

## Separability gap and large-deviation entanglement criterion

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For a given Hamiltonian  $H$  on a multipartite quantum system, one is interested in finding the energy  $E_0$  of its ground state. In the separability approximation, arising as a natural consequence of measurement in a separable basis, one looks for the minimal expectation value  $\lambda_{\min}^{\otimes}$  of  $H$  among all product states. For several concrete model Hamiltonians, we investigate the difference  $\lambda_{\min}^{\otimes} - E_0$ , called the separability gap, which vanishes if the ground state has a product structure. In the generic case of a random Hermitian matrix of the Gaussian orthogonal ensemble, we find explicit bounds for the size of the gap which depend on the number of subsystems and hold with probability one. This implies an effective entanglement criterion applicable for any multipartite quantum system: If an expectation value of a typical observable of a given state is sufficiently distant from the average value, the state is almost surely entangled.

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### I. INTRODUCTION

In describing complex many-body physical systems one often postulates a suitable Hamiltonian  $H$  and tries to find its ground-state energy  $E_0$ . From a mathematical perspective, one thus faces an optimization problem when searching for the minimal expectation value among all normalized pure states  $|\psi\rangle$ , that is to say,  $E_0(H) = \min_{\psi} \langle \psi | H | \psi \rangle$ . In principle, if a Hermitian Hamiltonian matrix  $H$  is provided, one can diagonalize it, find its spectrum, and thus easily identify the smallest eigenvalue  $E_0$ . Nevertheless, if the system in question consists of  $L$  interacting particles (e.g., spins), the dimension  $N$  of the matrix grows exponentially,  $N = 2^L$ , rendering this simplistic approach ineffective for  $L \gg 1$ .

Although heuristic algorithms for large systems exist [1,2], they are most likely to fail in the high-entanglement limit [3]. In such cases of practical importance, one applies various methods based on quantum annealing [4,5] and can depend on an increasing number of dedicated physical annealing systems [6–9]. Relying on this approach, however, one faces a variety of difficulties and challenges [10]. There is one particular drawback that is *not* readily evident. Namely, at the end of a quantum annealing, one measures the orientation of individual spins forming the system and obtains an approximation to the ground-state energy related to a product state  $\lambda_{\min}^{\otimes}(H) = \min_{\psi_{\text{sep}}} \langle \psi_{\text{sep}} | H | \psi_{\text{sep}} \rangle$ , where the minimum is taken over all product states  $|\psi_{\text{sep}}\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_L\rangle$ .<sup>1</sup> Such separable states, admitting the simplest tensor network structure with bond dimension being one [11], are physically associated with mean-field-like approximations.

Although for a system composed of  $L \sim 10^3$  spins selecting the optimal configuration of signs out of  $2^L$  possibilities is already a great achievement, in this way one cannot obtain any approximation for the ground-state energy better than the minimal product value  $\lambda_{\min}^{\otimes}(H)$ . The size of the separability gap  $\Delta_{\text{sep}}(H)$ , defined by the difference of both minima

$$\Delta_{\text{sep}}(H) = \lambda_{\min}^{\otimes}(H) - E_0(H), \quad (1)$$

depends clearly on the analyzed Hamiltonian  $H$ .

The aim of the present work is to investigate to what extent this issue poses a fundamental limitation to the near-term quantum annealing technology. In particular, we identify Hamiltonians for which the separability gap (1) becomes significant. For those Hamiltonians there exists a systematic upper bound for the precision of the separable state approximation commonly used by noisy intermediate-scale devices [12], quantum annealers in particular.

Since the latter devices are far from being perfect in many aspects [13], the measurement process they perform has not been put under theoretical scrutiny. However, as the quantum technology improves, this problem becomes more and more relevant for practical applications [14]. In this paper we show that for a generic Hamiltonian the separable state approximation leads to a significant and systematic error of the ground-state energy. Our findings allow us to formulate the large-deviation entanglement criterion based on a generic macroscopic observable that is applicable for any multipartite quantum system. The term “generic Hamiltonian” refers to a typical realization of a random Hermitian matrix pertaining to the Gaussian orthogonal ensemble of a fixed dimension.

We emphasize that it is the measurement process performed by current (and most likely also by near-term [15,16]) quantum annealers that serves as the main motivation behind our work. As far as we know, with these machines one can

<sup>1</sup>Measuring a complex system in a highly entangled energy basis (which may *a priori* be unknown) is practically impossible.

only measure individual spins in the computational basis. A primary example is the D-Wave 2000Q machine where all spins are measured in the  $z$  basis to reconstruct the final (classical) energy. Here we simply pinpoint far-reaching consequences of this fact, indicating the very limit of the underlying present-day technology.

## II. EXTREME SEPARABLE VALUES AND PRODUCT NUMERICAL RANGE

To tackle the aforementioned issue, we begin with basic notions and definitions concerning the spectrum of quantum systems. The set of possible expectation values of an operator  $H$  among all normalized states  $W(H) = \{z : z = \langle \psi | H | \psi \rangle\}$  is called the numerical range [17]. For any Hermitian matrix  $H = H^\dagger$  of order  $N$ , this set forms an interval along the real axis between the extreme eigenvalues  $W(H) = [E_0, E_{N-1}]$ , where the eigenvalues (possibly degenerated) are ordered  $E_0 \leq E_1 \leq \dots \leq E_{N-1}$ .

Assume now that (i)  $N = M^J$  so that the Hilbert space has a tensor structure  $\mathcal{H}_N = \mathcal{H}_M^{\otimes J}$  and (ii) the product states  $|\psi_{\text{sep}}\rangle$  are defined. By analogy, the set of expectation values of  $H$  among normalized product states  $W^\otimes(H) = \{z : z = \langle \psi_{\text{sep}} | H | \psi_{\text{sep}} \rangle\}$  is called the product normal range [18]. By definition it is a subset of  $W(H)$  and for a Hermitian  $H$  it forms an interval between extreme product values  $W^\otimes(H) = [\lambda_{\text{min}}^\otimes, \lambda_{\text{max}}^\otimes]$ . The product numerical range has found several applications in the theory of quantum information [19]. For instance, if the minimal product value of a Hermitian matrix  $H$  of size  $d^2$  is non-negative, then  $H$  represents an entanglement witness or a positive map useful for entanglement detection [20].

### A. Linear chain of interacting qubits

The model we are going to discuss first is motivated by the idea of finding the ground state of a physical system (consisting of interaction qubits) with spin-glass quantum annealers [6]. After the annealing cycle has been completed, just before the final measurement, the system Hamiltonian reads [5]

$$H = - \sum_{(i,j) \in \mathcal{E}} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \sum_{i \in \mathcal{V}} h_i \hat{\sigma}_i^z. \quad (2)$$

Here  $\hat{\sigma}_i^z$  is the  $z$ th component of the spin- $\frac{1}{2}$  operator (acting on a local Hilbert space  $\mathcal{H}_2$ ) associated with the  $i$ th qubit. The input parameters  $J_{ij}$  and  $h_i$  are defined on a graph  $\mathcal{G} = (\mathcal{E}, \mathcal{V})$ , specified by its edges and vertices. They encode the initial problem to be solved [6]. Clearly, this Hamiltonian is classical in the sense that all its terms commute. Thus, the final measurement can be carried out on individual qubits, in any order, without disturbing the system [21]. After that, the ground-state energy is easily reconstructed from the eigenvalues that were measured. This is of great practical importance. However, to become general purpose computing machines [12], near-term annealers will need to include interactions between the remaining components of the spin operator  $\sigma_i^x$  and  $\sigma_i^y$  [22].

General purpose computing machines are those that realize the gate model of quantum computation to which adiabatic

quantum computing is equivalent (with possible polynomial overhead) (cf. Ref. [22]). Although one cannot establish this equivalence with only ZZ interactions, it is sufficient to add only XX- or ZX-type interactions to the annealer Hamiltonian to demonstrate universality [23].

For the sake of argument, assume that the final measurement can be accomplished faithfully. Also, let the system be shielded from its environment for as long as it is necessary to perform computation. Even then, there exists a fundamental limitation on how much information can be extracted from the system by measuring it in the computational basis. We demonstrate this feature by studying a chain of  $L$  spins with a nearest-neighbor coupling: the one-dimensional (1D) Heisenberg model in the transverse magnetic field [24]

$$H = - \sum_{i=1}^{L-1} (\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x) - h \sum_{i=1}^L \hat{\sigma}_i^z. \quad (3)$$

Although for a general Hamiltonian it is hardly possible to evaluate the minimal product value analytically, it is doable in the case of vanishing magnetic field  $h = 0$ .

In order to simplify the matter, we assume spherical coordinates  $(\theta', \phi')$  on a Bloch sphere, rotated such that the main axis lies along the  $y$  axis of the standard Cartesian coordinates. Under such an assumption it can be shown that the expectation value on a separable state  $|\Psi'_{\text{sep}}\rangle = \bigotimes_{i=1}^L |\psi(\theta'_i, \phi'_i)\rangle$  yields

$$\langle \Psi'_{\text{sep}} | H | \Psi'_{\text{sep}} \rangle = \sum_{i=1}^{L-1} \sin \theta_i \sin \theta_{i+1} \cos(\phi_i - \phi_{i+1}), \quad (4)$$

and thus the minimal product value reads  $\lambda_{\text{min}}^\otimes = 1 - L$ .

A numerical simulation [cf. Fig. 1(a)] shows that the separability gap  $\Delta_{\text{sep}}$  plays a crucial role for any system size. For a large number of qubits the gap grows linearly with the system size  $\Delta_{\text{sep}} \approx CL$ , with  $C \approx 0.27$ . In the asymptotic limit  $L \rightarrow \infty$ , the ground-state energy of (3) is derived analytically,  $E_0/L = -4/\pi$ , for the same system with periodic boundary conditions [25,26]. As in this limit  $E_0$  does not depend on the boundary conditions, we arrive at the explicit result for the asymptotic separability gap

$$\Delta_{\text{sep}}(H) = \lambda_{\text{min}}^\otimes - E_0 \xrightarrow{L \rightarrow \infty} \left(\frac{4}{\pi} - 1\right)L. \quad (5)$$

This implies a systematic error if the ground-state energy is approximated by reconstructing the ground state by an optimal product state. To put it differently, in this case the true minimal energy of the system can never be reached by any annealing procedure.

The separability gap is maximal at  $h = 0$  and vanishes in the case of very strong fields  $|h| \gg 1$ , for which the interaction part of  $H$  can be neglected. Interestingly, this dependence is not monotonic, as the separability gap  $\Delta_{\text{sep}}$  exhibits its minimum at  $h \approx 2\sqrt{2}$ . At this value of the field the gap tends to zero, since the ground state of the system becomes a separable Néel product state [27].

### B. Toy model with interaction between all subsystems

Consider an arbitrary Hamiltonian  $H$  describing a system of  $L$  qudits and acting on the space of dimension  $d^L$ . If the

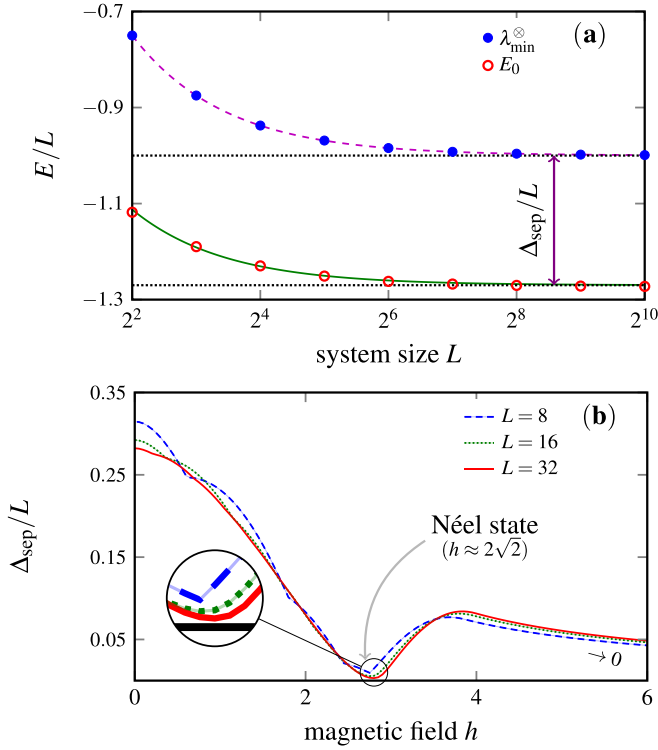


FIG. 1. Numerical solution obtained for the 1D Heisenberg model in Eq. (3). (a) Ground-state energy  $E_0$  and minimal reachable energy  $\lambda_{\min}^{\otimes}$  as a function of the system size  $L$ . Analytic calculations yield  $\lambda_{\min}^{\otimes} = 1/L - 1$  and the best fit results in  $E_0/L = 0.63/L - 1.27$ . (b) Separability gap  $\Delta_{\text{sep}}/L := (\lambda_{\min}^{\otimes} - E_0)/L$  versus the magnetic field  $h$ . The apparent local minimum at  $h \approx 2\sqrt{2}$  corresponds to a Néel product state.

eigenstate  $|\psi_0\rangle$  corresponding to the eigenvalue  $E_0$  is separable, the separability gap vanishes by definition. However, the reverse implication does not hold, as the gap  $\Delta_{\text{sep}}$  can be arbitrarily small even if two eigenstates with the smallest energies  $E_0$  and  $E_1$  are strongly entangled.

To investigate this problem consider a model Hamiltonian matrix representing a two-qubit system

$$H_2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & a & 0 \\ 0 & a & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} =: A(1, a, a, 1), \quad (6)$$

where  $A(x_1, \dots, x_N)$  denotes a matrix with the vector  $x$  at the antidiagonal and zero entries elsewhere. Then the Hamiltonian can be written as [25]

$$H_2 = (2 + 2a)\sigma_x^{\otimes 2} + (2a - 2)\sigma_y^{\otimes 2}. \quad (7)$$

We assume that  $a \in [0, 1]$ , so the ordered spectrum of  $H_2$  reads  $(-1, -a, a, 1)$  and  $E_0 = -1$ . In the nondegenerate case  $a \in (0, 1)$ , all the eigenvectors of  $H_2$  are maximally entangled and they form the Bell basis [28]. Due to the special form of  $H_2$ , it is possible to perform optimization over product states analytically. By assuming angular parametrization on the Bloch sphere  $|\psi(\theta_i, \phi_i)\rangle = (\cos \theta_i/2, e^{i\phi_i} \sin \theta_i/2)$  for each qubit, we arrive at the expectation value of  $H_2$  on a product

state  $|\psi_{\text{sep}}(\theta_1, \theta_2, \phi_1, \phi_2)\rangle \equiv |\psi_{\text{sep}}\rangle$ ,

$$\langle \psi_{\text{sep}} | H_2 | \psi_{\text{sep}} \rangle = \frac{1}{2} \sin \theta_1 \sin \theta_2 \times [\cos(\phi_1 + \phi_2) + a \cos(\phi_1 - \phi_2)], \quad (8)$$

which is to be minimized. By setting  $\theta_1 = \theta_2 = \pi/2$ ,  $\phi_1 + \phi_2 = \pi$ , and  $\phi_1 - \phi_2 = \pi$  we arrive at the minimal value  $\lambda_{\min}^{\otimes}(H_2) = -(1+a)/2$ . Note that the separability gap  $\Delta_{\text{sep}} = (1-a)/2$  is the largest for  $a = 0$  and vanishes for  $a = 1$ .

Analyzing the dimension of a subspace which contains at least a single separable state, one can show [18] that for a Hermitian matrix of order  $N = 4$  the minimal product value is not larger than the energy of the first excited state  $E_0 \leq \lambda_{\min}^{\otimes} \leq E_1$ , so in this case the separability gap is bounded  $\Delta_{\text{sep}} \leq \Delta_1 = E_1 - E_0$ . Hence, in the limit  $a \rightarrow 1$  the spectrum of  $H_2$  becomes degenerate and thus the separability gap vanishes.

Let us now generalize the above model for  $L$  qubits by considering a symmetric, antidiagonal real matrix of size  $N = 2^L$  such that  $(H_L)_{1,N} = (H_L)_{N,1} = 1$  and all other entries are equal to zero. This Hamiltonian captures an all-to-all type of interaction between qubits and can be written in a compact form  $H_L = \sigma_+^{\otimes L} + \sigma_-^{\otimes L}$ , where  $\sigma_{\pm} = \sigma_x \pm i\sigma_y$ . The only nonzero eigenvalues are  $\pm 1$  and thus  $E_0 = -1$ . To calculate the minimum value over the product states  $\lambda_{\min}^{\otimes}$ , we again resort to the polar coordinates on the Bloch ball and define state  $|\Psi_{\text{sep}}\rangle = \bigotimes_{i=1}^L |\psi(\theta_i, \phi_i)\rangle$ . Calculating the expectation value on such state yields

$$\langle \Psi_{\text{sep}} | H_L | \Psi_{\text{sep}} \rangle = 2^{1-L} \left( \prod_i \sin(\theta_i) \right) \cos \left( \sum_{j=1}^L \phi_j \right), \quad (9)$$

which is easily minimized with  $\theta_i = 0$  and  $\sum_{j=1}^L \phi_j = \pi$ . The resulting minimal separable expectation value  $\lambda_{\min}^{\otimes}(H_L) = 2^{1-L}$  tends to zero as  $L \rightarrow \infty$  (recall that  $E_0 = -1$ ). Similar conclusions can be drawn by analyzing a family of real symmetric and antidiagonal Hamiltonians with no more than  $2L$  nonzero entries,

$$(H'_L)_{i,j} = \begin{cases} a_k & \text{for } k = 0, \dots, L-1, \\ (i, j) = (1+k, N-k) \vee (i, j) = (N-k, 1+k) \\ 0 & \text{otherwise.} \end{cases}$$

In particular, setting  $a_1 = 1$ , one obtains  $E_0 = -1$ , and thus the support of the spectrum is  $[-1, 1]$ . On the other hand, one can show, using an analogous method to before, that

$$\lambda_{\min}^{\otimes}(H'_L) = 2^{1-L} \sum_{k=1}^L |a_k|. \quad (10)$$

Hence, the above model extends the family of Hamiltonians for which  $\lambda_{\min}^{\otimes}$  tends to zero in the case of a large number of qubits, despite the support of  $H_L$  being fixed.

As we will shortly see, this nonintuitive property is characteristic of generic Hamiltonians. This is an important result, especially since  $\lambda_{\min}^{\otimes}(H)$  cannot be calculated analytically in general [29] and furthermore all known numerical methods are restricted to small system sizes (cf. Appendix A).

### III. GENERIC HAMILTONIANS OF $L$ -QUBIT SYSTEMS

The situation in which separable states do not approximate well the ground state is in some sense generic (or typical). To substantiate this statement let us consider random Hermitian matrices drawn from the Gaussian orthogonal ensemble (GOE) of size  $N = 2^L$ , which describe Hamiltonians acting on  $L$  qubits. For each sample matrix  $H$  we wish to determine the minimal eigenvalue  $E_0$  and estimate the minimal separable expectation value  $\lambda_{\min}^{\otimes}$ . Due to the concentration of measure in the limit of a large system size, these quantities become self-averaging, so for a typical realization their values are close to the ensemble averages [30].

Generically, no product states are found in subspaces with dimension comparable to  $N$ . In the case of  $L$  qubits a subspace of dimension  $2^L - L - 1$  almost surely (a.s.) contains no product state [31]. It is therefore reasonable to expect that the range of expectation values of a GOE Hamiltonian over product states shrinks with increasing system size: Product states are superpositions of *almost all* eigenstates of the Hamiltonian. This behavior holds true as it is a consequence of the following two results.

*Proposition 1.* Consider a generic Hamiltonian represented by a GOE matrix  $H$  of size  $N = M^J$ , with  $M, J \gg 1$  normalized as  $\langle \text{Tr} H^2 \rangle = N$ , so that the minimal energy asymptotically reads  $E_0 \rightarrow -2$ .

Then the minimal value  $\lambda_{\min}^{\otimes}$  among all product states of the  $J$ -partite system satisfies both estimates

$$-\frac{2J}{\sqrt{N}}(1 + \epsilon_1) \leq_{\text{a.s.}} \lambda_{\min}^{\otimes} \leq_{\text{a.s.}} -\sqrt{\frac{4 \ln N}{N}}(1 - \epsilon_2), \quad (11)$$

understood as follows: Take arbitrary fixed positive constants  $\epsilon_1, \epsilon_2 > 0$ . Let  $A_N$  denote the following event: For a given  $N$  the number  $\lambda_{\min}^{\otimes}$  satisfies both inequalities (11). Then, for an arbitrary  $\delta > 0$  there exists such  $N^*$  that for all  $N > N^*$  the event occurs with probability  $P(A_N) > 1 - \delta$ .

*Proposition 2.* The above estimates work also for the partition of total space into  $L$  qubits. Let us assume that  $M = 2^K$  so that  $N = 2^L$  with  $L = K + J$ , and any state separable with respect to the partition  $\mathcal{H}_2^{\otimes L}$  is separable for splitting  $\mathcal{H}_M^{\otimes J}$  as well.

To derive the upper estimate note that the diagonal entries of  $H$  correspond to expectation values among product states  $|i_1 i_2, \dots, i_j\rangle$ . For any random GOE matrix of size  $N$ , its diagonal  $D = \text{diag} H$  is a sequence of  $N$  numbers independently drawn from the normal distribution  $\mathcal{N}(0, \sqrt{1/N})$ . Therefore, the typical minimal entry on diagonal  $\langle \min D \rangle_{\text{GOE}}$  behaves as  $-\sqrt{4 \ln N/N}$  [32] and leads to the second inequality in (11). The reasoning leading to the lower estimate relies partly on the use of the so-called replica trick and saddle-point approximation (cf. [33] and Appendixes B and C for a more detailed analysis).

Figure 2 presents histograms of the smallest separable expectation value  $\lambda_{\min}^{\otimes}$  obtained for a sample of  $10^3$  random Hamiltonians from the Gaussian orthogonal ensemble of size  $N = 2^L$ . Numerical data are obtained by the algorithm described in Appendix A or a standard optimization algorithm (shown by asterisks). The results obtained correlate with the bounds (11). The lower bound corresponds to a measurement of the energy in an optimized separable basis, while the upper

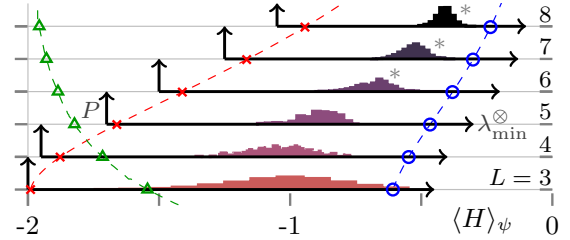


FIG. 2. Collection of six distributions  $P(\lambda_{\min}^{\otimes})$  of minimal separable expectation values for generic GOE Hamiltonians of dimension  $N = 2^L$  for  $L = 3, \dots, 8$ . Red crosses (blue circles) denote asymptotic lower (upper) bounds for  $\lambda_{\min}^{\otimes}$  obtained in Eqs. (11) and (B15) and with fixed  $M = 4$  and green triangles represent the average ground-state energy  $E_0$ . Dashed lines are plotted to guide the eye.

one corresponds to a measurement carried out in the fixed separable basis.

Proposition 1 implies that for a typical random matrix  $H$  acting on an  $L$ -qubit system,  $\lambda_{\min}^{\otimes}(H) \rightarrow 0$  with probability one, although  $E_0(H) \rightarrow -2$ . This observation implies that for a large system described by a generic Hamiltonian, the separability gap is constant,  $\Delta_{\text{sep}} \rightarrow 2$ , so it is not possible to obtain an accurate estimation of the ground-state energy if the measurement is performed in *any* separable basis.

It is worth emphasizing that the above observation has key consequences for the theory of multipartite entanglement in large quantum systems: Measuring any generic observable  $A$  of a composed system of total dimension  $N$  in a separable state yields an outcome close to the average of eigenvalues  $\bar{A} = \text{Tr} A/N$ . This statement can be connected to earlier results of Wieśniak *et al.* [34], who proposed that macroscopic quantities, such as magnetic susceptibility, should be considered as entanglement witnesses. In fact, our observation can be formulated in a similar spirit.

Any generic Hermitian observable  $A$  of order  $N = M^J$  allows one to construct two dual entanglement witnesses, corresponding to both wings of the semicircular spectrum  $W_{\pm}(A) := \mathbb{I} \pm c_{\pm} A$  such that any negative expectation value  $\text{Tr} \rho W_{\pm} < 0$  implies entanglement of the state  $\rho$ . The actual value of the parameter  $c_{\pm} = N/(J\sqrt{\text{Tr} A^2} \mp \text{Tr} A)$ , as a function of the total system size  $N$ , number of parties  $J$ , mean value, and the variance of  $A$ , follows from the bound (11), since it implies that the matrix  $W_{\pm}$  is positive among all states separable with respect to the partition  $\mathcal{H}_N = \mathcal{H}_M^{\otimes J}$ . The above result can be reformulated into the following simple yet very general large-deviation entanglement criterion. Namely, if an expectation value of a typical observable  $A$  of order  $N = M^J$  in the state  $\rho$  is sufficiently distant from the barycenter of the spectrum  $\bar{A} = \text{Tr} A/N$ , that is, when

$$|\text{Tr} A \rho - \bar{A}| > 2J\sqrt{\text{Tr} A^2}/N^2, \quad (12)$$

then the state  $\rho$  is almost surely entangled with respect to the partition into  $J$  subsystems with  $M$  levels each.

Hence this criterion belongs to the class of double-sided entanglement witnesses 2.0 recently analyzed in [35]. Note that the reasoning holds in one direction only, as there exist also entangled states for which the expectation value is close to the mean  $\bar{A}$ . However, numerical computations confirm a

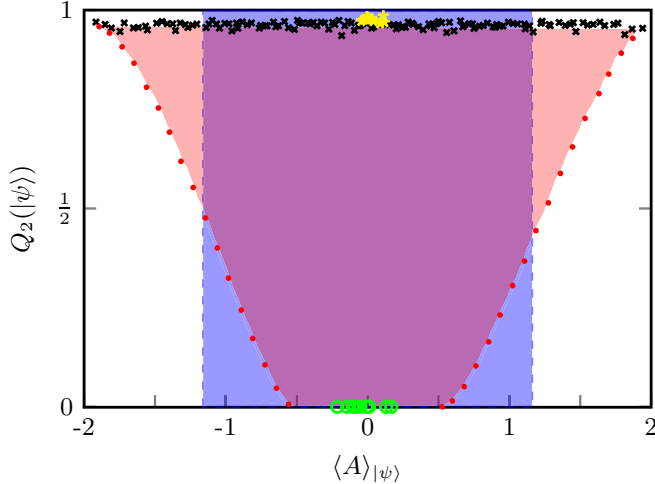


FIG. 3. Range of allowed values for pure states of the system consisting of  $L = 7$  qubits in the plane spanned by the expectation value  $\langle A \rangle_{|\psi\rangle}$  of a GOE observable  $A = H$  of size  $N = 2^L$  and the Meyer-Wallach measure  $Q_2$  of entanglement defined in Eq. (13). Black crosses denote eigenstates of  $H$ , the red region is the numerically determined range attained by pure states, and the shaded blue region denotes the bound  $|\text{Tr}A\rho - \bar{A}| \leq 2L\sqrt{\text{Tr}A^2}/N^2$  implied by Eq. (12), beyond which the states are entangled. In addition, yellow stars represent a sample of ten random pure states and green circles ten random product states.

natural conjecture that the larger the absolute value of the deviation  $\delta = |\langle \phi|A|\phi\rangle - \bar{A}|$ , the larger the average entanglement of the analyzed state  $|\phi\rangle$  (cf. numerical results presented in Fig. 3). To quantify entanglement of pure states of an  $L$ -qubit system, we used the family of measures introduced by Meyer and Wallach [36], which are based on the linear entropy of reduced states averaged over all possible reductions consisting of  $k$  subsystems,

$$Q_k(|\psi\rangle) = \frac{2^k}{2^k - 1} \binom{L}{k}^{-1} \sum_{X:|X|=k} S_{\text{lin}}(\rho_X), \quad (13)$$

where  $S_{\text{lin}}(\rho) = 1 - \text{Tr}\rho^2$  is the linear entropy of a state  $\rho$  of dimension  $2^k$ . This function captures the mean entanglement of  $k$ -qubit subsystems with the rest of the system. Although Fig. 3 depicts data obtained for  $Q_2$ , similar results were also analyzed for other measures of entanglement, including quantities  $Q_k$ , with  $k = 1, \dots, L$ . All these results support the statement that the deviation of the expectation value  $\langle A \rangle_{|\psi\rangle}$  beyond the bounds (12) can be used to quantify the degree of entanglement of the analyzed state  $|\psi\rangle$ .

For comparison, Fig. 3 contains also data for random separable states and generic random states, which are known to be highly entangled [37,38]. The set of separable pure states has a lower dimension and carries zero measure in the entire set of all pure states, so its projection  $W^{\otimes}(A)$  onto an axis determined by the observable  $A$  is typically much smaller than the entire range  $W(A)$ . Asymptotically, in the limit of large dimension  $N$  of the Hilbert space, the ratio of the volumes of both sets tends to zero.

#### IV. DISCUSSION AND OUTLOOK

In this work we have investigated to what extent the near-term quantum annealing technology may become fundamentally limited by its intrinsic measurement process allowing one to ask only *yes* or *no* questions of individual qubits. This type of polling on a quantum system is probably the most natural one and definitely the easiest to realize experimentally. Unfortunately, as we have argued, it does *not* allow one to extract all relevant information from the system in question.

In particular, we analyzed the separability gap and showed that it is nonzero for several model Hamiltonians acting on multipartite quantum systems. Moreover, we studied Hamiltonians constructed by random matrices from the Gaussian orthogonal ensemble and demonstrated that for such a generic Hamiltonian involving  $L$  qubits the minimal value of energy  $\lambda_{\text{min}}^{\otimes}$  among all product states is significantly larger than the ground-state energy  $E_0$ . Thus, making use of near-term quantum annealers, in which the final result is obtained by independent measurements of each of  $L$  qubits and corresponds to a product state, cannot provide a reliable approximation for the ground-state energy of a typical problem. Furthermore, we formulated an entanglement criterion based on the expectation value of a generic observable  $A$  among an arbitrary state  $\rho$  of a composed quantum system and showed that  $\text{Tr}\rho A$  provides direct information concerning the degree of entanglement of the investigated state  $\rho$ .

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#### APPENDIX A: NUMERICAL TECHNIQUE TO ESTIMATE $\lambda_{\text{min}}^{\otimes}(H)$

We briefly sketch here the approach employed in this work to calculate the separability gap for a random Hamiltonian pertaining to the GOE, in the case of a small system size (up to  $N = 2^8$ ). The ground-state energy  $E_0$  can be obtained easily in this case. The algorithm used for calculation of minimal separable expectation  $\lambda_{\text{min}}^{\otimes}$ , on the other hand, utilizes the divide and conquer strategy [39]. To begin with, let us consider a general case of minimizing expectation value of  $\langle \alpha \otimes \beta | H | \alpha \otimes \beta \rangle$ , where  $|\alpha\rangle \in \mathcal{H}_2$  is a qubit state and  $|\beta\rangle$  belongs to a  $d$ -dimensional space  $\mathcal{H}_d$ . The expectation value can be rewritten as

$$\langle \alpha \otimes \beta | H | \alpha \otimes \beta \rangle = \langle \alpha | H_{|\beta\rangle} | \alpha \rangle, \quad (A1)$$

where  $H_{|\beta\rangle} = \text{Tr}_B[H(1 \otimes |\beta\rangle\langle\beta|)]$  is a matrix of size 2. If  $|\beta\rangle$  is fixed, further optimization over  $|\alpha\rangle$  is trivial: The result is a

minimal eigenvalue of the  $2 \times 2$  Hermitian matrix  $H_{|\beta\rangle}$ ,

$$\min_{|\alpha\rangle} \langle \alpha | H_{|\beta\rangle} | \alpha \rangle = \frac{\text{Tr } H_{|\beta\rangle}}{2} - \sqrt{\left(\frac{\langle H_{|\beta\rangle} \rangle}{2}\right)^2 - \det H_{|\beta\rangle}}. \quad (\text{A2})$$

This expression can be written in a more succinct form. Let  $H_i = \text{Tr}_A[H(\sigma_i \otimes 1)]$  (with  $\sigma_0 = 1_2$ ). Then the expression (A2) becomes

$$\frac{\langle H_0 \rangle}{2} - \frac{1}{2} \sqrt{\langle H_1 \rangle^2 + \langle H_2 \rangle^2 + \langle H_3 \rangle^2}, \quad (\text{A3})$$

where all averages are taken over the  $d$ -dimensional vector  $|\beta\rangle$ . The minimization of  $\langle \alpha \otimes \beta | H | \alpha \otimes \beta \rangle$  can be now interpreted as minimization of the convex function over a four-dimensional convex set of simultaneous expectation values called the numerical range:

$$W(H_0, H_1, H_2, H_3) = \text{conv}\{(\langle H_0 \rangle, \langle H_1 \rangle, \langle H_2 \rangle, \langle H_3 \rangle)_{|\beta\rangle} : |\beta\rangle \in \mathcal{H}_d\}. \quad (\text{A4})$$

This problem is easily solved numerically with arbitrarily high accuracy.

The solution of the  $\mathcal{H}_2 \otimes \mathcal{H}_d$  case can be leveraged to the more general  $\mathcal{H}_2^{(\otimes k)} \otimes \mathcal{H}_d$ , where  $k \in \mathbb{N}$ : Using the procedure described above, it is possible to determine an arbitrarily close approximation of the set

$$W^{\otimes}(H_0, H_1, H_2, H_3) = \text{conv}\{(\langle H_0 \rangle, \langle H_1 \rangle, \langle H_2 \rangle, \langle H_3 \rangle)_{|\gamma\rangle} : |\gamma\rangle \in \mathcal{H}_2 \otimes \mathcal{H}_d, |\gamma\rangle = |\alpha \otimes \beta\rangle\}. \quad (\text{A5})$$

This (convex) set  $W^{\otimes}$  can then be used in place of  $W$  in the calculation of  $\lambda_{\min}^{\otimes}$ ; the result is minimal energy over separable states in the tripartite case. This result can be similarly used further; the recursive structure provides natural extensions. The complexity of the algorithm is exponential, owing to the NP-completeness of the problem, but it is possible to determine certified lower and upper bounds of  $\lambda_{\min}^{\otimes}$  this way in deterministic time and linear space complexity.

### APPENDIX B: LOWER ESTIMATE IN PROPOSITION 1

In this Appendix we provide reasoning which leads to the left-hand side of Eq. (11) in the main text for any generic Hamiltonian  $H$  of order  $N = M^J$ , where  $M$  denotes a high ( $M \gg 1$ ), but otherwise arbitrary dimension of each subsystem, while  $J$  stands for their number. The method used relies upon the use of the replica trick, which is a powerful but not fully rigorous method of theoretical physics.

We wish to show that the minimal separable expectation value  $\lambda_{\min}^{\otimes}(H)$  vanishes in the large-system limit  $N \rightarrow \infty$ . Here we analyze separability with respect to partition of the system into  $J$  subsystems of size  $M$  each. Due to the effect of concentration of measure [see a more detailed discussion below after Eq. (B14)] the above quantity is self-averaging, which means that its distribution becomes strongly localized around the expectation value. Therefore, it is sufficient to study the average value and demonstrate that

$$\langle \lambda_{\min}^{\otimes} \rangle \sim -2J/\sqrt{N}, \quad (\text{B1})$$

where the angular brackets denote the ensemble average and

$$\lambda_{\min}^{\otimes} = \min_{|w_{\otimes}\rangle} \langle w_{\otimes} | H | w_{\otimes} \rangle, \quad (\text{B2})$$

with  $w_{\otimes} := w_1 \otimes \dots \otimes w_J$ . To this end, we assume a Hermitian Hamiltonian  $H$  drawn from the GOE with scale parameter  $a$  such that  $\langle \text{Tr } H^2 \rangle = aN$ .

To begin with, we introduce the partition function [40,41]

$$\mathcal{Z}_{\beta} = \int \exp(-\beta \langle w_{\otimes} | H | w_{\otimes} \rangle) dw_{\otimes}, \quad (\text{B3})$$

where  $\beta$  plays the role of the inverse temperature. Here  $dw_i$  denotes the integration measure over a single-qubit space. Then the typical separable expectation value (B1) can be found as the zero-temperature limit of the associated free energy

$$\langle \lambda_{\min}^{\otimes} \rangle = - \lim_{\beta \rightarrow \infty} \frac{\ln \mathcal{Z}_{\beta}}{\beta}. \quad (\text{B4})$$

To calculate the latter limit, consider the function defined for a positive integer  $n$ ,

$$\mathcal{Z}_{\beta}^n = \int \exp\left(-\beta \sum_{i=1}^n \langle w_{\otimes}^{(i)} | H | w_{\otimes}^{(i)} \rangle\right) \prod_{i=1}^n dw_{\otimes}^{(i)}, \quad (\text{B5})$$

which is the  $n$ th power of  $\mathcal{Z}_{\beta}$ . Then we can formally write

$$\langle \ln \mathcal{Z}_{\beta} \rangle = \lim_{n \rightarrow 0} \left\langle \frac{\mathcal{Z}_{\beta}^n - 1}{n} \right\rangle = \frac{d}{dn} \langle \mathcal{Z}_{\beta}^n \rangle \Big|_{n=0}, \quad (\text{B6})$$

which is interpreted as a derivative of an analytic continuation of  $\langle \mathcal{Z}_{\beta}^n \rangle$ . This average can be further simplified using the equality which holds for any matrix  $X$ ,

$$\langle \exp(-\beta \text{Tr } HX) \rangle = \exp[a\beta^2 (\text{Tr } X_H^2)/2], \quad (\text{B7})$$

with  $a$  being the scaling parameter of the GOE. Here  $X_H$  denotes a Hermitian part of a matrix  $X$ . Therefore,

$$\langle \mathcal{Z}_{\beta}^n \rangle = \int \exp\left(\frac{1}{2} a \beta^2 \sum_{i,j=1}^n \langle w_{\otimes}^{(i)} | w_{\otimes}^{(j)} \rangle^2\right) \prod_{i=1}^n dw_{\otimes}^{(i)}. \quad (\text{B8})$$

By introduction of a collection of matrices  $Q_k^{(i,j)} = \langle u_k^{(i)} | u_k^{(j)} \rangle$  one can use them as new integration variables which incur a Jacobian, so that following the method of [42], we have

$$\prod_{i=1}^n du_{\otimes}^{(i)} = C(n, M)^J \prod_{i,j=1,\dots,n}^{k=1,\dots,J} dQ_k^{(i,j)} \left( \prod_{k=1}^J \det Q_k \right)^{(M-n-1)/2}, \quad (\text{B9})$$

where the number  $C(n, M)$  does not depend on  $J$  [furthermore,  $C(0, M) = 1$ ] and the domain of integration over matrices  $Q$  goes over positive-definite matrices of size  $n$  with diagonal entries fixed to be unity. After choosing a nonstandard GOE scaling  $a = M = N^{1/J}$ , the resulting integral can be written in the form

$$\langle \mathcal{Z}_{\beta}^n \rangle = \int \exp \left\{ \frac{M}{2} \left[ \beta^2 \sum (Q_1^{(i,j)} \dots Q_J^{(i,j)})^2 + \sum \ln \det Q_k \right] \right\} \times C(n, M)^J \prod dQ_k^{(i,j)} \left( \prod \det Q_k \right)^{-(n+1)/2} \quad (\text{B10})$$

suitable for the saddle-point–Laplace-method asymptotic approximation [33,43]. Namely, in the limit of large  $M \gg 1$  the integral is dominated by the maximum of the exponent argument, which eventually implies, when combined with (B6) to the leading order,

$$\langle \ln \mathcal{Z}_\beta \rangle \approx \lim_{n \rightarrow 0} \frac{M \Phi(Q_{\text{optim}})}{2n}. \quad (\text{B11})$$

Henceforth, we solve the optimization problem assuming the so-called replica-symmetric ansatz amounting to searching for the optimum on the manifold of  $n \times n$  matrices  $Q_1 = \dots = Q_J := Q$ , where the matrix  $Q$  is parametrized with a single parameter  $q$  as

$$Q(q) = \begin{pmatrix} 1 & q & \dots & q \\ q & 1 & \dots & q \\ \vdots & \vdots & \ddots & \vdots \\ q & q & \dots & 1 \end{pmatrix}. \quad (\text{B12})$$

Such an ansatz is only the simplest among many possible choices compatible with properties of the maximal  $\Phi[Q(q)]$  (and eventually  $n \rightarrow 0$ ) at low temperature (high values of  $\beta$ ) (see Appendix C). It is well known that optimizing in this class gives, strictly speaking, only an upper bound for the true free energy. Checking whether optimizing in a more general class of matrices built by the so-called hierarchical Parisi ansatz [44] can provide a lower ground state is a subject left for future investigation.

Thus the problem within the replica-symmetric ansatz amounts to the optimization of

$$\begin{aligned} \Phi[Q(q)] &= \beta^2 \sum (Q^{oJ})_{i,j}^2 + \sum \ln \det Q_k \\ &= \text{const} + \beta^2 \frac{n(n-1)}{2} q^{2J} \\ &\quad + J\{(n-1) \ln[1-q] + \ln[1+q(n-1)]\}, \end{aligned} \quad (\text{B13})$$

where  $\circ$  denotes the Hadamard (i.e., elementwise) product of matrices. After some computation, one determines the optimal value of  $q$  in the limit  $n \rightarrow 0$  and  $\beta \gg 1$  is to be given by  $q = 1 - 1/\beta + o(1/\beta)$ . Therefore, the following estimate holds:

$$\begin{aligned} \langle \ln \mathcal{Z}_\beta \rangle &\sim \frac{M}{2} \left\{ \frac{\beta^2}{2} (1 - q^{2J}) + J \left( \frac{q}{1-q} + \ln[1-q] \right) \right\} \\ &\approx \frac{M}{2} J [2\beta - \ln \beta]. \end{aligned} \quad (\text{B14})$$

This immediately implies, after taking the limit  $\beta \rightarrow \infty$  in Eq. (B4), that  $\langle \lambda_{\min}^\otimes \rangle \sim -MJ$ , with  $M = N^{1/J}$ , where  $N$  is the total system size,  $J$  is the number of partitions, and  $M$  is their local dimension. Moreover, following [41], one can study fluctuations of the random quantity  $\lambda_{\min}^\otimes$  around its mean value. Namely, defining  $\epsilon := \lambda_{\min}^\otimes / N^{1/J}$ , one can show that the probability density for  $\epsilon$  must have the large-deviation form  $P(\epsilon) \sim \exp\{-N^{1/J} \mathcal{I}(\epsilon)\}$  where the rate function  $\mathcal{I}(\epsilon)$  has its unique minimum at  $\epsilon = -J$ . This quantifies the concentration of measure phenomenon mentioned at the beginning of this Appendix.

Since we have worked with the scaling  $a = M$ , the ensemble average  $\langle \lambda_{\min}^\otimes \rangle$  needs to be compared to the average

minimal eigenvalue  $E_0$ . Then we arrive at the desired expression

$$\frac{\langle \lambda_{\min}^\otimes \rangle}{E_0} = \frac{-JN^{1/J}}{-N^{(1+J^{-1})/2}} = JN^{-(1-J^{-1})/2}. \quad (\text{B15})$$

We have assumed that  $M \gg 1$  such that the saddle-point method can be used. Let us now consider the case of  $N \rightarrow \infty$ ;  $M \gg 1$  is kept constant and  $L \rightarrow \infty$ . In this limit the following holds:

$$\frac{\langle \lambda_{\min}^\otimes \rangle}{E_0} = \frac{\log_M N}{\sqrt{N}}. \quad (\text{B16})$$

This demonstrates that the estimate (B1) holds for  $J \gg 1$ , which completes the reasoning concerning Proposition 1. Therefore, when the dimension  $N = M^J$  increases, the minimal separable expectation value  $\lambda_{\min}^\otimes$  of a generic Hamiltonian of size  $N$  with respect to partition  $\mathcal{H}_M^{\otimes J}$  approaches 0.

Let us now proceed to Proposition 2. Formally, to conduct the proof we require that  $M = N^{1/J} \gg 1$ . Let us now assume that the local dimension forms a power of 2,  $M = 2^K$ , so the total dimension reads  $N = M^J = 2^L$  with  $L = K + J$ . Any state  $|\psi\rangle$  entangled with respect to the partition of the entire system into  $J$  subsystems of size  $M$  is also entangled with respect to the finer partition into  $L$  qubits. Therefore, the estimate (B16) holds also for the physically motivated partition  $\mathcal{H}_N = \mathcal{H}_2^{\otimes L}$  and implies that the ratio  $\langle \lambda_{\min}^\otimes \rangle / E_0$  tends to zero in the limit  $N \rightarrow \infty$ .

### APPENDIX C: MOTIVATION FOR SYMMETRIC-REPLICA ANSATZ

In this Appendix we present heuristic arguments in favor of using the symmetric-replica ansatz. In the low-temperature limit  $\beta \rightarrow \infty$ , the subexponentials have limited importance, provided they are nonpositive in a set of measure zero which does not contain the maximum of the exponential function. First, let us analyze the behavior of the exponent in this limit (the subexponential terms will be taken care of later):

$$\exp\left(\frac{1}{2} a \beta^2 \sum (Q_1^{(i,j)} \dots Q_L^{(i,j)})^2\right). \quad (\text{C1})$$

The term  $\sum_{i,j} (Q_1^{(i,j)} \dots Q_L^{(i,j)})^2$  has a simple interpretation using Hadamard products, i.e., elementwise product of matrices  $(A \circ B)_{i,j} = A_{i,j} B_{i,j}$ . Let us denote by  $X$  a Hadamard product of  $L$  terms, from  $Q_1$  through  $Q_L$ ,

$$X = Q_1 \circ Q_2 \circ \dots \circ Q_L. \quad (\text{C2})$$

Every positive-semidefinite  $X$  can be attained this way. By  $\mathcal{M}$  we denote the set of positive-semidefinite matrices with unit diagonal and by  $J$  a matrix of ones,  $J_{ab} = 1$ . Trivially  $J \in \mathcal{M}$  and  $J \circ \mathcal{M} = \mathcal{M}$ , so  $\mathcal{M} \circ \mathcal{M} \supset \mathcal{M}$ . Due to the Schur product theorem,  $\mathcal{M} \circ \mathcal{M} \subset \mathcal{M}$ , so  $\mathcal{M} \circ \dots \circ \mathcal{M} = \mathcal{M}$ .

Since the diagonal of  $X$  is composed of ones, the positivity condition ensures that  $|X_{i,j}| \leq 1$ . In such a case the maximum of the exponent argument in Eq. (C1) is attained on  $X$  such that  $X \circ X = J$ . The only positive-semidefinite matrix  $X$  with this property is a matrix of ones: Since  $X \circ X = J$ , elements of  $X$  can only be  $\pm 1$  and any sign flip leads to a negative eigenvalue.

We cannot apply this result directly in the calculation of the integral (C5) while using the saddle-point method; subexponential terms are zero at this point and even if we omit them and the limit in  $\beta \rightarrow \infty$  exists, the derivative  $d/dn$  is ill-defined at  $n = 0$ . We know however that  $X = J$  is the limit of the saddle points as  $\beta \rightarrow \infty$ . Making use of this fact, let us write the position of the saddle point as

$$Q_i = J + \mathcal{E}_i(\beta). \quad (\text{C3})$$

In the limit  $\beta \rightarrow \infty$ , the matrices  $\mathcal{E}_i$  tends to zero. Using this, let us expand Eq. (C2) and keep the terms linear in  $\mathcal{E}_i$  only:

$$X = (J + \mathcal{E}_1) \circ (J + \mathcal{E}_2) \circ \dots \circ (J + \mathcal{E}_L) = J + \sum_{i=0}^L \mathcal{E}_i + O(\mathcal{E}^2). \quad (\text{C4})$$

Now the integral (C5) clearly separates:

$$\begin{aligned} ((\mathcal{Z}_\beta^{(H)})^n)_{\text{GOE}} &= C \int \exp\left[\frac{1}{2} a \beta^2 (n^2)\right] \prod_k \left[ \exp\left(2 \sum \mathcal{E}_k^{(i,j)}\right) \right. \\ &\quad \left. \times \det(J + \mathcal{E}_k)^{(M-n-1)/2} d\mathcal{E}_k \right]. \end{aligned} \quad (\text{C5})$$

Because of the separation, all  $\mathcal{E}_i$  are optimized independently and therefore are equal. Now we will argue that due to symmetries of the integral, the optimal matrix  $\mathcal{E}$  has a special form captured by the replica-symmetric ansatz.

The term  $\sum \mathcal{E}^{(i,j)}$  can be interpreted as  $\langle o | \mathcal{E} | o \rangle$ , where  $|o\rangle = (1, 1, \dots, 1)^T$ . If  $\mathcal{E}' = O \mathcal{E} O^T$  for an orthogonal  $O$  such

that  $O|o\rangle = |o\rangle$ , both the determinant  $\det J + \mathcal{E}'$  and  $\sum \mathcal{E}^{(i,j)}$  do not change;  $\mathcal{E}'$  is optimal as well.

Let  $\mathcal{E}'' = (\mathcal{E} + \mathcal{E}')/2$ . The argument of exponent for  $\mathcal{E}''$  is the same. The determinant changes however; due to Minkowski determinant inequality,

$$\begin{aligned} \left(\det \frac{\mathcal{E} + \mathcal{E}'}{2}\right)^{1/n} &\geq \left(\det \frac{\mathcal{E}}{2}\right)^{1/n} + \left(\det \frac{\mathcal{E}'}{2}\right)^{1/n} \\ &= \left(\det \frac{\mathcal{E}}{2}\right)^{1/n}, \end{aligned} \quad (\text{C6})$$

so

$$\det \frac{\mathcal{E} + O \mathcal{E} O^T}{2} \geq \det \mathcal{E}. \quad (\text{C7})$$

This fact holds for every orthogonal matrix  $O$  leaving  $|o\rangle$  unchanged: If  $n < L$ , this implies that either  $\mathcal{E}$  is not optimal (a contradiction) or  $\mathcal{E} = \mathcal{E}'$ . Thus,  $\mathcal{E}$  lies on the set invariant under rotations leaving  $|o\rangle$  unchanged. This implies that  $\mathcal{E} \propto (|o\rangle\langle o| - \mathbb{1})$  and we can parametrize  $Q$  as in Eq. (B12).

Strictly speaking, the above reasoning is valid if the objects  $Q_1, \dots, Q_L$  appearing in the expressions below are square matrices of a definite integer dimension  $n$ . However, during the calculation presented in Appendix B, a formal limit of the analytically extended integral value is taken at  $n \rightarrow 0$ . Therefore, our argumentation is not entirely conclusive, but only suggests that the final results obtained this way still hold true.

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