nonclassical* correlations in the ground state, that is, the *ground-state entanglement*. Some recent work on this problem, with further references, includes Refs. [1–15,32]. This work has been motivated by the remarkable recent progress in using entanglement as a physical resource to accomplish feats such as quantum computation and quantum teleportation.[1]

In this paper we connect the phenomenon of ground-state entanglement to a well-known idea in condensed-matter physics, that of *frustration*, which we now briefly review. More detailed introductions may be found in Ref. [18]. A typical example of a frustrated spin system is shown in Fig. 1. It consists of a triangular arrangement of three spin-$\frac{1}{2}$ particles, each pair being coupled by a classical antiferromagnetic coupling ($+J\sigma_z\sigma_z$, with positive coupling strength $J$). The antiferromagnetic coupling means that neighbors prefer to be antialigned in order to minimize their interaction energies. However, a little thought shows that it is impossible for all three spins to simultaneously be antialigned with each of their neighbors. It is therefore not possible to simultaneously minimize all three interaction energies, and the system is said to be *frustrated* for this reason. The ground state of the Hamiltonian is a compromise between the minimum-energy states of the interaction terms.

Let us consider an analogous example in which frustration arises not from the difficulty of choosing simultaneously compatible spin configurations, but rather from choosing simultaneously compatible *bases* for Hilbert space. For example, consider a system of two spin-$\frac{1}{2}$ particles with Hamiltonian $H=-g(\sigma_x^1+\sigma_x^2)-\sigma_z^1\sigma_z^2$, where the superscripts indicate which spin the operators act on, and $\sigma_x$, $\sigma_y$, and $\sigma_z$ are the usual Pauli spin operators. The ground state of this system arises as the result of a competitive process between minimizing the contribution to the energy from the local Hamiltonian, $-g(\sigma_x^1+\sigma_x^2)$, and from the interaction Hamiltonian, $-\sigma_z^1\sigma_z^2$. Of course, because these two Hamiltonians do not have common eigenvectors, the actual ground state cannot possibly minimize both simultaneously, and must be a compromise between the respective ground states of the local and interaction Hamiltonians.

This example suggests a connection between the ground-state entanglement and a generalized concept of frustration. If the interaction term in the Hamiltonian were turned off,

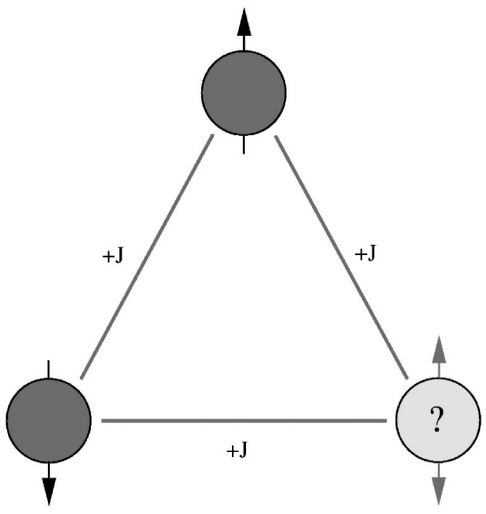


FIG. 1. A system containing three spin-$\frac{1}{2}$ particles, coupled by a classical antiferromagnetic coupling ($+J\sigma_z\sigma_z$, with positive coupling strength $J$) favoring antialignment. There is no way all the competing coupling energies can be simultaneously minimized; for this reason we say the system is *frustrated*.

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[1]See, Refs. [16,17] for reviews and further references.

 

the system would sit in an unentangled state—the ground state of the local Hamiltonian. As the interaction term is turned on, it causes the local Hamiltonian to become frustrated. As a result, the ground state sits in a basis which is a compromise between the unentangled basis of the local Hamiltonian, and the basis for the interaction Hamiltonian. Provided the interaction was chosen appropriately, the result will be an entangled ground state. Furthermore, it is clear that the more frustrated the local Hamiltonian is by the interaction, the greater the potential entanglement in the ground state.

The main result of this paper is a bound that makes these intuitive ideas quantitatively precise. Our paper thus illustrates a general idea discussed in Refs. [1,14,19–22], namely, that quantum information science provides tools and perspectives for understanding the properties of complex quantum systems, complementary to the existing tools of quantum many-body physics.

We begin in Sec. II by reviewing some basic material on quantitative measures of entanglement. In Sec. III we prove a general, nonperturbative bound on the ground-state entanglement, relating it to the extent to which the interaction Hamiltonian frustrates the local Hamiltonian. We call this the "entanglement-frustration" bound. The proof of the bound is conceptually and mathematically extremely simple. Its interest lies in illustrating quantitatively a connection between two apparently disparate physical phenomena, and in the consequences which follow from this connection, to be discussed in later sections.

In Sec. IV we apply the entanglement-frustration bound to an illustrative example. Using this example, we determine necessary conditions for the bound to saturate the ground-state entanglement. It is then shown by construction that it is possible to come arbitrarily close to saturation for all possible values of the ground-state entanglement, and we conclude that the entanglement-frustration bound is thus the strongest possible bound of its type.

Aside from its intuitive appeal and immediate relevance, the entanglement-frustration bound has an elegant corollary described in Sec. V. Intuitively, it is clear that the ground-state entanglement of a Hamiltonian $H=H_L+H_I$ is small if the size of the interaction $H_I$ is small compared with some appropriate local energy scale associated with $H_L$. Indeed, it is straightforward to use perturbation theory to demonstrate a bound along these lines, valid in the limit when $H_I$ is a small perturbation. The entanglement-frustration bound allows us to prove a general nonperturbative bound quantifying this intuition. This corollary is proved in Sec. V. Section VI generalizes these results so that they apply to *arbitrary* eigenstates of the Hamiltonian, not just the ground state. This is done using methods quite different from those used in Sec. V, using a variant on a powerful theorem from linear algebra known as the Davis-Kahan theorem.

The results in Secs. III–V provide a compelling picture of how ground-state entanglement arises as the result of frustration between competing local and interaction terms in the system Hamiltonian. Section VI generalizes some of these results to apply to other energy eigenstates as well. The paper concludes in Sec. VII with a discussion of some possible extensions to this work.

## II. BACKGROUND ON ENTANGLEMENT MEASURES

To make our ideas precise we must introduce a quantitative measure of the amount of entanglement in the ground state of a quantum system. A major focus of research in quantum information science over the past few years has been developing such a theory of entanglement,[2] and several good candidate measures exist. We shall use a measure of entanglement introduced in Refs. [25,26]. For an $n$-body quantum system in a state $\psi$ this entanglement measure is defined by[3]

$$E(\psi) \equiv 1 - \max_{\psi_1,\ldots,\psi_n} |\langle\psi|\psi_1 \otimes \cdots \otimes \psi_n\rangle|^2. \tag{1}$$

That is, $E(\psi)$ measures the maximal overlap $\psi$ has with a product state $\psi_1 \otimes \cdots \otimes \psi_n$ of the $n$ bodies making up the system.

What makes $E(\psi)$ a good entanglement measure? References [25,26] investigated the properties of $E(\psi)$ and found that it has many properties that make it a good measure of entanglement. These properties include the fact that: (i) $E(\psi)$ can only decrease, never increase, under local operations and classical communication, i.e., it is an entanglement monotone; and (ii) $E(\psi)$ is zero if and only if $\psi$ is unentangled, and otherwise is positive. In addition, an interesting connection has been found [27] between $E(\psi)$ and the theory of quantum algorithms, with $E(\psi)$ being related to the probability of success of an algorithm whose initial state is equivalent to $\psi$, up to a local unitary transformation.

## III. ENTANGLEMENT-FRUSTRATION BOUND

The general scenario we consider is an $n$-body quantum system with Hamiltonian $H=H_L+H_I$. $H_L$ is a *local Hamiltonian* consisting of single-body or *local* terms, and therefore has an eigenbasis of unentangled states. $H_I$ contains all the remaining terms in the Hamiltonian, and is called the *interaction Hamiltonian*.

We let $E_0$ be the global ground-state energy, i.e., the ground-state energy of $H$, with $|E_0\rangle$ any corresponding ground state. Similarly $E_0^L$ and $E_0^I$ are defined to be the local and interaction ground-state energies, respectively, for $H_L$ and $H_I$. We define the *frustration energy* of the system as $E_f \equiv E_0 - E_0^L - E_0^I$. The frustration energy thus measures the extent to which the global ground state fails to simultaneously minimize the local and interaction energies. It is easily shown from matrix eigenvalue inequalities that $E_0 \geqslant E_0^L + E_0^I$, so $E_f$ is always a non-negative quantity, and is equal to zero if and only if $H_L$ and $H_I$ have a common ground state.

Our aim is to relate the amount of entanglement in the ground state, $E(|E_0\rangle)$, to the frustration energy $E_f$. Of course, to relate the dimensionless quantity $E(|E_0\rangle)$ to $E_f$, which has

[2] See e.g., Refs. [23,24] for an introduction and further references on the theory of entanglement.

[3] Note that this measure is a slightly rescaled version of that in Refs. [25,26], but has essentially the same properties. In the present context the rescaled definition turns out to be easier to work with.

TABLE I. Quantities important in derivation of the entanglement-frustration bound.

| Quantity | Description |
|---|---|
| $E_j$, $\|E_j\rangle$ | $j$th energy eigenvalue and corresponding eigenvector of the total Hamiltonian $H$ |
| $E_j^L$, $\|E_j^L\rangle$ | $j$th energy eigenvalue and eigenvector of the local Hamiltonian $H_L$ |
| $E_j^I$, $\|E_j^I\rangle$ | $j$th energy eigenvalue and eigenvector of the interaction Hamiltonian $H_I$ |
| $\Delta E^l$ | Excitation gap between the ground and first excited energies of the $l$th subsystem Hamiltonian $H_l$ |
| $\Delta E_{\text{ent}}$ | Minimum energy required to excite at least two subsystems of $H_L$, equal to the second smallest of the $\Delta E^l$ above |
| $E_f$ | Frustration energy $E_f = E_0 - E_I - E_L$ |

units of energy, we require another energy scale in the system. The relevant energy scale turns out to be associated with local excitations of the system. Suppose we decompose $H_L$ as $H_1 + H_2 + \cdots + H_n$, where $H_l$ is the contribution to the local Hamiltonian from the $l$th subsystem. The energy scale we will refer to is the gap between the ground and first excited energies. The term "gap" is often used in two different senses, in some cases it refers to the energy difference between the ground state and the first excited state with a strictly higher energy. We will use the alternative sense where the gap $\Delta E^l$ is zero if $H_l$ has a degenerate ground state.

Now let $\Delta E^l$ denote the gaps between the ground and first excited energies for each $H_l$, and let $\Delta E_{\text{ent}}$ be the *second smallest* of these energies. That is, suppose we choose $l_0, l_1, \ldots$ such that $\Delta E^{l_0} \leqslant \Delta E^{l_1} \leqslant \cdots$. Then $\Delta E_{\text{ent}} = \Delta E^{l_1}$. For the convenience of the reader we have placed brief descriptions of these quantities in Table I.

Physically, $\Delta E_{\text{ent}}$ is the energy we need to put into a system with Hamiltonian $H_L$ in order to cause an excitation from the ground state into an excited state of either system $l_0$ *or* system $l_1$. It is thus the minimal amount of energy that we would need to put into the system in order to cause entanglement in the ground state, since merely exciting one system, while leaving the others alone, leaves the system still in a product state.

Our result relating the ground-state entanglement to the frustration energy and $\Delta E_{\text{ent}}$ is the inequality

$$E(|E_0\rangle) \leqslant \frac{E_f}{\Delta E_{\text{ent}}}. \tag{2}$$

We call this the *entanglement-frustration* bound. This bound tells us that when the frustration energy is small compared with $\Delta E_{\text{ent}}$, there cannot possibly be much entanglement in the ground state of the system. Thus it is only systems in which the interaction and local terms substantially frustrate one another that it is possible to have a highly entangled ground state.

The first step in the proof of the entanglement-frustration bound, Eq. (2), is to prove that

$$\langle E_0|H_L|E_0\rangle - E_0^L \leqslant E_f. \tag{3}$$

Physically, this is just the obvious statement that the extent to which the local Hamiltonian is frustrated is no larger than the total frustration in the system. The proof is simply to split the frustration energy into a sum of contributions from the local and interaction frustration energies:

$$E_f = \langle E_0|H|E_0\rangle - E_0^L - E_0^I \tag{4}$$

$$= (\langle E_0|H_L|E_0\rangle - E_0^L) + (\langle E_0|H_I|E_0\rangle - E_0^I). \tag{5}$$

The inequality of Eq. (3) now follows from the observation that $\langle E_0|H_I|E_0\rangle \geqslant E_0^I$.

The second step in the proof of the entanglement-frustration bound is to expand $|E_0\rangle$ in terms of the eigenstates $|E_j^L\rangle$ of $H_L$, $|E_0\rangle = \Sigma_j\, \alpha_j |E_j^L\rangle$. We assume that the local energies are ordered so that $E_0^L \leqslant E_1^L \leqslant \cdots$. We now split the expansion of $|E_0\rangle$ into terms with energies below $E_0^L + \Delta E_{\text{ent}}$, and into terms with energies at least $E_0^L + \Delta E_{\text{ent}}$, that is,

$$|E_0\rangle = \sum_{j=0}^{k} \alpha_j |E_j^L\rangle + \gamma |E_\perp\rangle, \tag{6}$$

where (i) $k$ is the largest integer such that $E_k^L < E_0^L + \Delta E_{\text{ent}}$, and thus $E_{k+1}^L = E_0^L + \Delta E_{\text{ent}}$; (ii) $|E_\perp\rangle$ is a normalized state containing all the terms of energy at least $E_0^L + \Delta E_{\text{ent}}$, and thus is orthogonal to the lower energy terms; and (iii) $\gamma$ is the amplitude for $|E_\perp\rangle$, and thus satisfies $|\gamma|^2 = 1 - \Sigma_{j=0}^{k} |\alpha_j|^2$.

For later use it is important to note that $\Sigma_{j=0}^{k} \alpha_j |E_j^L\rangle$ is a product state, as all the terms $|E_j^L\rangle$ involve excitations of the *same subsystem* (system $j_0$, to return to the notation used earlier in defining $\Delta E_{\text{ent}}$). Furthermore, its overlap squared with $|E_0\rangle$ is given by $\Sigma_{j=0}^{k} |\alpha_j|^2$.

Returning to the main line of the proof, from Eq. (6) we have

$$\langle E_0|H_L|E_0\rangle = \sum_{j=0}^{k} |\alpha_j|^2 E_j^L + |\gamma|^2 \langle E_\perp|H_L|E_\perp\rangle. \tag{7}$$

But $E_j^L \geqslant E_0^L$, $\langle E_\perp|H_L|E_\perp\rangle \geqslant E_0^L + \Delta E_{\text{ent}}$, and $|\gamma|^2 = 1 - \Sigma_{j=0}^{k} |\alpha_j|^2$, so

$$\langle E_0|H_L|E_0\rangle \geqslant \sum_{j=0}^{k} |\alpha_j|^2 E_0^L + \left(1 - \sum_{j=0}^{k} |\alpha_j|^2\right)(E_0^L + \Delta E_{\text{ent}}). \tag{8}$$

Rearrangement of this inequality gives

$$\langle E_0|H_L|E_0\rangle - E_0^L \geqslant \left(1 - \sum_{j=0}^{k} |\alpha_j|^2\right) \Delta E_{\text{ent}}. \tag{9}$$

Combining Eqs. (3) and (9) we have

$$\left(1-\sum_{j=0}^{k}|\alpha_j|^2\right)\leqslant\frac{E_f}{\Delta E_{\text{ent}}}. \tag{10}$$

Our desired result, Eq. (2), will follow if we can establish that $E(|E_0\rangle)\leqslant(1-\Sigma_{j=0}^{k}|\alpha_j|^2)$. This follows immediately from the definition of the entanglement measure, Eq. (1), and the observation we made earlier in the proof, that $|E_0\rangle$ and the product state $\Sigma_{j=0}^{k}\alpha_j|E_j^L\rangle$ have overlap squared $\Sigma_{j=0}^{k}|\alpha_j|^2$.

## IV. APPLICATION AND SATURATION OF THE ENTANGLEMENT-FRUSTRATION BOUND

In this section we consider two separate but related issues. First, in Sec. IV A we apply the entanglement-frustration bound to an illustrative and physically relevant Hamiltonian, the two-spin transverse Ising model. This example is used to develop insight into the question of when the entanglement-frustration bound is saturated. Building on these insights, we analyze this question in more generality in Sec. IV B, showing that the entanglement-frustration bound can be saturated for all possible values of the ground-state entanglement. Thus there is a sense in which the entanglement-frustration bound is the best possible bound of its type.

### A. Two-spin transverse Ising model

As an illustrative example, consider a system of two spin-$\frac{1}{2}$ particles evolving under a transverse Ising Hamiltonian,

$$H=-g(\sigma_x^1+\sigma_x^2)-\sigma_z^1\sigma_z^2. \tag{11}$$

In this model, the two particles are coupled magnetically along their $z$ axes, and interact with an external magnetic field of strength $g$ directed along the $x$ axis. For the purposes of this example we take $g\geqslant 0$. The $g<0$ analysis is similar, but it simplifies the discussion to pick a definite value for the sign of $g$.

Note that while the two-spin transverse Ising model is mathematically rather trivial, it has genuine physical interest. Furthermore, we will find that it is surprisingly informative as a way of understanding the conditions under which the entanglement-frustration bound is saturated. For these reasons we describe the results in some detail.

Physically, $g\to 0$ is the strong-coupling limit, where we expect the ground state to become quite entangled. We will see in detail below that it becomes maximally entangled in this limit, i.e., $E(|E_0\rangle)\to\frac{1}{2}$, for our entanglement measure. In contrast, $g\to\infty$ is the weak-coupling limit, and we expect that the ground state should be a product state in that limit, $E(|E_0\rangle)\to 0$.

The ground-state energy of Eq. (11) is easily found to be $E_0=-\sqrt{1+4g^2}$, and the ground state is

$$|E_0\rangle=\frac{1}{\sqrt{N}}[(2g+\sqrt{1+4g^2})|++\rangle+|--\rangle], \tag{12}$$

where $N=1+(2g+\sqrt{1+4g})^2$ is a normalization constant, and $|\pm\rangle\equiv(|0\rangle\pm|1\rangle)/\sqrt{2}$. Note that $|E_0\rangle$ is in its Schmidt form, with largest Schmidt coefficient[4] $\lambda_0=(2g+\sqrt{1+4g^2})/\sqrt{N}$. The ground-state entanglement is given by $1-\lambda_0^2$, which simplifies to

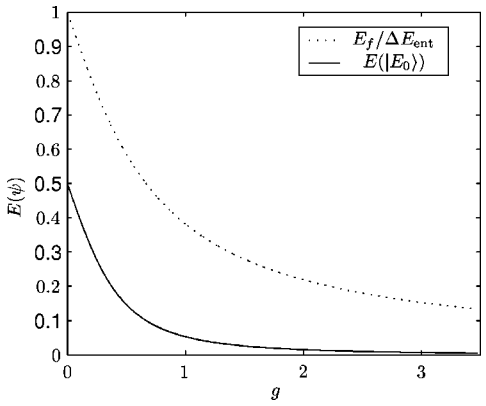


FIG. 2. The ground-state entanglement and entanglement-frustration bound for the transverse Ising Hamiltonian (11) plotted against the parameter $g$.

$$E(|E_0\rangle)=\frac{1}{2}-\frac{g}{\sqrt{1+4g^2}}. \tag{13}$$

To calculate the entanglement-frustration bound we must first split the Hamiltonian into a local and interaction part, $H_L=-g(\sigma_x^1+\sigma_x^2)$, and $H_I=-\sigma_z^1\sigma_z^2$. With these choices we find that $E_0^L=-2g$ and $E_0^I=-1$. The two spin systems each have the same local energy spectrum with the gap between the ground and excited states being $2g$, so we have $\Delta E_{\text{ent}}=2g$. This gives the entanglement-frustration bound

$$\frac{E_f}{\Delta E_{\text{ent}}}=\frac{1+2g-\sqrt{1+4g^2}}{2g}. \tag{14}$$

A comparison of the quantities appearing in Eqs. (13) and (14) is shown in Fig. 2. Both the ground-state entanglement and the entanglement-frustration bound decrease sharply as $g$ increases from 0. For these small values of $g$ the bound is approximately double the entanglement. As $g$ increases further the ground-state entanglement decreases rapidly to 0, while the bound decreases to 0 more slowly. The entanglement-frustration bound is clearly not very tight in this case, although the qualitative behavior of the bound and the actual ground-state entanglement is similar.

We can identify two reasons for the failure to saturate the entanglement-frustration bound in this example. First, in the language of Sec. III, the quantity $\langle E_\perp|H_L|E_\perp\rangle$ is strictly larger than $E_0^L+\Delta E_{\text{ent}}$. We see from Eq. (12) that $|E_\perp\rangle=|--\rangle$, and thus $\langle E_\perp|H_L|E_\perp\rangle=E_0^L+2\Delta E_{\text{ent}}$. It follows that

$$\langle E_0|H_L|E_0\rangle=\lambda_0^2E_0^L+(1-\lambda_0^2)(E_0^L+2\Delta E_{\text{ent}}) \tag{15}$$

and upon substitution into Eq. (5) this gives

[4]By contrast, if $g<0$ the largest Schmidt coefficient is $\lambda_0=1/\sqrt{N}$. This is the main difference between the $g<0$ and $g\geqslant 0$ cases.

$$E_f = 2\Delta E_{\text{ent}}(1-\lambda_0^2) + \langle E_0|H_I|E_0\rangle - E_0^I \tag{16}$$

or

$$\frac{E_f}{\Delta E_{\text{ent}}} = 2E(|E_0\rangle) + \frac{\langle E_0|H_I|E_0\rangle - E_0^I}{\Delta E_{\text{ent}}}. \tag{17}$$

The entanglement-frustration bound is therefore at least twice the ground-state entanglement with this choice of $H_L$, for all values of $g$.

The second contribution to the excess is the term $(\langle E_0|H_I|E_0\rangle - E_0^I)/\Delta E_{\text{ent}}$. Physically, this is the ratio of the frustration of the interaction energy to the local energy scale. The excess sharply increases from 0 for small $g$, and decreases slowly as $g\to\infty$. For $g$ greater than about 2 the ground-state entanglement is close to 0 and the entanglement-frustration bound is composed almost entirely of this excess term.

### B. Saturation of the entanglement-frustration bound

When, if ever, is the entanglement-frustration bound saturated? We will show in this section that for all possible values of $E(|E_0\rangle)$ we can find a Hamiltonian $H$ whose ground state has that amount of entanglement, and saturates the entanglement-frustration bound as closely as desired.

Interestingly, it turns out that it is not possible to *exactly* saturate the entanglement-frustration bound except in the extreme cases $E(|E_0\rangle)=0$ and $E(|E_0\rangle)=1$. However, as we show in this section, it is always possible to saturate the bound to as good an approximation as desired.

To see that exact saturation is not possible, consider the necessary condition for saturation $\langle E_0|H_I|E_0\rangle = E_0^I$ identified in the previous section. This condition implies that $|E_0\rangle$ is a ground state of $H_I$, and therefore also an eigenstate of $H_L = H - H_I$. Entanglement in an eigenstate of a local Hamiltonian is only possible if there is an associated degeneracy. If $|E_0\rangle$ is a ground state of $H_L$ then we conclude that $\Delta E_{\text{ent}}=0$, the entanglement-frustration bound is undefined, and so saturation certainly does not occur. On the other hand, if $|E_0\rangle$ is an excited state of $H_L$ corresponding to some eigenvalue $E_j^L$ then

$$\langle E_0|H_L|E_0\rangle - E_0^L = E_j^L - E_0^L. \tag{18}$$

But since $|E_0\rangle$ is entangled, by assumption, we must have $E_j^L - E_0^L \geqslant \Delta E_{\text{ent}}$. Combining this with the result $E_f \geqslant \langle E_0|H_L|E_0\rangle - E_0^L$ gives $E_f/\Delta E_{\text{ent}} \geqslant 1$. In contrast the maximum values of $E(|E_0\rangle)$ for qubits is $\frac{1}{2}$, and more generally for pairs of $d$-dimensional systems it is $1-1/d$. We conclude that it is not possible for the entanglement-frustration bound to exactly saturate, except when $E(|E_0\rangle)=0$ or 1.

The above analysis, however, says nothing for $|E_0\rangle$ arbitrarily close to a ground state of $H_I$, and in these cases it is possible that the bound approaches saturation.

Before dealing directly with the issue of saturation, it is helpful to address another issue, the question of how a given many-body Hamiltonian $H$ is to be split into local and interaction parts. Consider, for example, the transverse Ising Hamiltonian $H=-g(\sigma_x^1+\sigma_x^2)-\sigma_z^1\sigma_z^2$. In our earlier analysis we set $H_L=-g(\sigma_x^1+\sigma_x^2)$ and $H_I=-\sigma_z^1\sigma_z^2$.

However, there is a certain arbitrariness in the splitting into local and interaction Hamiltonians. From a mathematical point of view, there is nothing to stop us from splitting $H$ up as $H=H_L'+H_I'$, where $H_L'$ is *any* desired local Hamiltonian, and we simply choose $H_I' \equiv H - H_L'$. So, for example, we could choose $H_L'=-g\sigma_x^1$ and $H_I'=-g\sigma_x^2-\sigma_z^1\sigma_z^2$. The reason for this ambiguity is that while the class of local Hamiltonians is perfectly well defined, there is no similar definition of what it means for a Hamiltonian to be an interaction Hamiltonian. Failing to have such a definition, we are free to choose $H_L$ however we like, compensating by choosing an appropriate interaction Hamiltonian.

This freedom to choose a splitting into local and interaction parts is reflected in the fact that the entanglement-frustration bound holds for any choice of splitting $H=H_L+H_I$. Of course, while $E(|E_0\rangle)$ is not affected by the splitting chosen, the quantities $\Delta E_{\text{ent}}$ and $E_f$ are. As a result the exact value of the entanglement-frustration bound depends on the particular splitting chosen. We will use this freedom in choosing a splitting to engineer saturation in the entanglement-frustration bound.

Physically, of course, there is often a reason to favor one splitting into local and interaction parts over another. For example, if we regard the transverse Ising Hamiltonian as a model of two magnetically coupled spins placed in an external magnetic field, then there is a clearly defined physical sense in which $-g(\sigma_x^1+\sigma_x^2)$ ought to be regarded as the local term in the Hamiltonian and $-\sigma_z^1\sigma_z^2$ as the interaction term.

However, the same model Hamiltonian may describe many quite different physical systems, and it is not at all clear that the splitting into local and interaction Hamiltonians will necessarily be the same for all these physical systems. *A priori* it does not seem that the mathematics of quantum mechanics distinguishes any special subclass of interaction Hamiltonians, and this makes it impossible to define a unique splitting of $H$ into local and interaction parties on purely mathematical grounds. More importantly, from our point of view, the entanglement-frustration bound holds for any splitting whatsoever, regardless of its physical (or unphysical) origin, and it is interesting to address the question of which splitting gives the best value for the entanglement-frustration bound.

Let us return now to the question of saturation, and to a closer investigation of the example of the transverse Ising model considered in the previous section. In this example the decomposition of $|E_0\rangle$ into eigenstates of the local Hamiltonian $H_L$ is equivalent to the Schmidt decomposition, and the largest Schmidt coefficient is given by $|\langle E_0^L|E_0\rangle|$. Furthermore, the inequality

$$\langle E_\perp|H_L|E_\perp\rangle \geqslant E_0^L + \Delta E_{\text{ent}} \tag{19}$$

is strict because $|E_\perp\rangle = |--\rangle$ is an excitation of *both* subsystems, whereas $E_0^L + \Delta E_{\text{ent}}$ is the energy of a *single* excited subsystem. The excess is therefore the energy gap of the remaining subsystem.

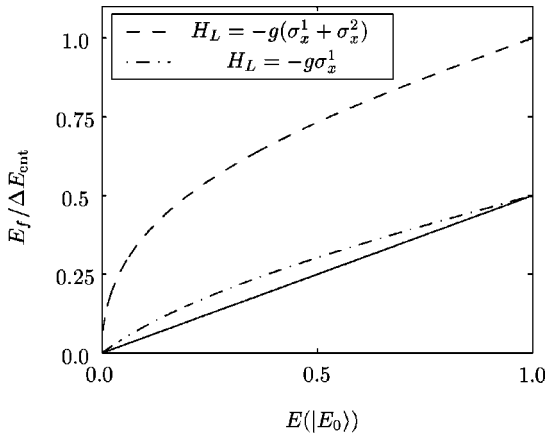


FIG. 3. Comparison of the ground-state entanglement and entanglement-frustration bounds for two choices of splitting in the transverse Ising model. The solid line denotes the ideal case of saturation.

On the other hand, if we take advantage of the possibility of different splittings of $H$ to choose $H_L=-g\sigma_x^1$ then there is zero energy associated with an excitation of the second subsystem and Eq. (19) becomes an equality. The interaction Hamiltonian is determined by the choice of local Hamiltonian, $H_I=H-H_L=-g\sigma_x^2-\sigma_z^1\sigma_z^2$, and we calculate a second entanglement-frustration bound

$$\frac{E_f}{\Delta E_{\rm ent}} = \frac{1}{2} - \left( \frac{\sqrt{1+4g^2} - \sqrt{1+g^2}}{2g} \right). \tag{20}$$

The two bounds Eq. (14) and Eq. (20) are plotted against the ground-state entanglement in Fig. 3. It is clear that this second choice for $H_L$ provides a substantially tighter bound, as we expect.

Let us generalize this example further. Suppose $H$ is an arbitrary bipartite Hamiltonian acting on two $d$-dimensional systems, with ground state Schmidt decomposition

$$|E_0\rangle = \lambda |a_0 b_0\rangle + \sum_{j=1}^{d-1} \lambda_j |a_j b_j\rangle, \tag{21}$$

where we have chosen labels so that $\lambda$ is the largest Schmidt coefficient. In order to ensure that Eq. (19) is saturated we choose a splitting of $H$ with $H_L$ as follows:

$$H_L = -\gamma |a_0\rangle\langle a_0| \otimes I, \tag{22}$$

where $\gamma > 0$ is a parameter that will be chosen later in order to best saturate the bound. It is clear that Eq. (21) is an expansion of $|E_0\rangle$ in an energy eigenbasis of $H_L$, of the same form as used in Eq. (6), and thus that

$$\langle E_\perp | H_L | E_\perp \rangle = 0 = E_0^L + \Delta E_{\rm ent}. \tag{23}$$

It follows that for this choice of local Hamiltonian,

$$E(|E_0\rangle) = \frac{E_f}{\Delta E_{\rm ent}} + (\langle E_0|H_I|E_0\rangle - E_0^I)/\Delta E_{\rm ent}, \tag{24}$$

i.e., the amount by which the entanglement exceeds the entanglement-frustration bound is composed entirely of the second term identified earlier in Eq. (17).

To minimize this excess we choose $\gamma$ small and positive. Observing that $H_I=H-H_L$ we may do perturbation theory in $\gamma$ to show:

$$E_0^I = E_0 - \langle E_0|H_L|E_0\rangle + O(\gamma^2) \tag{25}$$

$$= \langle E_0|H_I|E_0\rangle + O(\gamma^2), \tag{26}$$

where we used $H_I=H-H_L$ in the second line. Using this fact and the observation $\Delta E_{\rm ent}=\gamma$, we have

$$\frac{\langle E_0|H_I|E_0\rangle - E_0^I}{\Delta E_{\rm ent}} = O(\gamma). \tag{27}$$

Taking the limit as $\gamma \to 0$ we see that the entanglement-frustration bound approaches the ground-state entanglement.

In summary, we have shown:

*Proposition 1.* Let $H$ be an arbitrary bipartite Hamiltonian. Then there exists a local Hamiltonian $H_L$ and corresponding interaction Hamiltonian $H_I$ such that the entanglement-frustration bound derived from the splitting $H=H_L+H_I$ is arbitrarily close to the ground-state entanglement of $H$.

This shown that, in principle, the entanglement-frustration bound may be arbitrarily close to saturation for all possible values of the ground-state entanglement $E(|E_0\rangle)$. We therefore conclude that the entanglement-frustration bound cannot be strengthened without using more detailed knowledge of the system properties.

Our results show that saturation of the entanglement-frustration bound is always possible with an appropriate choice of splitting. They do not, of course, tell us what splitting ought to be used, except in the unusual situation where one knows virtually everything about the ground state already, in which case one may as well calculate the ground-state entanglement directly. Thus the content of Proposition 1 is not that we ought to expect to calculate ground-state entanglement exactly, merely by choosing the appropriate splitting for the Hamiltonian. Rather, Proposition 1, and the methods that lead to it, tell us that the entanglement-frustration bound is the best possible, and provide some physical guidance as to how to choose the splitting into local and interaction Hamiltonians in order to achieve the best possible values for the entanglement frustration bound.

In the case of $n$-partite Hamiltonians, Proposition 1 can be applied by taking a bipartite split between any single subsystem and the remaining subsystems, and is possible in this manner to gain some indication of the distribution of entanglement within the ground state. This problem is discussed further in Sec. VII.

## V. GROUND-STATE ENTANGLEMENT AND THE RATIO OF INTERACTION STRENGTH TO THE LOCAL ENERGY SCALE

The inequality Eq. (2) has a nice corollary that is easily proved, relating the ground-state entanglement to a ratio of the interaction strength with the local energy scale of the system. Suppose we define $E^I_{\max}$ to be the largest eigenvalue of $H_I$, and let $E^I_{\rm tot} \equiv E^I_{\max} - E^I_0$ be the total energy scale for the interaction Hamiltonian, i.e., the difference between the largest and the smallest energies. It follows that

$$E_0 \leqslant \langle E^L_0|H|E^L_0\rangle \tag{28}$$

$$= \langle E^L_0|H_L|E^L_0\rangle + \langle E^L_0|H_I|E^L_0\rangle \tag{29}$$

$$\leqslant E^L_0 + E^I_{\max}. \tag{30}$$

Rearranging this inequality we obtain $E_f \leqslant E^I_{\rm tot}$. Combining with Eq. (2) then gives

$$E(|E_0\rangle) \leqslant \frac{E^I_{\rm tot}}{\Delta E_{\rm ent}}. \tag{31}$$

The inequality Eq. (31) is an interesting result. Intuition, experience, and perturbation theory tell us that if we start with a local Hamiltonian and slowly turn on an interaction, the ground-state entanglement will depend on how strong the interaction is, compared with the local terms in the Hamiltonian, which tend to keep the ground state unentangled. Equation (31) is a precise, completely general statement of this intuition, a statement that holds even nonperturbatively.

## VI. HIGHER-ENERGY EIGENSTATES AND THE RATIO OF INTERACTION STRENGTH TO THE LOCAL ENERGY SCALE

In Sec. V we proved a bound, Eq. (31), quantifying the intuition that when an interaction term is switched on in a many-body system, the ground-state entanglement will depend on how strong the interaction is compared with the strength of the local Hamiltonian. Of course, a similar intuition applies also for higher-energy eigenstates. Unfortunately, the strategy used to prove Eq. (31) cannot be applied directly to energy eigenstates other than the ground and most excited states.[5] The reason is that the proof of Eq. (31) relied on the entanglement-frustration bound, Eq. (2), and there is no natural analog of this bound—or even a definition of frustration energy—for states other than the ground and most excited states.

In this section we prove a bound validating this intuition for all energy eigenstates. The bound is proved in two steps.

First, suppose $A = B + C$, where $A$ and $B$ are normal matrices. We will prove a general *eigenspace perturbation theorem* making precise the intuition that $A$ and $B$ have similar eigenspaces when $C$ is sufficiently small. Our eigenspace perturbation theorem is a variant on a celebrated theorem of linear algebra, the Davis-Kahan theorem [28].[6]

A detailed discussion of how our eigenspace perturbation theorem compares to the Davis-Kahan theorem is given below. Summarizing, the major differences are that (i) our proof is simpler, (ii) our conclusions are more powerful, but (iii) our hypotheses are more specialized. For these reasons, we believe our eigenspace perturbation theorem is of substantial independent interest in its own right.

The second step in the proof of the bound is to apply our eigenspace perturbation theorem to understand how the entanglement in an energy eigenstate depends on the relationship between the strength of the local and the interaction Hamiltonians.

Let us begin with the eigenspace perturbation theorem.

*Theorem 1 (Eigenspace perturbation theorem).* Let $A$, $B$, and $C$ be matrices such that $A = B + C$, with $A$ and $B$ normal matrices. Let $a$ be an eigenvalue of $A$, and suppose $P_a$ is any projector that projects onto some subspace of the corresponding eigenspace. ($P_a$ may, for example, project onto the entire eigenspace.) Let $\beta$ be some subset of the eigenvalues of $\beta$, and let $Q_b$ be a projector onto an arbitrary subspace of the eigenspace corresponding to $b \in \beta$. Define $Q \equiv \Sigma_{b\in\beta} Q_b$. Then

$$|P_a Q| \leqslant \frac{|P_a C Q|}{\Delta_a} \leqslant \frac{U|C|U^\dagger}{\Delta_a}, \tag{32}$$

where $S \leqslant T$ denotes a matrix inequality, i.e., $T - S$ is a positive matrix, $|S| \equiv \sqrt{SS^\dagger}$, $\Delta_a \equiv \min_{b\in\beta}|a-b|$ is the distance from $a$ to the set $\beta$, and $U$ is some unitary matrix.

The interpretation of these inequalities in terms of eigenspace perturbation is perhaps not immediately clear. Rather than describe this interpretation immediately, we defer the description until after the proof of the theorem and a discussion of how this result relates to the Davis-Kahan theorem.

*Proof:* We begin by proving the first inequality. Multiplying $A = B + C$ on the left by $P_a$ and on the right by $Q_b$, we obtain $aP_aQ_b = bP_aQ_b + P_aCQ_b$, which may be rearranged to give

$$P_a Q_b = \frac{P_a C Q_b}{a - b}. \tag{33}$$

Observe that $|P_aQ|^2 = P_aQP_a = \Sigma_b P_aQ_bQ_bP_a$. Substituting Eq. (33) and its adjoint gives

$$|P_a Q|^2 = \sum_b \frac{P_a C Q_b C^\dagger P_a}{|a-b|^2} \tag{34}$$

$$\leqslant \sum_b \frac{P_a C Q_b C^\dagger P_a}{\Delta_a^2}, \tag{35}$$

where we used $|a-b|^2 \geqslant \Delta_a^2$. Summing out $b$ gives

[5] We only proved Eq. (31) for the ground state. An analogous result for the most excited state may be proved by applying Eq. (31) to the Hamiltonian $-H$.

[6] For an account of the Davis-Kahan theorem, see Theorem VII.3.1 on page 211 of Ref. [29], and the surrounding discussion in Chap. VII of that work.

$$|P_a Q|^2 \leq \frac{|P_a CQ|^2}{\Delta_a^2}. \tag{36}$$

The conclusion follows by using the operator monotonicity[7] of the square root function, i.e., the fact that if $S \leq T$ then $\sqrt{S} \leq \sqrt{T}$.

To prove the second inequality in the statement of the theorem, it obviously suffices to prove $|P_a CQ| \leq U|C|U^\dagger$. Note first that $P_a CQC^\dagger P_a \leq P_a CC^\dagger P_a$. But $P_a CC^\dagger P_a$ and $C^\dagger P_a C$ are positive operators with the same eigenvalues, so there exists a unitary $V$ such that $P_a CC^\dagger P_a = VC^\dagger P_a CV^\dagger \leq VC^\dagger CV^\dagger$. Putting these observations together gives $P_a CQC^\dagger P_a \leq VC^\dagger CV^\dagger$, from which it follows that $P_A CQC^\dagger P_a \leq UCC^\dagger U^\dagger$ for some unitary $U$. The result now follows by using the operator monotonicity of the square-root function. ■

The conclusion of Theorem 1 has a nice implication in terms of matrix norms. Suppose $|||\cdot|||$ is a *unitarily invariant* matrix norm, i.e., $|||USV||| = |||S|||$ for any unitaries $U$ and $V$. (Most of the familiar norms in common use in quantum information, including all the $l_p$ norms, are easily shown to be unitarily invariant.) Using the polar decomposition we see that $S = |S|U$ for some unitary $U$, and thus Eq. (32) implies that

$$|||P_a Q||| \leq \frac{|||P_a CQ|||}{\Delta_a} \leq \frac{|||C|||}{\Delta_a}, \tag{37}$$

for any unitarily invariant norm $|||\cdot|||$.

Let us compare the eigenspace perturbation theorem, Theorem 1, with the Davis-Kahan theorem. The Davis-Kahan theorem is as follows:

*Theorem 2 Davis-Kahan theorem.* Let $A$, $B$, and $C$ be matrices such that $A = B + C$, with $A$ and $B$ normal matrices. Let $\alpha$ and $\beta$ be subsets of the eigenvalues of $A$ and $B$, respectively. Let $P$ (respectively $Q$) project onto the space spanned by all the eigenspaces of $A$ (respectively $B$) corresponding to elements of $\alpha$ (respectively $\beta$). Suppose furthermore that $\alpha$ and $\beta$ are separated by an annulus of width $\delta$ in the complex plane, e.g., with $\alpha$ inside the annulus, and $\beta$ outside the annulus. Then for any unitarily invariant norm $|||\cdot|||$,

$$|||PQ||| \leq \frac{|||PCQ|||}{\delta} \leq \frac{|||C|||}{\delta}. \tag{38}$$

There are three interesting differences between the Davis-Kahan theorem and Theorem 1. First, Theorem 1 is more specialized than Davis-Kahan, in that it applies only for a single eigenvalue of $A$, not for multiple eigenvalues. We have tried and failed to extend our proof to the more general case. A second difference is that Theorem 1 gives an operator inequality that implies the corresponding inequalities for unitarily invariant norms, but which is not implied by those inequalities. Finally, our proof of Theorem 1 seems to be substantially simpler than known proofs of the Davis-Kahan theorem.

To better understand how Theorems 1 and 2 relate to eigenspace perturbations, suppose that $P_a$ projects onto a subspace $\mathcal{P}_a$ spanned by a single eigenstate $|a\rangle$ of $A$, and $Q$ projects onto a subspace $\mathcal{Q}$ spanned by eigenstates $|b\rangle$, $b \in \beta$. The norm $|||P_a Q|||$ turns out to measure the orthogonality of these two subspaces. For example, in the special case when $Q$ is a rank-1 projector, $Q = |b\rangle\langle b|$, we have

$$|||P_a Q||| = ||||a\rangle\langle a|b\rangle\langle b|||| = |\langle a|b\rangle|||||a\rangle\langle b|||| \tag{39}$$

which is proportional to the cosine of the angle between $|a\rangle$ and $|b\rangle$. (Note that $||||a\rangle\langle b|||| $ is a constant independent of $|a\rangle$ and $|b\rangle$, due to unitary invariance of the norm.) Thus Theorems 1 and 2 tell us that this cosine is very small (and thus $|a\rangle$ and $|b\rangle$ are close to orthogonal) whenever the ratio of the size of the perturbation $|||C|||$ to the distance $\Delta_a$ is small. It follows that provided $|||C|||$ is sufficiently small, all the eigenvectors of $A$ and $B$ are nearly orthogonal, except for a single nearly parallel eigenvector.

More generally, the singular values of $P_a Q$ are the cosines of what are known as the *canonical angles* between the subspaces $\mathcal{P}$ and $\mathcal{Q}$.[8] If $|||P_a Q|||$ is small then the cosines of the canonical angles are small, and it can be shown that all vectors in $\mathcal{P}$ are very nearly orthogonal to all vectors in $\mathcal{Q}$.

Let us return now to the problem of bounding the entanglement in an arbitrary eigenstate $|E_j\rangle$ of a many-body Hamiltonian $H$. $H$ is split into a local part, $H_L$, and an interaction part, $H_I$, as before. Our starting point is again the expansion of $|E_j\rangle$ in terms of the eigenstates $|E_k^L\rangle$ of $H_L$. Associated to any local Hamiltonian we can identify some natural subspaces that contain no entanglement. These subspaces are spanned by a set of eigenstates $|E_m^L\rangle$ related to each other by *excitations or de-excitations of a single subsystem*. Any superposition of such states factors into a product state, and for convenience we will refer to such a subspace as a *product subspace*. Our use of this term should not be confused with the more general (and more common) use of the term product subspace, to mean any vector subspace containing no entanglement; our use of the term is specific to a particular $H_L$, and refers to those subspaces spanned by sets of eigenstates $|E_m^L\rangle$ which are all related by excitations or de-excitations of a single subsystem.

We will see later that for each $|E_j\rangle$ there is a natural way to choose a corresponding product subspace from the eigenstates of $H_L$. For now let $\mathcal{K}$ be any such product subspace and expand $|E_j\rangle$ in the energy eigenbasis of $H_L$ as follows:

$$|E_j\rangle = \sum_{k, |E_k^L\rangle \in \mathcal{K}} \alpha_k |E_k^L\rangle + \gamma |E_\perp\rangle, \tag{40}$$

where $|E_\perp\rangle$ is orthogonal to all states in $\mathcal{K}$. It follows from Eq. (1) that

[7] A review of operator monotonicity may be found in Chap. V of Ref. [29].

[8] For an introduction to the canonical angles, see Chap. VII of Ref. [29], especially the first section. We do not need to use any properties of the canonical angles in this paper.

$$E(|E_j\rangle) \leqslant 1 - \sum_k |\alpha_k|^2 = |\gamma|^2. \tag{41}$$

Our strategy is to apply Theorem 1 to obtain a bound on $|\gamma|^2 = 1 - \Sigma_k |\alpha_k|^2$.

Define $P_j$ to be the projector onto $|E_j\rangle$. We're trying to bound the amplitude squared $|\gamma|^2$ of the component of $|E_j\rangle$ orthogonal to $\mathcal{K}$, so let $\mathcal{K}_\perp$ denote the subspace spanned by all eigenstates $|E_l^L\rangle$ of $H_L$ not in $\mathcal{K}$ and define $Q_{\mathcal{K}_\perp}$ to be the corresponding projector. Theorem 1 implies that

$$|||P_j Q_{\mathcal{K}_\perp}||| \leqslant \frac{|||H_I|||}{\Delta E_{j,\mathcal{K}_\perp}}, \tag{42}$$

where $\Delta E_{j,\mathcal{K}_\perp} = \min_{|E_l^L\rangle \in \mathcal{K}_\perp} |E_j - E_l^L|$. Next we must show how $|||P_j Q_{\mathcal{K}_\perp}|||$ is related to the entanglement $E(|E_j\rangle)$.

It is easily seen from Eq. (40) that $Q_{\mathcal{K}_\perp}|E_j\rangle = |E_\perp\rangle$ and so

$$|||P_j Q_{\mathcal{K}_\perp}||| = ||||E_j\rangle\langle E_j|Q_{\mathcal{K}_\perp}||| \tag{43}$$

$$= |\gamma|||E_j\rangle\langle E_\perp|||. \tag{44}$$

As remarked earlier, the value of $||||v\rangle\langle w||||$ for any normalized vectors $|v\rangle$ and $|w\rangle$ is a constant that depends only upon the norm $|||\cdot|||$. Without loss of generality we may assume that $||||v\rangle\langle w||| = 1$, since multiplying a unitarily invariant norm by a constant gives another unitarily invariant norm. We will say any norm satisfying this condition is *normalized*. [Examples of normalized unitarily invariant norms include the operator norm $\|A\| = \sup_{\||v\rangle\|=1} \|A|v\rangle\|$ and the Hilbert-Schmidt norm $\|A\|_2 = \sqrt{\mathrm{tr}(AA^\dagger)}$.]

Assuming that $|||\cdot|||$ is normalized we see that

$$|||P_j Q_{\mathcal{K}_\perp}||| = |\gamma|, \tag{45}$$

and it follows from Eqs. (41) and (42) that

$$E(|E_j\rangle) \leqslant \frac{|||H_I|||^2}{(\Delta E_{j,\mathcal{K}_\perp})^2}. \tag{46}$$

For any normalized, unitarily invariant norm $|||\cdot|||$ we have $\|S\| \leqslant |||S|||$ where $\|\cdot\|$ is the operator norm and $S$ any operator [29]. The strongest bound of this form is therefore

$$E(|E_j\rangle) \leqslant \frac{\|H_I\|^2}{(\Delta E_{j,\mathcal{K}_\perp})^2}. \tag{47}$$

Different choices of the product subspace $\mathcal{K}$ provide us with a different bound in Eq. (47). Ideally we would like to choose $\mathcal{K}$ so that the quantity $\Delta E_{j,\mathcal{K}_\perp}$ is as large as possible. If $E_j$, or a good approximation to $E_j$, is known then we would ensure that $\mathcal{K}$ contained $|E_k^L\rangle$ where $|E_k^L - E_j|$ is minimal. More typically $E_j$ is unknown, and this is not possible. However, there is still a natural way for us to choose $\mathcal{K}$. Importantly this choice also allows us to obtain a lower bound for $\Delta E_{j,\mathcal{K}_\perp}$ in terms of relatively simple quantities that depend only on $H_L$ and $H_I$, not on typically difficult-to-calculate quantities associated with the total Hamiltonian $H$.

Let $|E_j^L\rangle$ be the $j$th excited eigenstate of the local Hamiltonian. We choose the product subspace $\mathcal{K}$ so that the expression

$$\Delta E_{j,\mathrm{ent}} = \min_{|E_k^L\rangle \in \mathcal{K}_\perp} |E_j^L - E_k^L| \tag{48}$$

is maximized. $\Delta E_{j,\mathrm{ent}}$ is a generalization of $\Delta E_{\mathrm{ent}}$ in Sec. III, in that it is the energy required to excite or de-excite at least two subsystems from the state $|E_j^L\rangle$. Note that the calculation of $\Delta E_{j,\mathrm{ent}}$ is tedious, but in principle straightforward provided that the energy spectrum of $H_L$ is known: simply enumerate the possible product subspaces given the spectrum of $H_L$ (a long, but finite list), and then calculate the minimum by inspection.

Now for each $|E_k^L\rangle \in \mathcal{K}_\perp$ we have by the triangle inequality

$$|E_k^L - E_j| \geqslant |E_k^L - E_j^L| - |E_j^L - E_j| \tag{49}$$

$$\geqslant \Delta E_{j,\mathrm{ent}} - |E_j^L - E_j|. \tag{50}$$

Furthermore, it is straightforward to show that $|E_j - E_j^L| \leqslant |E_{\max}^I|$ and so

$$\Delta E_{j,\mathcal{K}_\perp} = \min_{|E_k^L\rangle \in \mathcal{K}_\perp} |E_k^L - E_j| \geqslant \Delta E_{j,\mathrm{ent}} - |E_{\max}^I|. \tag{51}$$

Substituting into Eq. (47) we obtain a result in terms of the spectrum of $H_L$ and the strength of $H_I$ alone.

*Proposition 2*. Let $H = H_L + H_I$ with $H_L$ a local Hamiltonian, and suppose $\Delta E_{j,\mathrm{ent}} > |E_{\max}^I|$. Then the entanglement in the $j$th excited eigenstate $|E_j\rangle$ of $H$, as measured using the definition of Eq. (1), is bounded above by

$$E(|E_j\rangle) \leqslant \frac{\|H_I\|^2}{(\Delta E_{j,\mathrm{ent}} - |E_{\max}^I|)^2}. \tag{52}$$

Noting that $|E_{\max}^I| \leqslant \|H_I\|$ this can be restated in a slightly weaker but perhaps more elegant form, supposing $\Delta E_{j,\mathrm{ent}} \geqslant \|H_I\|$:

$$E(|E_j\rangle) \leqslant \frac{\|H_I\|^2}{(\Delta E_{j,\mathrm{ent}} - \|H_I\|)^2} = \frac{1}{\left(\dfrac{\Delta E_{j,\mathrm{ent}}}{\|H_I\|} - 1\right)^2}. \tag{53}$$

Equations (52) and (53) confirm and quantify our intuition that when the nonentangled energy scale associated with $|E_j^L\rangle$ is large compared to the strength of the interaction Hamiltonian we expect little entanglement in the excited state $|E_j\rangle$ of the total Hamiltonian.

Equation (52) should be compared with the earlier result Eq. (31) for the ground-state entanglement. We see that the present result is equivalent to the earlier result, except for the presence of the term $-|E_{\max}^I|$ in the denominator of Eq. (52), which makes the present result weaker.

## VII. CONCLUSION

We have introduced the frustration energy $E_f$ as a measure of the degree of frustration between local and interaction terms in the Hamiltonian $H = H_L + H_I$ of a many-body quan-

tum system. This measure, when related to a local energy scale, allowed us to derive the entanglement-frustration bound on the ground-state entanglement in the system. An interesting feature of this bound is that it depends only on spectral properties of the Hamiltonians $H$, $H_L$, and $H_I$. Ground-state entanglement properties can therefore be easily inferred directly from the spectra alone.

The entanglement-frustration bound has, in turn, been used to prove a bound, Eq. (31), relating the ground-state entanglement to a ratio of the strength of the interactions and an appropriate local energy scale. This bound involves only the eigenvalues of the local and interaction Hamiltonians, which are typically much easier to calculate than the eigenvalues of the full Hamiltonian, and thus this bound is more likely to be useful in practice. A similar bound for an arbitrary energy eigenstate is proved in Eqs. (52) and (53).

Ultimately it would be useful to have many powerful general techniques enabling us to infer ground-state entanglement properties of a Hamiltonian by considering the interplay between its constituent terms. This is not always easy. For example, consider the following system of three spin-$\frac{1}{2}$ particles:

$$H = g_a H_A + g_b H_B + g_c H_C + H_{AB} + H_{BC}, \tag{54}$$

where $A,B,C$ label the three particles. $H_A,H_B,H_C$ are local Hamiltonians, $H_{AB},H_{BC}$ are interaction Hamiltonians on the appropriate subsystem, and $g_A,g_B,g_C$ control the respective strengths of the local Hamiltonians. The bound Eq. (31) derived from the entanglement-frustration bound tells us that if $g_b$ is relatively large then there is little entanglement between particle $B$ and the rest of the system $AC$. From this we may deduce that if there is any entanglement in the ground state then it must be between particles $A$ and $C$. To some extent, then, the entanglement-frustration bound allows us to determine the distribution of entanglement. In cases where all three local energy scales are small compared to the interactions, however, we are unable to directly deduce anything using the techniques in this paper.

Throughout this paper we have defined frustration to occur when it is not possible to find a simultaneous ground state for some local and interaction part of a Hamiltonian. This is based on an analogy to the usual definition of frustration, which involves competition between interactions, as discussed in the Introduction, and illustrated in Fig. 1. (An insightful review of classical and quantum frustration in this sense may be found in Ref. [30].) Both these points of view suggest interesting extensions of the investigations in the present paper.

For example, we believe that quantum frustration suggests interesting parallels with the phenomenon of *entanglement sharing* [31] which places restrictions on the distribution of entanglement amongst many particles. In particular, we expect nontrivial distributions of entanglement in the ground state of two overlapping interactions. For example, consider a Hamiltonian acting on three spin-$\frac{1}{2}$ particles as before,

$$H = H_{AB} + H_{BC}, \tag{55}$$

and suppose that $H_{AB}$ and $H_{BC}$ have nondegenerate, maximally entangled ground states. It is impossible for entanglement to be distributed in a way that would provide a ground state for $H$ that is a simultaneous ground state of $H_{AB}$ and $H_{BC}$. The system is therefore necessarily frustrated. We might ask what happens to the ground-state entanglement distribution in systems such as this, and whether there are any properties of the constituent Hamiltonians that allow us to prove quantitative bounds relating the distribution of two-party, GHZ-type and W-type entanglement in this system.

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[1] H. L. Haselgrove, M. A. Nielsen, and T. J. Osborne, Phys. Rev. A **69**, 032303 (2004).
[2] H. L. Haselgrove, M. A. Nielsen, and T. J. Osborne, Phys. Rev. Lett. **91**, 210401 (2003).
[3] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
[4] J. I. Latorre, E. Rico, and G. Vidal, Quantum Inf. Comput. **4**, 48 (2004).
[5] T. Tessier, I. H. Deutsch, A. Delgado, and I. Fuentes-Guridi, Phys. Rev. A **68**, 062316 (2003).
[6] T. A. Costi and R. H. McKenzie, Phys. Rev. A **68**, 034301 (2003).
[7] A. P. Hines, R. H. McKenzie, and G. J. Milburn, Phys. Rev. A **67**, 013609 (2003).
[8] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).
[9] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).
[10] S. Scheel, J. Eisert, P. L. Knight, and M. B. Plenio, J. Mod. Opt. **50**, 881 (2002).
[11] X. Wang and P. Zanardi, Phys. Lett. A **301**, 1 (2002).
[12] K. M. O'Connor and W. K. Wootters, Phys. Rev. A **63**, 052302 (2001).
[13] D. Gunlycke, V. M. Kendon, V. Vedral, and S. Bose, Phys. Rev. A **64**, 042302 (2001).
[14] M. A. Nielsen, Ph.D. thesis, University of New Mexico, 1998.
[15] A. N. Jordan and M. Büttiker, quant-ph/0311647.
[16] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
[17] J. Preskill, *Physics 229: Advanced Mathematical Methods of Physics—Quantum Computation and Information* (California Institute of Technology, Pasadena, CA, 1998), http://www.theory.caltech.edu/people/preskill/ph229/
[18] G. Aeppli and P. Chandra, Science **275**, 177 (1997).
[19] M. A. Nielsen, Sci. Am. (Int. Ed.) **287**, 66 (2002).

[20] G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003).
[21] T. J. Osborne, Ph.D. thesis, The University of Queensland, 2002.
[22] J. Preskill, J. Mod. Opt. **47**, 127 (2000).
[23] M. Horodecki, Quantum Inf. Comput. **1**, 3 (2001).
[24] B. M. Terhal, Theor. Comput. Sci. **287**, 313 (2002).
[25] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight, Phys. Rev. Lett. **78**, 2275 (1997).
[26] V. Vedral and M. B. Plenio, Phys. Rev. A **57**, 1619 (1998).
[27] O. Biham, M. A. Nielsen, and T. J. Osborne, Phys. Rev. A **65**, 062312 (2002).
[28] C. Davis and W. M. Kahan, SIAM (Soc. Ind. Appl. Math.) J. Numer. Anal. **7**, 1 (1970).
[29] R. Bhatia, *Matrix Analysis* (Springer-Verlag, New York, 1997).
[30] M. M. Wolf, F. Verstaete, and J. I. Cirac, quant-ph/0311051.
[31] V. Coffman, J. Kundu, and W. K. Wootters, Phys. Rev. A **61**, 052306 (2000).
[32] I. Bose and W. E. Chattopadadhyay, Phys. Rev. A **66**, 062320 (2002).