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

Christopher M. Dawson[1, 2, *] and Michael A. Nielsen[1, 2, 3, †]

[1] *School of Physical Sciences, The University of Queensland, Brisbane Queensland 4072, Australia*
[2] *Institute for Quantum Information, California Institute of Technology, Pasadena CA 91125, USA*
[3] *School of Information Technology and Electrical Engineering, The University of Queensland, Brisbane Queensland 4072, Australia*

(Dated: February 1, 2008)

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.

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 *non-classical* correlations in the ground state, that is, the *ground-state entanglement*. Some recent work on this problem, with further references, includes [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. 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 [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 anti-ferromagnetic coupling ($+J\sigma_z\sigma_z$, with positive coupling strength J). The anti-ferromagnetic coupling means that neighbours prefer to be anti-aligned in order to minimize their interaction energies. However, a little thought shows that it is impossible for all three spins to simultaneously be anti-aligned with each of their neighbours. 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.

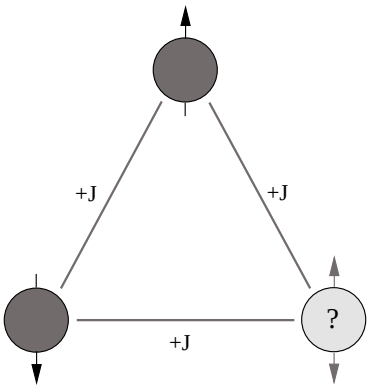

FIG. 1: A system containing three spin-$\frac{1}{2}$ particles, coupled by a classical anti-ferromagnetic coupling ($+J\sigma_z\sigma_z$, with positive coupling strength J) favouring anti-alignment. There is no way all the competing couplings can be simultaneously satisfied; for this reason we say the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

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 $H = -g\left(\sigma_x^1 + \sigma_x^2\right) - \sigma_z^1\sigma_z^2$, where the superscripts indicate which spin the operators act on, and σ_x, σ_y, and σ_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, $-g\left(\sigma_x^1 + \sigma_x^2\right)$, 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

*Electronic address: dawson@physics.uq.edu.au
†Electronic address: nielsen@physics.uq.edu.au; URL: www.qinfo.org/people/nielsen

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

ground-state entanglement and a generalized concept of frustration. If the interaction term in the Hamiltonian were turned off, 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 [1, 14, 19, 20, 21, 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, non-perturbative 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 non-perturbative bound quantifying this intuition. This corollary is proved in Sec. V. Sec. 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. Sec. 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 [25, 26]. For an n-body quantum system in a state ψ this entanglement measure is defined by[3]:

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

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

What makes $E(\psi)$ a good entanglement measure? [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: (a) $E(\psi)$ can only decrease, never increase, under local operations and classical communication, i.e., it is an entanglement monotone; and (b) $E(\psi)$ is zero if and only if ψ 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 ψ, up to a local unitary transformation.

III. THE 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*.

---

[2] See, e.g., [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 [25, 26], but has essentially the same properties. In the present context the rescaled definition turns out to be easier to work with.

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 $E_0 \geq E_0^L + E_0^I$, 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 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 $H_1 + H_2 + \ldots + H_n$, where H_j is the contribution to the local Hamiltonian from the jth system. Let ΔE_j be the gap between the ground and first excited energies[4] of H_j. Let $\Delta E_{\rm ent}$ be the *second smallest* of these energies. That is, suppose we choose $j_0, j_1, \ldots$ such that $\Delta E_{j_0} \leq \Delta E_{j_1} \leq \ldots$. Then $\Delta E_{\rm ent} = \Delta E_{j_1}$.

Physically, $\Delta E_{\rm ent}$ 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 j_0 *or* system j_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 $\Delta E_{\rm ent}$ is the inequality:

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

We call this the *entanglement-frustration* bound. This bound tells us that when the frustration energy is small compared with $\Delta E_{\rm ent}$, there can't 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

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

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:

$$\begin{aligned} E_f &= \langle E_0|H|E_0\rangle - E_0^L - E_0^I & (4)\\ &= \left(\langle E_0|H_L|E_0\rangle - E_0^L\right) + \left(\langle E_0|H_I|E_0\rangle - E_0^I\right). & (5)\end{aligned}$$

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

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, $|E_0\rangle = \sum_j \alpha_j |E_j^L\rangle$. We assume that the local energies are ordered so that $E_0^L \leq E_1^L \leq \ldots$. We now split the expansion of $|E_0\rangle$ into terms with energies below $E_0^L + \Delta E_{\rm ent}$, and into terms with energies at least $E_0^L + \Delta E_{\rm ent}$, that is,

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

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

For later use it is important to note that $\sum_{j=0}^{k} \alpha_j |E_j^L\rangle$ is a product state, as all the terms $|E_j^L\rangle$ involve excitations of the *same subsystem*[5]. Furthermore its overlap squared with $|E_0\rangle$ is given by $\sum_{j=0}^{k} |\alpha_j|^2$.

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

$$\begin{aligned} \langle E_0|H_L|E_0\rangle \;\geq\; & \sum_{j=0}^{k} |\alpha_j|^2 E_0^L \\ & + \left(1 - \sum_{j=0}^{k} |\alpha_j|^2\right) \left(E_0^L + \Delta E_{\rm ent}\right). \end{aligned} \tag{8}$$

Rearrangement of this inequality gives

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

[4] *Note for clarity:* The term "gap" may be used in two different senses. Sometimes it means the energy difference between the ground state and the first excited state with a strictly higher energy. We use the term in the other sense, where the gap ΔE_j is zero if H_j has a degenerate ground state.

[5] System j_0, to return to the notation used earlier in defining $\Delta E_{\rm ent}$.

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

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

Our desired result, Eq. (2), will follow if we can establish that $E(|E_0\rangle) \leq \left(1 - \sum_{j=0}^{k} |\alpha_j|^2\right)$. 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 $\sum_{j=0}^{k} \alpha_j |E_j^L\rangle$ have overlap squared $\sum_{j=0}^{k} |\alpha_j|^2$.

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 analyse 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. The 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 $g \geq 0$. 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 the ground state should be a product state in that limit, $E(|E_0\rangle) \to 0$.

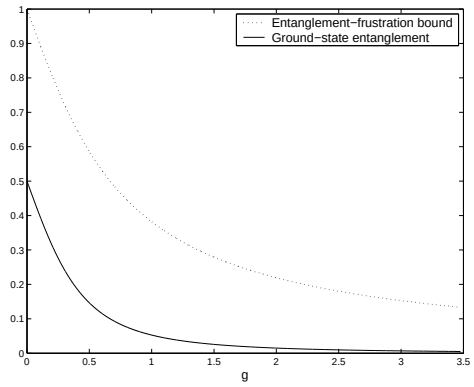

FIG. 2: The ground-state entanglement and entanglement-frustration bound for the transverse Ising Hamiltonian (11) plotted against the parameter g.

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

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

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[6] $\lambda_0 = \left(2g + \sqrt{1+4g^2}\right)/\sqrt{N}$. The ground-state entanglement is given by $1 - \lambda_0^2$, which simplifies to

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

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 $\Delta E_{\rm ent} = 2g$. This gives the entanglement-frustration bound

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

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

[6] 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 $g \geq 0$ cases.

to 0 more slowly. The entanglement-frustration bound is clearly not very tight in this case, although the qualitative behaviour 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 $E_0^L + \Delta E_{\rm ent}$. We see from Eq. (12) that $|E_\perp\rangle = |--\rangle$, and thus $\langle E_\perp|H_L|E_\perp\rangle = E_0^L + 2\Delta E_{\rm ent}$. It follows that

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

and upon substitution into Eq. (5) this gives

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

or

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

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 $(\langle E_0|H_I|E_0\rangle - E_0^I)/\Delta E_{\rm ent}$. 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 $\Delta E_{\rm ent} = 0$, 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

$$\langle E_0|H_L|E_0\rangle - E_0^L = E_j^L - E_0^L. \quad (18)$$

But since $|E_0\rangle$ is entangled, by assumption, we must have $E_j^L - E_0^L \geq \Delta E_{\rm ent}$. Combining this with the result $E_f \geq \langle E_0|H_L|E_0\rangle - E_0^L$ gives $E_f/\Delta E_{\rm ent} \geq 1$. 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 $1 - \frac{1}{d}$. 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 a 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 $\Delta E_{\rm ent}$ 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 favour 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

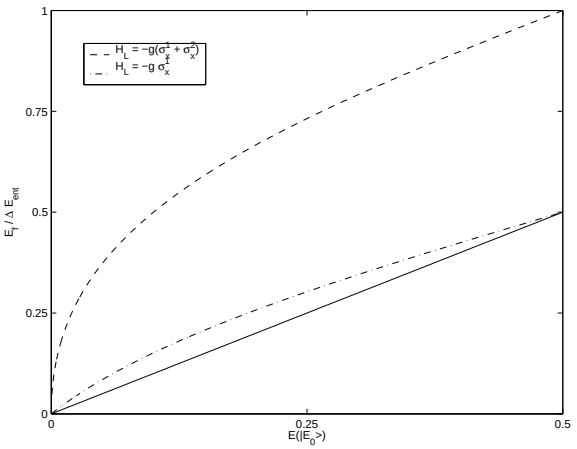

FIG. 3: Comparison of the ground-state entanglement and entanglement-frustration bounds for two choices of splitting in the transverse Ising model. The solid line denotes the ideal case of saturation.

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

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

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

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 λ 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,

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

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 γ small and positive. Observing that $H_I = H - H_L$ we may do perturbation theory in γ to show:

$$\begin{aligned} E_0^I &= E_0 - \langle E_0|H_L|E_0\rangle + O(\gamma^2) &(25)\\ &= \langle E_0|H_I|E_0\rangle + O(\gamma^2). &(26)\end{aligned}$$

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.

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

$$\begin{aligned} E_0 &\leq \langle E^L_0|H|E^L_0\rangle && (28)\\ &= \langle E^L_0|H_L|E^L_0\rangle + \langle E^L_0|H_I|E^L_0\rangle && (29)\\ &\leq E^L_0 + E^I_{\max}. && (30)\end{aligned}$$

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

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

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. Eq. (31) is a precise, completely general statement of this intuition, a statement that holds even non-perturbatively.

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[7]. The reason is that the proof of Eq. (31) relied on the entanglement-frustration bound, Eq. (2), and there is no natural analogue 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][8].

A detailed discussion of how our eigenspace perturbation theorem compares to the Davis-Kahan theorem is given below. Summarizing, the major differences are that (a) our proof is simpler, (b) our conclusions are more powerful, but (c) 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 $\beta = \{b\}$ be some subset of the eigenvalues of B, and let Q_b be projectors projecting onto any subspaces of the corresponding eigenspaces of B. Define $Q \equiv \sum_{b\in\beta} Q_b$. Then*

$$|P_a Q| \leq \frac{|P_a C Q|}{\Delta_a} \leq \frac{U|C|U^\dagger}{\Delta_a}, \quad (32)$$

where $S \leq T$ 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

[7] 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 $-H$.

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

the distance from a to the set β, 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

$$P_aQ_b = \frac{P_aCQ_b}{a-b}. \tag{33}$$

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

$$|P_aQ|^2 = \sum_b \frac{P_aCQ_bC^\dagger P_a}{|a-b|^2} \tag{34}$$

$$\leq \sum_b \frac{P_aCQ_bC^\dagger P_a}{\Delta_a^2}, \tag{35}$$

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

$$|P_aQ|^2 \leq \frac{|P_aCQ|^2}{\Delta_a^2}. \tag{36}$$

The conclusion follows by using the operator monotonicity[9] 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 $|P_aCQ| \leq U|C|U^\dagger$. Note first that $P_aCQC^\dagger P_a \leq P_aCC^\dagger P_a$. But $P_aCC^\dagger P_a$ and $C^\dagger P_aC$ are positive operators with the same eigenvalues, so there exists a unitary V such that $P_aCC^\dagger P_a = VC^\dagger P_aCV^\dagger \leq VC^\dagger CV^\dagger$. Putting these observations together gives $P_aCQC^\dagger P_a \leq VC^\dagger CV^\dagger$, from which it follows that $P_ACQC^\dagger P_a \leq UCC^\dagger U^\dagger$ for some unitary U. The result now follows by using the operator monotonicity of the square root function.

QED

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

$$|||P_aQ||| \leq \frac{|||P_aCQ|||}{\Delta_a} \leq \frac{|||C|||}{\Delta_a}, \tag{37}$$

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 α and β be subsets of the eigenvalues of A and B, respectively. Let P (resp. Q) project onto the space spanned by all the eigenspaces of A (resp. B) corresponding to elements of α (resp. β). Suppose furthermore that α and β are separated by an annulus of width δ in the complex plane, e.g., with α inside the annulus, and β 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 $|||P_aQ|||$ 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

$$|||P_aQ||| = ||| \, |a\rangle\langle a|b\rangle\langle b| \, ||| = |\langle a|b\rangle| \, ||| \, |a\rangle\langle b| \, ||| \tag{39}$$

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 Δ_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_aQ are the cosines of what are known as the *canonical angles* between the subspaces $\mathcal{P}$ and $\mathcal{Q}$[10]. If $|||P_aQ|||$ is small then

[9] A review of operator monotonicity may be found in Chapter V of [29].

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

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

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

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

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

$$|||P_j Q_{\mathcal{K}_\perp}||| \leq \frac{|||H_I|||}{\Delta_{j,\mathcal{K}_\perp}} \tag{42}$$

where $\Delta_{j,\mathcal{K}_\perp} = \min_{|E_l^L\rangle\in\mathcal{K}_\perp} |E_j - E_l^L|$. 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

$$\begin{aligned} |||P_j Q_{\mathcal{K}_\perp}||| &= ||| \,|E_j\rangle\langle E_j| Q_{\mathcal{K}_\perp}||| && (43)\\ &= |\gamma|\, ||| \,|E_j\rangle\langle E_\perp|\,|||. && (44)\end{aligned}$$

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

$$E(|E_j\rangle) \leq \frac{|||H_I|||^2}{\left(\Delta_{j,\mathcal{K}_\perp}\right)^2}. \tag{46}$$

In Appendix A we show that for any normalized unitarily invariant norm $|||\cdot|||$ we have $\|S\| \leq |||S|||$, where $\|\cdot\|$ is the operator norm and S any operator. The strongest form of the bound is therefore:

$$E(|E_j\rangle) \leq \frac{\|H_I\|^2}{\left(\Delta_{j,\mathcal{K}_\perp}\right)^2}. \tag{47}$$

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 $\Delta_{j,\mathcal{K}_\perp}$ 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 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

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

is maximized. $\Delta E_{j,\mathrm{ent}}$ is a generalization of ΔE_{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

$$\begin{aligned} |E_k^L - E_j| &\geq |E_k^L - E_j^L| - |E_j^L - E_j| && (49)\\ &\geq \Delta E_{j,\mathrm{ent}} - |E_j^L - E_j|. && (50)\end{aligned}$$

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

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

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 $\Delta_{j,\mathrm{ent}} > |E^I_{\max}|$. Then the entanglement in the jth excited eigenstate $|E_j\rangle$ of H, as measured using the definition of Eq. (1), is bounded above by:*

$$E(|E_j\rangle) \leq \frac{\|H_I\|^2}{\left(\Delta E_{j,\mathrm{ent}} - |E^I_{\max}|\right)^2} \tag{52}$$

Noting that $|E^I_{\max}| \leq \|H_I\|$ this can be restated in a slightly weaker but perhaps more elegant form, supposing $\Delta_{j,\mathrm{ent}} \geq \|H_I\|$:

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

Eqs. (52) and (53) confirm and quantify our intuition that when the non-entangled energy scale associated with $|E^L_j\rangle$ 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.

Eq. (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 $-|E^I_{\max}|$ 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 quantum 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. A novel 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 useful definition of frustration, which involves competition between interactions, as discussed in the introduction, and illustrated Fig. 1. (An insightful review of classical and quantum frustration in this sense may be found in [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 non-trivial 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 non-degenerate, 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.

Acknowledgments

We thank Henry Haselgrove and Guifre Vidal for enjoyable and encouraging discussions. Much of this work was completed at the Institute for Quantum Information

at Caltech, and we thank the Institute for their hospitality.

APPENDIX A: UNITARILY INVARIANT NORMS AND THE SUP NORM

In this Appendix we prove that for any normalized unitarily invariant norm $|||\cdot|||$, $\|S\| \leq |||S|||$, where $\|\cdot\|$ is the usual matrix norm. This result is an easy corollary of the following theorem, proved as Theorem 3.5.5 on page 204 of [32]:

Theorem 3. *Let $|||\cdot|||$ be a unitarily invariant norm on the space of $n \times n$ matrices. Then there exists a compact set M in $\Re^n$ whose elements are decreasing sequences of positive real numbers, and such that*

$$|||S||| = \max_{m \in M} \sum_{j=1}^{n} m_j \sigma_j(S), \tag{A1}$$

where $\sigma_j(S)$ are the singular values of S, arranged into decreasing order.

For a normalized unitarily invariant norm we have $||| |s\rangle\langle s| ||| = 1$, where $|s\rangle$ is any normalized state. It follows from the theorem that there exists $m \in M$ such that $m_1 = 1$. It follows that for any S, $|||S||| \geq \sigma_1(S) = \|S\|$, as we set out to prove.

[1] H. L. Haselgrove, M. A. Nielsen, and T. J. Osborne, arXiv:quant-ph/0308083 (2003).
[2] H. L. Haselgrove, M. A. Nielsen, and T. J. Osborne, Phys. Rev. Lett. **91**, 052311 (2003), arXiv:quant-ph/0303022.
[3] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003), arXiv:quant-ph/0211074.
[4] J. I. Latorre, E. Rico, and G. Vidal, arXiv:quant-ph/0304098 (2003).
[5] T. Tessier, I. H. Deutsch, A. Delgado, and I. Fuentes-Guridi, arXiv:quant-ph/0306015 (2003).
[6] T. A. Costi and R. H. McKenzie, Phys. Rev. A **68**, 034301 (2003), arXiv:quant-ph/0302055.
[7] A. P. Hines, R. H. McKenzie, and G. J. Milburn, Phys. Rev. A **67**, 013609 (2003), arXiv:quant-ph/0209122.
[8] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature **416**, 608 (2002), arXiv:quant-ph/0202029.
[9] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002), arXiv:quant-ph/0202162.
[10] S. Scheel, J. Eisert, P. L. Knight, and M. B. Plenio, J. Mod. Opt. **50**, 881 (2002), arXiv:quant-ph/0207120.
[11] X. Wang and P. Zanardi, Phys. Lett. A **301**, 1 (2002), arXiv:quant-ph/0202108.
[12] K. M. O'Connor and W. K. Wootters, Phys. Rev. A **63**, 052302 (2001), 0009041.
[13] D. Gunlycke, V. M. Kendon, V. Vedral, and S. Bose, Phys. Rev. A **64**, 042302 (2001), arXiv:quant-ph/0102137.
[14] M. A. Nielsen, Ph.D. thesis, University of New Mexico (1998), arXiv:quant-ph/0011036.
[15] A. N. Jordan and M. Büttiker (2003), arXiv:quant-ph/0311647.
[16] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information* (Cambridge University Press, Cambridge, 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. **287**, 66 (2002).
[20] G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003), arXiv:quant-ph/0301063.
[21] T. J. Osborne, Ph.D. thesis, The University of Queensland (2002).
[22] J. Preskill, J. Mod. Opt. **47**, 127 (2000), arXiv:quant-ph/9904022.
[23] M. Horodecki, Quantum Information and Computation **1**, 3 (2001).
[24] B. M. Terhal, Theoretical Computer Science **287**, 313 (2002), arXiv:quant-ph/0101032.
[25] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight, Phys. Rev. Lett. **78**, 2275 (1997), arXiv:quant-ph/9702027.
[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 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 (2003), arXiv:quant-ph/0311051.
[31] V. Coffman, J. Kundu, and W. K. Wootters, Phys. Rev. A **61**, 052306 (2000), arXiv:quant-ph/9907047.
[32] R. A. Horn and C. R. Johnson, *Topics in matrix analysis* (Cambridge University Press, Cambridge, 1991).