# Typicality in Ensembles of Quantum States: Monte Carlo Sampling versus Analytical Approximations[†]

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Random quantum states are presently of interest in the fields of quantum information theory and quantum chaos. Moreover, a detailed study of their properties can shed light on some foundational issues of the quantum statistical mechanics such as the emergence of well-defined thermal properties from the pure quantum mechanical description of large many-body systems. When dealing with an ensemble of pure quantum states, two questions naturally arise, what is the probability density function on the parameters which specify the state of the system in a given ensemble, and does there exist a "most typical" value of a function of interest in the considered ensemble? Here, two different ensembles are considered, the random pure state ensemble (RPSE) and the fixed expectation energy ensemble (FEEE). By means of a suitable parametrization of the wave function in terms of populations and phases, we focus on the probability distribution of the populations in these ensembles. A comparison is made between the distribution induced by the inherent geometry of the Hilbert Space and an approximate distribution derived by means of the minimization of the informational functional. While the latter can be analytically handled, the exact geometrical distribution is sampled by a Metropolis–Hastings algorithm. The analysis is made for an ensemble of wave functions describing an ideal system composed of *n* spins of 1/2 and reveals the salient differences between the geometrical and the approximate distributions. The analytical approximations are proven to be useful tools in order to obtain an ensemble-averaged quantity. In particular, we focus on the distribution of the Shannon entropy by providing an explanation of the emergence of a typical value of this quantity in the ensembles.

## 1. Introduction

The characterization of thermodynamic properties and the study of the dynamics of many-body quantum systems are central issues of physical chemistry which should be treated within a suitable statistical framework. The need for a statistical approach to these long-standing problems can be understood from various points of view. On a methodological ground, there are no doubts that statistical methods are the right conceptual tools to build the bridge between a pure (quantum) mechanical description of complex systems and their characterization in terms of thermodynamic quantities or relaxation behavior. Still, from a more practical standpoint, one has to face the difficulties in performing efficient numerical simulations of large quantum systems due to the well-known exponential scaling of the required computation resources with the system dimension.[1] Moreover, although several schemes have been developed in order to increase the quantum simulation performances,[2–4] one should also consider a more subtle difficulty which finds its roots in some foundational aspects of the standard quantum statistical mechanics.[5,6] In particular, the following question arises, how do statistical mechanics emerge from the underlying quantum mechanical description? There is no obvious answer to this question. Even if we could perform a simulation of a large many-body quantum system in analogy to a classical molecular dynamics experiment, there is not a straightforward relation between the results of such a calculation, that is, the time-dependent wave function of the isolated system, and the standard quantum statistical description based on the statistical density matrix. Of course, one could identify the latter quantity

with the time average of the instantaneous density matrix determined by the wave function, but in such a case, it is not clear why an evolving isolated system should necessarily leads to the microcanonical statistical density matrix.[7]

Recently, the possibility of investigating single-molecule or single-spin observables,[8,9] as well as the necessity of a better understanding of the mechanisms underlying quantum dynamics in order to obtain nanoscale devices and nanostructured materials suitable for quantum computing tasks,[10–12] has revived the interest in the foundations of quantum statistical mechanics. Important contributions in this field[13–15] invite one to look at quantum statistical mechanics from a different standpoint. One of the key ingredients of this new perspective consists of shifting the focus from the ensemble averages of the traditional quantum statistics back to the role and predictability of one single realization of a system and its environment described by a quantum mechanical pure state associated with a wave function.

Within this perspective, the concept of typicality[16] as the key to the emergence of standard statistical equilibrium behavior has recently been discussed in various works.[13–15] In its widest meaning, the term typicality indicates that by selecting a set of states on the basis of some conventional rules, one obtains a very narrow distribution of some relevant features, which become, actually, typical among those states. In particular, it has been shown that a quantum subsystem which is part of a much bigger system described by a pure state can be very likely described by a typical reduced density matrix, which is the canonical one under certain conditions.[14] Nonetheless the emergence of typical values for a large class of observables is not restricted to a small subsystem, as discussed by Reimann in ref 15.

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The main goal of the present contribution is the development of methodologies for the study of statistical ensembles of quantum pure states. These methodologies are useful tools for the analysis of typicality not only of asymptotically large systems but also for finite systems amenable to exact numerical computations. They include the following items: (i) the derivation of the probability density (distribution) for ensembles of quantum pure states on the basis of the geometrical measure in the Hilbert space given a suitable parametrization of the wave function, (ii) for a given probability density, the generation of a numerical sampling of the ensemble, which allows one to calculate the distribution of any property of the quantum system and, in particular, to assess its typicality, and (iii) the derivation of approximate probability distributions leading to a direct calculation of the averages within the ensemble without the need for the numerical sampling. We emphasize the importance of the third item for the study of large quantum systems whose characterization through numerical sampling is not feasible. Obviously, the evaluation of typicality for asymptotically large systems falls in such a category of problems. On the other hand, a stronger confidence on the applicability of the invoked approximations could derive from the comparison with the exact numerical results for finite systems.

In the present paper, these new methodological tools will be applied to two different ensembles of quantum pure states. In the first one, we consider quantum pure states chosen at random with respect to the uniform measure on the unit sphere in a finite dimensional Hilbert space.[17] They are a much studied subject in the field of quantum information science since they are a resource for a variety of quantum information protocols.[18,19] For example, their entanglement properties have been studied by many authors,[20−23] and several schemes have been proposed for generating them efficiently.[24] Furthermore, ensembles of random states have been previously considered in several studies of the foundations of statistical mechanics.[14,25,26] A statistical sample of states drawn according to such a distribution will be called the random pure state ensemble (RPSE).

In the second type of ensembles, the wave functions are chosen at random but with the constraint of having a common expectation value of some observable. We specifically consider the case of fixed expectation value of the energy, but the methodology used by us to obtain the corresponding probability density is rather general, and it can be employed to generate any ensemble of this kind.[27] The statistical sample for such a distribution will be denoted as the fixed expectation energy ensemble (FEEE). This type of distribution has been recently proposed as the quantum counterpart of the classical microcanonical ensemble.[28−30]

In order to test the capability of these methods to quantify the typicality of a given observable, we shall explicitly consider the Shannon entropy as an important collective property of the quantum system. We emphasize, however, that the same methods can be applied to any chosen property of the quantum system.

In section 2, we introduce a suitable parametrization of the wave function in terms of populations and phases and derive the corresponding probability density from the inherent geometry of the Hilbert space. In section 3, the distributions for the considered ensembles are investigated by employing Monte Carlo sampling techniques. Albeit we consider systems of noninteracting spins for the sake of simplicity, the procedure can be easily applied to arbitrary quantum systems. In section 4, we shall derive and discuss approximations of probability distributions for the ensembles, which can be analytically

handled, and their validity can be assessed by comparison with the Monte Carlo results.

## 2. Theory

**2.1. Definition of the Ensembles.** Before providing the formal definition of the examined ensembles of pure states, it is worth spending some words to clarify how the concept of ensemble is intended in the following. By ensemble, we always mean an abstract construction for the statistical sampling of the possible pure states (each of them described by a wave function) of an isolated quantum system. Once the states (wave functions) have been properly parametrized, one can introduce the probability density with respect to these parameters, and the ensemble becomes simply a realization for the statistical sampling of the probability distribution.

A given isolated quantum system is characterized by its time-independent Hamiltonian $H$, which defines the corresponding eigenenergy (orthonormal) basis $\{e_k, k = 1, ..., N\}$, where $N$ denotes the dimension of the Hilbert space $\mathcal{H}$ of the system. Here, we shall consider a Hilbert space of arbitrary large but finite dimension. Thus, any wave function $\psi$ in such a space can be specified as the superposition of the eigenenergy vectors

$$\psi = \sum_{k=1}^{N} c^k e_k \qquad (1)$$

The $N$-dimensional complex vector $c \equiv (c^1, c^2, ..., c^N) \in \mathbb{C}^N$ can be written as a $2N$ dimensional real vector $x \equiv (\text{Re } c, \text{Im } c) \in \mathbb{R}^{2N}$, and in the latter representation, the norm of the state vector is given as Euclidean norm

$$\psi = \sqrt{\langle \psi | \psi \rangle} = \sqrt{\sum_{j}^{2N} (x^j)^2} \qquad (2)$$

Thus, the $\mathbb{R}^{2N}$ space "contains" all of the possible non-normalized state vectors.

We define the RPSE as the set of normalized wave functions which are uniformly distributed in the Hilbert space $\mathcal{H}$ of the system. The normalization condition

$$\langle \psi | \psi \rangle = 1 \qquad (3)$$

defines, according to eq 2, a $(2N − 1)$-dimensional sphere embedded in the $(2N)$-dimensional $\mathbb{R}^{2N}$ space

$$S^{2N-1} = \{x \in \mathbb{R}^{2N} | \sum_{j=1}^{2N} (x^j)^2 = 1\} \qquad (4)$$

For the set of pure states, there is a unique measure which is invariant under all unitary transformations,[17] in correspondence to the uniform distribution over the $S^{2N-1}$ unit sphere defined above.

Recently, a generalized microcanonical ensemble has been proposed,[28,29] with the microcanonical energy identified with the expectation value of the Hamiltonian

$$E = \langle \psi | H | \psi \rangle = \sum_{k=1}^{N} E_k c^k \qquad (5)$$

$E_k$ being the $k$th Hamiltonian eigenvalue, $He_k = E_k e_k$. We define the FEEE in correspondence with the set of all of the normalized wave functions in $\mathscr{H}$, which are characterized by a given value $E$ of the expectation energy according to eq 5.

For the geometrical analysis of the previously defined ensembles, it is convenient to introduce the following parametrization of the wave functions

$$\psi = \sum_{k=1}^{N} \sqrt{P_k} \exp[i\alpha_k] e_k \qquad (6)$$

where the complex coefficients of eq 1 are written in their polar form. We shall refer to the absolute squares of the coefficients as "populations", $P_k \equiv |c_k|^2$, while the "phases" $\alpha_k$ are defined as the inverse tangent of the ratio between the imaginary and the real part of the coefficients, $\alpha_k \equiv \tan^{-1}(\text{Im } c_k/\text{Re } c_k)$. It should be emphasized that in the space $\mathbb{R}^{2N}$, the set of populations is not normalized, $\sum_k P_k \neq 1$, unless $\|\psi\| = 1$.

**2.2. Probability Distribution on the Ensembles.** In this section, we shall sketch the derivation of the ensemble probability distributions on a chosen coordinate set which specifies the wave function. The natural underlying assumption is that the probability of a certain set of wave functions is proportional to the measure of the set of their representative points in the space where the ensemble is defined.

Let us start by recalling that in the $\mathbb{R}^{2N}$ space, the state vector has a Euclidean norm, eq 2, when the set of coordinates $x \equiv (\text{Re } c, \text{Im } c)$ is used. Therefore, for such a representation, a Euclidean geometry can be assumed with a unit metric tensor[31]

$$g_{ij}(x) = \delta_{ij} \qquad (7)$$

and the measure of any region is obtained by integration of the elementary volume element $dV = dx = dx^1 dx^2 ... dx^{2N}$. The invariance of the volume measure allows one to write the volume element in arbitrary coordinates $y = (y^1, y^2, ..., y^{2N})$ as

$$dV = \sqrt{|g(y)|} dy \qquad (8)$$

where $dy = dy^1 dy^2 ... dy^{2N}$ and $g(y)$ is the determinant of the metric tensor $g_{ij}(y)$ in the $y$ representation

$$g_{ij}(y) = \sum_{i',j'=1}^{2N} \frac{\partial x^{i'}}{\partial y^i} g_{i'j'}(x) \frac{\partial x^{j'}}{\partial y^j} = \sum_{j'=1}^{2N} \frac{\partial x^{i'}}{\partial y^i} \frac{\partial x^{i'}}{\partial y^j} \qquad (9)$$

The explicit use of the metric tensor is convenient because it permits determination of the proper volume element of any surface embedded in the original Euclidean space.[31] In general, $n$ conditions on the coordinates $y$ of a $2N$-dimensional space define an hypersurface of dimension $K = 2N - n$. In the neighborhoods of any nonsingular point of the surface, one can introduce a local set of coordinates $z = (z^1, ..., z^K)$ which parametrically determines the location of a point on the surface, $y^i(z)$ for $i = 1, 2, ..., 2N$. The metric tensor induced on the surface is then given by

$$g_{kk'}(z) = \sum_{ij=1}^{2N} \frac{\partial y^i}{\partial z^k} g_{ij}(y) \frac{\partial y^j}{\partial z^{k'}} \qquad (10)$$

where $k,k' = 1, ..., K$. Once the metrics on the surface is known, like in eq 8, one can specify the corresponding volume element as $dV = |g(z)|^{1/2} dz$ with $dz = dz^1 dz^2 ... dz^K$.

Since both ensembles, RPSE and the FEEE, are defined by constraints which define hypersurfaces embedded in the $\mathbb{R}^{2N}$ space, one can apply the above-mentioned scheme to obtain the corresponding volume element $dV$. Then, because of the assumed proportionality between the probability that the state vector belongs to a given set and its geometrical measure, one can specify the probability density $p(z)$ with respect to coordinates $z$ according to the relation

$$p(z)dz = \frac{dV}{\int_D dV} \qquad (11)$$

where the normalization is calculated as the total volume of the set D for the allowed pure states. In this way, from the measure, one derives the probability density of the surface points

$$p(z) = \frac{\sqrt{|g(z)|}}{\int_D \sqrt{|g(z)|} dz} \qquad (12)$$

The representation of the $\mathbb{R}^{2N}$ space by means of populations and phases, $y = (P, \alpha)$, where $P = (P_1, P_2, ..., P_N)$ and $\alpha = (\alpha_1, \alpha_2, ..., \alpha_N)$, is particularly convenient since the constraints of state vector normalization eq 3 and fixed expectation energy eq 5 involve populations only

$$\sum_k P_k = 1 \qquad (13)$$

$$\sum_k P_k E_k = E \qquad (14)$$

This implies that the set of populations is statistically independent of the phases and also that each phase variable is characterized by a uniform distribution in the corresponding definition domain $[0, 2\pi)$ (see Appendix A for the details). Thus, the probability density on the populations $P$ and phases $\alpha$ can be factored as

$$p(P, \alpha) = p(P)p(\alpha) = p(P)/(2\pi)^N \qquad (15)$$

For the RPSE, only the condition in eq 13 has to be considered, and thus, one can use all of the set of phases $\alpha$ and the $(N - 1)$-independent populations $P = (P_1, ..., P_{N-1})$ as coordinates $z$ on the corresponding surface. Appendix A describes in detail the calculation of the determinant $g(z)$ of the metric tensor leading to the following RPSE probability density on the populations

$$p_{\text{RPSE}}(P_1, ..., P_{N-1}) = (N - 1)! \qquad (16)$$

The set of populations which characterizes wave functions in the FEEE has to satisfy both eqs 13 and 14. If the two constraints are used to determine the populations $P_N$ and $P_{N-1}$, then as described in Appendix A, one derives the following explicit form for the probability distribution

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$$p_{\text{FEEE}}(P_1, ..., P_{N-2}) = \frac{1}{C}\left[\sum_{j=1}^{N-2} P_j(1 + a_j)a_j - \left(\frac{E - E_{N-1}}{E_N - E_{N-1}}\right)^2 + \left(\frac{E - E_{N-1}}{E_N - E_{N-1}}\right)\right]^{1/2} \quad (17)$$

with coefficients $a_j = (E_{N-1} - E_j)/(E_N - E_{N-1})$ and the constant $C$ determined by the normalization of the probability density.

By using the ensemble distribution, eq 15, with the corresponding probability density on populations, eq 16 or 17, one can obtain in principle the ensemble average of any function of a quantum state $a(|\psi\rangle) = a(P,\alpha)$

$$\langle a \rangle = \int_D a(\alpha, P)p(\alpha, P)\mathrm{d}P\mathrm{d}\alpha \quad (18)$$

as well as the average of its higher moments

$$\langle a^n \rangle = \int_D a(\alpha, P)^n p(\alpha, P)\mathrm{d}P\mathrm{d}\alpha \quad (19)$$

Among the possible functions, one can include the expectation value $a = \langle\psi|A|\psi\rangle$ of an operator $A$ defined in the Hilbert space. It should be emphasized that, if these averages are available, then one can quantify the typicality of a property described by a real function $a(P,\alpha)$ by examining its variance

$$\sigma_a \equiv \sqrt{\langle a^2 \rangle - \langle a \rangle^2} \quad (20)$$

In conclusion, for the two types of ensembles introduced here, we have derived the corresponding probability distributions, which in principle allow the calculation of the average of any property and characterization of the typicality as well. This, however, requires the evaluation of multidimensional integrals that rarely can be performed directly. Therefore, in order to characterize the statistical behavior of a property within an ensemble, one has to introduce a suitable approximation of the probability distribution that allows an analytical estimate of the averages or to perform a statistical sampling for the given probability distribution. The first route will be tackled in section 4, while in the next section, we address the issue of the statistical sampling. Albeit the procedures we present are general enough to analyze the typicality of any property, in order to provide specific examples of their application, we shall consider the following entropy function

$$S = -\sum_{k=1}^{N} P_k \ln P_k \quad (21)$$

It corresponds to the Shannon entropy in the energy representation, which is usually interpreted as a measure of the lack of information about the outcome of the measurement of the energy. In the present framework, we do not consider the measurement process, so that the function in eq 21 is rather interpreted as a measure of the degree of disorder of a quantum pure state in relation to its decomposition into the Hamiltonian eigenstates. In particular, a vanishing entropy would be recovered only for a stationary state, $\psi \propto e_k$, for a given eigenstate $e_k$. It should be noted that several theoretical entropy measures for quantum systems have been discussed in the literature;[32-34] nonetheless, the issue of the relation between such informational measure and the thermodynamic entropy is still the subject of a lively debate and active research.[35-38]

## 3. Monte Carlo Ensemble Sampling and Typicality

We shall employ Monte Carlo sampling techniques in order to draw a statistical sample of population sets and study the corresponding ensemble distributions of the populations and of the entropy function eq 21. Ensembles of spins are convenient systems for investigations of quantum statistical behavior since one has to consider a finite dimensional Hilbert space. This kind of model systems is the subject of a continuously increasing attention either from a theoretical[11,39] or an experimental perspective[8,9,40] because it represents the natural test bed for quantum information protocols. We thus consider a system composed of $n$ noninteracting 1/2 spins, each spin having its Zeeman frequency $\omega_k$, so that the total number of states of the system is $N = 2^n$.

**3.1. Population and Entropy Distribution in the RPSE.** In order to study the RPSE, one has to draw samples from the uniform probability distribution on the $N - 1$ simplex, eq 16, of the populations. The problem can be solved by introducing an auxiliary set of variables $\xi \equiv (\xi_1, ..., \xi_{N-1})$ uniformly distributed in (0,1]. It is easily shown[26,41] that the set of populations calculated as

$$P_1 = 1 - \xi_1^{1/(N-1)}, ......, \quad P_J = \left(1 - \xi_J^{1/(N-J)}\right)\prod_{i=1}^{J-1} \xi_i^{1/(N-i)}, ......,$$

$$P_N = \prod_{i=1}^{N-1} \xi_i^{1/(N-i)} \quad (22)$$

is a realization from the RPSE distribution, eq 16. This allows one to efficiently generate a statistical sample of the population set for the RPSE and thus the corresponding distribution of the entropy through the definition in eq 21.

Figure 1 shows the marginal distribution of a single population obtained as a (normalized) histogram of the statistical sample numerically generated from the geometrical distribution, eq 16. It should be evident that RPSE, whose probability distribution is invariant with respect to the exchange of population variables, does not privilege any population and, therefore, leads to the same marginal distribution for all of the populations. It is also clear that an increase of the number of spins moves the marginal distribution to lower values of the population variable. This is a direct consequence of the dependence of the average population $\langle P_k \rangle = 1/N$ on the dimension $N$ of the Hilbert space, simply deriving from the population normalization. A less obvious behavior which appears evident from the diagrams of Figure 1 is that the population distribution has a width $\sigma_{P_k}$ always comparable to the population average $\langle P_k \rangle$. Such a feature, which will be rationalized in section 4, brings the conclusion that within RPSE, the populations do not display typicality.

On the other hand, from the standard quantum statistical mechanics, one has the intuition that at least some functions of the state of the system, such as the entropy, should not depend on the details which specify the state, that is, on a particular choice of the population set but only on "gross properties" of the quantum state. In Figure 2, the ensemble distribution of the entropy per spin, that is, $S/n$, for systems composed of different numbers of spins is reported. The histograms resulting from the sampling are well fitted by Gaussian distributions. In the inset of the figure, the standard deviations of the fitting
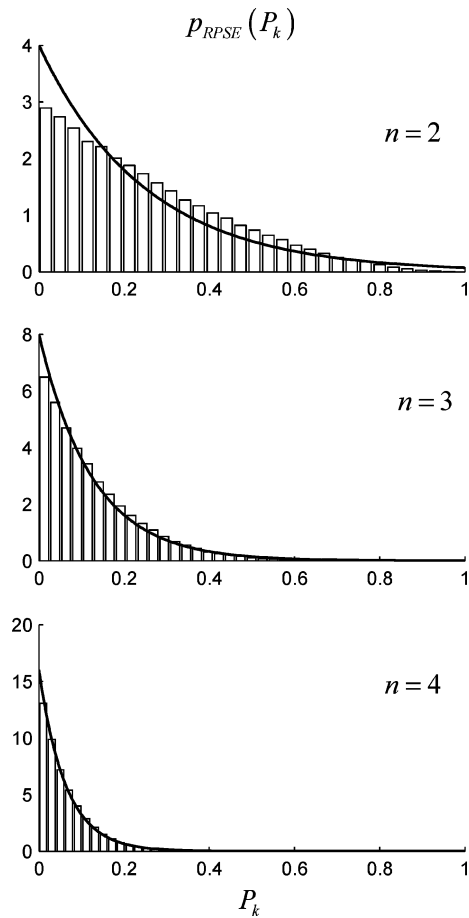
$p_{RPSE}(P_k)$



**Figure 1.** Marginal distribution of a population in the RPSE: the (normalized) histograms refers to the statistical sample of $10^5$ points (in 30 bins) generated by the algorithm described in the text for a system composed of $n = 2$, 3, and 4 spins respectively. The continuous lines represent the exponential distribution, eq 29, discussed in section 4.1.
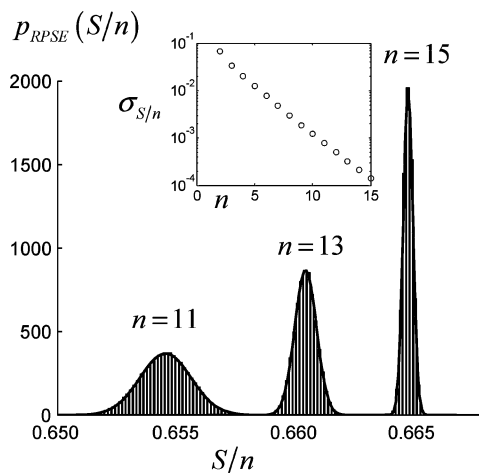
$p_{RPSE}(S/n)$



**Figure 2.** Distribution of the entropy per spin $S/n$ for different numbers of spins as obtained by numerical sampling ($10^5$ sampled points) of the RPSE distribution of systems composed of $n = 11$, 13, and 15 spins as indicated in the figure. In the inset, the standard deviation of the fitting Gaussian distributions is reported as a function of the number of spins which constitute the system.

distributions are reported as a function of the number of spins in the system.

The main point which emerges from these calculations is the existence of a typical value of the entropy per spin in the

considered ensemble of pure states. Indeed, as the number of spins increases, the entropy distribution becomes a sharper and sharper function peaked around a typical value which can be identified with the average entropy. Such a property, which is called typicality, has been recently used to explain the emergence of the canonical state for a subsystem which is part of a much bigger system described by a pure state.[13,14] Reimann[15] has proven that under certain hypotheses, the property of typicality also holds for the expectation value of a generic observable. Our results on the RPSE distribution of the entropy have to be interpreted as evidence of the property of typicality. In other words, as the size of the system increases, the vast majority of the different pure states which belong to the RPSE are characterized by nearly the same value of the entropy function even if each of them is defined by a different set of populations.

**3.2. Population and Entropy Distribution in the FEEE.** For studying the FEEE, we need to generate a statistical sample from the probability density eq 17. Since the normalization constant is unknown and we deal with a multivariate probability distribution, the use of a Markov chain becomes convenient. Our sampling of the FEEE has been performed by means of a Metropolis−Hastings algorithm.[42,43] In particular, a random walk updating scheme[44] has been implemented.[7]

The algorithm is basically made up by the following steps:

(1) Start at an arbitrary point $X$ which belong to the domain of the target distribution $p_{FEEE}(P_1, ..., P_{N-2})$, with $p_{FEEE}(X) > 0$.

(2) Generate a random variable $Y$ from an arbitrary but fixed proposal distribution $q(X,Y)$; this represents a proposed move from the state $X$ to the state $Y$. In the random walk updating scheme, the proposed new value $Y$ equals the current values $X$ incremented by a random variable $Z$, $Y = X + Z$. In this case, $q(X,Y) = g(Y - X) = g(Z)$ is the probability density associated with the random variable $Z$. We have used the multivariate Gaussian distribution

$$g(Z) = \frac{1}{(2\pi)^{N/2}(\det \Sigma)^{1/2}} \exp\left[-\frac{1}{2}Z^T\Sigma^{-1}Z\right] \quad (23)$$

where $\Sigma$ is the covariance matrix. A diagonal covariance matrix is used, with each entry proportional to the average populations calculated on the basis of the approximate distributions introduced in section 4

$$\Sigma_{kk'} \propto \delta_{kk'}(\lambda + \mu E_k)^{-1} \quad (24)$$

where the $\lambda$ and $\mu$ parameters are defined in eq 36. The variance of the proposal distribution can be thought of as a set of tuning parameters to be adjusted to get an optimal sampling of the target distribution.

(3) Calculate what can be termed the probability of move

$$\alpha(X, Y) = \min\left[1, \frac{p_{FEEE}(Y)}{p_{FEEE}(X)}\right] \quad (25)$$

(4) Generate a random variable $u$ uniformly from [0,1]. If $u < \alpha$, accept the proposal and move to state $Y$; otherwise, reject the proposal and remain in $X$, to be considered as the new sample. Repeat 1−4.

In order to determine the FEEE target distribution, one has to specify the energy spectrum of the considered system. Let $|M\rangle = |m_1^M m_2^M ... m_n^M\rangle$ be an eigenenergy state of the system
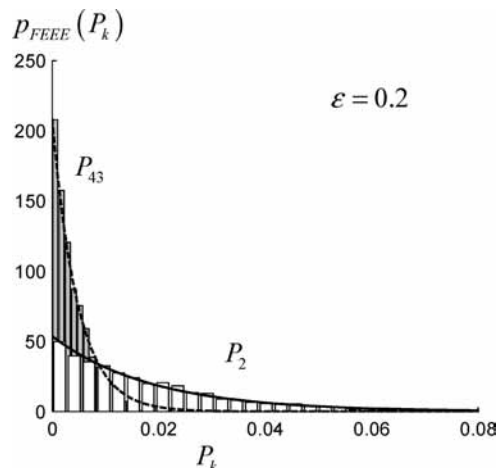
**Figure 3.** Marginal distributions of $P_2$, corresponding to the energy eigenvalue $E_2 = 1$, and those of $P_{43}$, corresponding to the energy eigenvalue $E_{43} = 4$, obtained from the numerical sampling ($2 \times 10^5$ sampled points) of the FEEE for a system of $n = 6$ spins. The expectation energy per spin is set to $\varepsilon = 0.2$. The solid lines represent the approximate distributions discussed in section 4.2.
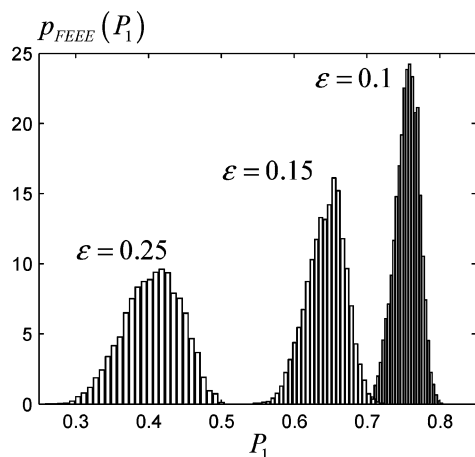


**Figure 4.** Marginal distributions of the first population $P_1$ corresponding to the ground state. The calculations refer to the FEEE ($2 \times 10^5$ sampled points) of a system composed of $n = 6$ spins for three different values of the expectation energy per spin as reported in the figure.

composed of $n$ noninteracting 1/2 spins. Thus, the corresponding energy is given as $E_M = \sum_{k=1}^{n} \hbar\omega_k m_k^M$, where $m_k^M = \mp 1/2$ and $\omega_k$ is the Zeeman frequency of the $k$th spin. We have to study the distribution of the populations and that of the entropy as a function of the expectation energy $E = \sum_{M=1}^{N} P_M E_M$. In practice, it is convenient to employ the energy per spin $\varepsilon = E/n$ as the only independent parameter which defines the FEEE of a given system. For the sake of simplicity, the distributions reported here refer to a system of $n$ identical spins, that is, $\omega_k = \omega_0$ for all $k$; however, it has been verified that the general features of resulting distributions do not depend on such a particular assumption. In the following, $\hbar\omega_0$ will be used as the energy unit, and we conventionally set the zero of the energy scale in correspondence to the ground state, that is, $E_1 = 0$. Figures 3 and 4 report the distributions of single populations obtained from the numerical sampling. Due to the presence of the expectation energy constraint, the populations corresponding to different energy levels are not statistically equivalent. In Figure 3, the distributions of the population $P_2$, corresponding to $E_2 = 1$, and those of the population $P_{43}$, corresponding to the energy eigenvalue $E_{43} = 4$, are shown. These calculations refer to a system composed of $n = 6$ spins with energy per spin equal to
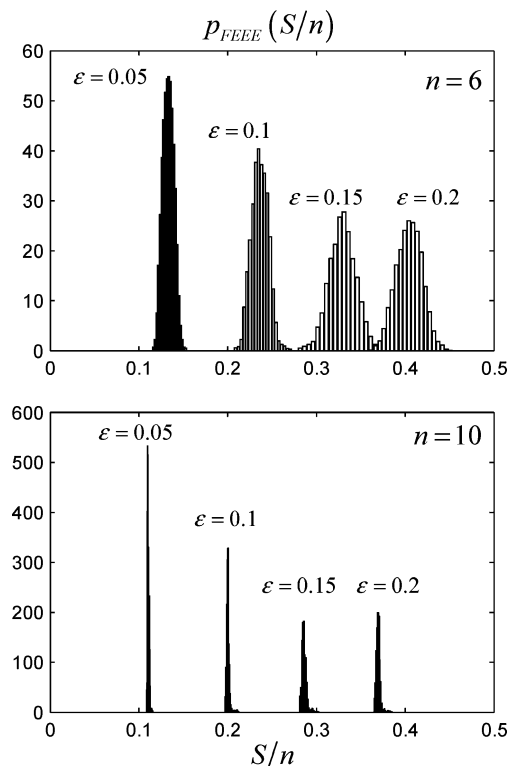


**Figure 5.** FEEE distributions of the Shannon entropy per spin for a system composed of $n = 6$ (upper panel) and 10 spins (lower panel). The (normalized) histograms refer to different values of the expectation energy per spin as reported in the figure.

$\varepsilon = 0.2$. Even if the populations are not statistically equivalent, each marginal distribution has an exponential-like profile like that in the RPSE. This is generally true for all of the populations and for all the possible values of the energy parameter $\varepsilon$, with the notable exception of the ground-state population. As it is evident from Figure 4, the ground-state population has a distribution with a peaked profile, at least for not too large expectation energies. Furthermore, the center of such a distribution moves toward the unity with a decrease of its width for $\varepsilon \rightarrow 0$. Indeed, to attain such a limit, the ground-state population should increase up to reach its maximum value.

Figure 5 shows the FEEE distribution of the entropy per spin obtained from the Monte Carlo sampling for different values of the expectation energy per spin. The upper panel refers to a system of $n = 6$ spins, while the lower panel is the sampling for $n = 10$ spins. These results clearly show that the entropy distribution is concentrated around a typical value. Furthermore, the comparison of the distributions for $n = 6$ and 10 cases clearly demonstrates that the enlargement of the system size produces a narrowing of the entropy distribution, like that for the RPSE distributions previously examined. The main difference is that for FEEE, the distribution of the entropy and its typical value (i.e., the distribution maximum) depends on the expectation energy.

## 4. Approximate Distributions from Minimization of the Information Functional

**4.1. Approximate Distribution for the RPSE.** An approximate form of the distribution for the RPSE has been proposed by Wootters.[45] Such a distribution is very useful since it allows straightforward estimates of the averages in the ensemble, which result to be rather accurate in the comparison with the numerical results of the Monte Carlo calculations. We

shall derive the same approximate distribution by following a different method based on the information functional, which can be easily generalized to ensembles different from the RPSE, like the FEEE, as shown in the following.

The key methodological ingredient of the Wootters (and our) method is the replacement of the populations, which in the RPSE should satisfy the normalization constraint, $\sum_{k=1}^{N} P_k = 1$, with a set of $N$ random variables $\eta = (\eta_1, \eta_2, ..., \eta_N)$, each of them defined in the domain $[0,\infty]$, with a distribution characterized through the probability density $W(\eta)$ normalized as

$$\int d\eta\, W(\eta) = \int_0^\infty d\eta_1 \int_0^\infty d\eta_2... \int_0^\infty d\eta_N W(\eta) = 1 \tag{26}$$

and which allows the determination of the average $\langle f(\eta)\rangle$ of any function $f(\eta)$ of the stochastic variables $\eta$. The important point to emphasize is that, in general, variables $\eta$ do not satisfy the normalization condition, $\sum_{k=1}^{N} \eta_k \neq 1$, and therefore, they cannot be identified with populations. However, the distribution function $W(\eta)$ is chosen in such a way that their average is normalized

$$\sum_{k=1}^{N} \langle \eta_k \rangle = 1 \tag{27}$$

Thus, we require that these random variables satisfy approximately (that is, on average) the condition for the RPSE, with a posteriori check of the goodness of such an approximation.

The conditions in eqs 26 and 27 do not determine a unique probability distribution function $W(\eta)$. The general problem of the specification of the probability function in the absence of information for its full characterization is as old as the theory of probability itself. The "Principle of Insufficient Reason" of Laplace was an attempt to supply a criterion of choice for the probability if no other stronger reasons were available. The development of information theory and statistical inference has led to the maximum entropy principle, as the rule which permits determination of the least biased distribution according to our initial information.[46] This principle states that among the infinite set of functions $W(\eta)$ which satisfy the given constraints, it is reasonable to choose the one which minimizes the informational functional

$$I[W] = \int d\eta\, W(\eta) \ln W(\eta) \tag{28}$$

where $I[W]$ denotes a functional dependence of the information content $I$ on the distribution $W(\eta)$. The minimum information (maximum entropy) principle selects the distribution, being compatible with the given constraints, which has the maximum random character in relation to the smoothest dependence of $W(\eta)$ on the stochastic variables $\eta$.

The minimization of the functional in eq 28 under the constraints of eqs 26 and 27 is easily performed by means of the Lagrange multiplier method. The resulting distribution is factored into identical exponential distributions for all of the components of the random vector $\eta$

$$W_{RPSE}(\eta) = \prod_{k=1}^{N} w_{RPSE}(\eta_k) \qquad w_{RPSE}(\eta_k) = N e^{-N\eta_k} \tag{29}$$
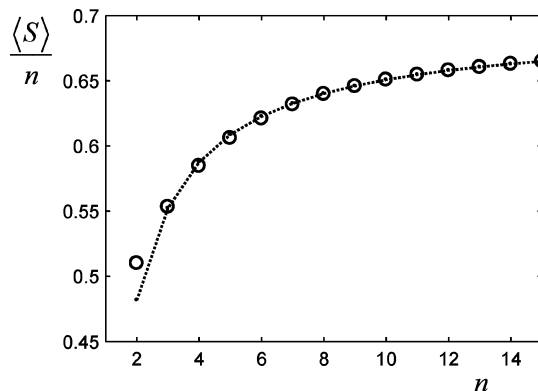


**Figure 6.** Average entropy per spin as a function of the number of spins. Circles: numerical sampling of RPSE; dotted line: approximation of eq 31.

In conclusion, the random variables (associated with the populations) result in being statistically independent, with an exponential distribution for each variable. In Figure 1, one can compare these approximate distributions $w_{RPSE}(\eta_k)$ drawn as continuous lines with the exact marginal distribution of populations deriving from the numerical sampling of RPSE. The convergence of the approximate distribution toward the exact ones clearly emerges for increasing dimensions of the spin system.

On the basis of this result, it is interesting to look at the statistical behavior of the sum $X = \sum_{k=1}^{N} \eta_k$ of the $N$ random variables $\eta$, whose average is unitary, $\langle X \rangle = 1$, because of the constraint of eq 27. One can apply the central limit theorem[47] to conclude that $X$ is a normally distributed random variable with a variance decreasing with the dimension $N$ of the Hilbert space, as one can explicitly derive from the distribution in eq 29

$$\langle (X - \langle X \rangle)^2 \rangle = \langle X^2 \rangle - 1 =$$
$$\sum_{k=1}^{N} \langle \eta_k^2 \rangle + \sum_{k,k'\neq k}^{N(N-1)} \langle \eta_k \eta_{k'} \rangle - 1 = \frac{1}{N} \tag{30}$$

In other words, as $N$ become very large, the condition of normalization on average, eq 27, becomes effectively a condition on the normalization of each realization of the set. However, the exact equivalence is found only in the limit $N \to \infty$.

From the statistical independence of the variables in the approximate distribution, eq 29, one can also justify the Gaussian distribution of the entropy as recovered from the numerical sampling reported in Figure 2. Indeed, if $N$ is large enough, this is the prediction of the central limit theorem when applied to the sum of eq 21, which defines the entropy function. Furthermore, one can directly calculate the average value of the entropy as

$$\langle S \rangle = N \int_0^\infty d\eta_k\, w_{RPSE}(\eta_k) \eta_k \ln \eta_k = \ln N - (1 - \gamma) \tag{31}$$

where $\gamma \cong 0.5772$ is the Euler constant. In order to provide direct evidence of the accuracy of the approximate result of eq 31 also for small-size systems, in Figure 6, we have compared it with the exact numerical values of the average entropy as a function of the number $n$ of spins. Furthermore,

by explicitly calculating the second moment of the entropy distribution, one can shown that at the leading order in $N$

$$\frac{\sigma_S}{\langle S \rangle} \simeq \frac{1}{\sqrt{N}} \qquad (32)$$

This is equivalent to proving the typicality of the entropy in the RPSE, as long as by increasing the dimension of the Hilbert space, the width of the entropy distribution within the ensemble, when compared to its average, tends to vanish.

**4.2. Approximate Distributions for the FEEE.** In order to obtain the approximate distribution for the FEEE, the minimization of the informational functional eq 28 has to be performed under the additional constraint on the average of the energy expectation value

$$\sum_{k=1}^{N} \langle \eta_k \rangle E_k = E \qquad (33)$$

Like for the constraint on the population normalization, within such an approximation, the constraint on the expectation energy is taken into account in the mean by replacing the populations $P_k$ in eq 14 with the averages $\langle \eta_k \rangle$ of the stochastic variables. In the following, we shall assume that the energy eigenvalues are ordered in magnitude, $E_k \leq E_{k+1}$, and that the origin of the energy scale is chosen in correspondence of the lowest-energy eigenvalue, $E_1 = 0$. The result, by applying the Lagrange multipliers method, is again a distribution factored in $N$-independent exponential distributions

$$W_{\text{FEEE}}(\eta) = \prod_{k=1}^{N} w_{\text{FEEE}}(\eta_k)$$

$$w_{\text{FEEE}}(\eta_k) = (\lambda + \mu E_k) e^{-(\lambda + \mu E_k)\eta_k} \qquad (34)$$

but now, the averages of the random variables depend on the corresponding energy eigenvalues

$$\langle \eta_k \rangle = (\lambda + \mu E_k)^{-1} \qquad (35)$$

The Lagrange parameters $\lambda$ and $\mu$ are implicitly determined by the following equations

$$\sum_{k=1}^{N} \frac{1}{(\lambda + \mu E_k)} = 1 \qquad \sum_{k=1}^{N} \frac{E_k}{(\lambda + \mu E_k)} = E \qquad (36)$$

Notice that when the energy expectation value $E$ approaches the value corresponding to all of the energy levels equally populated, $E^* = \sum_{k=1}^{N} E_k/N$, then these parameters tend to the limiting values $\lambda \rightarrow N$ and $\mu \rightarrow 0$. Correspondingly, the population distribution $W_{\text{FEEE}}(\eta)$ tends to the RPSE population distribution of eq 29.

The distribution of eq 29 for the RPSE and that of eq 34 for the FEEE are exactly the distributions proposed by Wootters[45] on the basis of different types of considerations. An important feature of these distributions is their factorization into single-variable distributions whose domains are the entire positive real axis. Thus, the ensemble average of any function of the quantum state can be analytically calculated. For example, according to
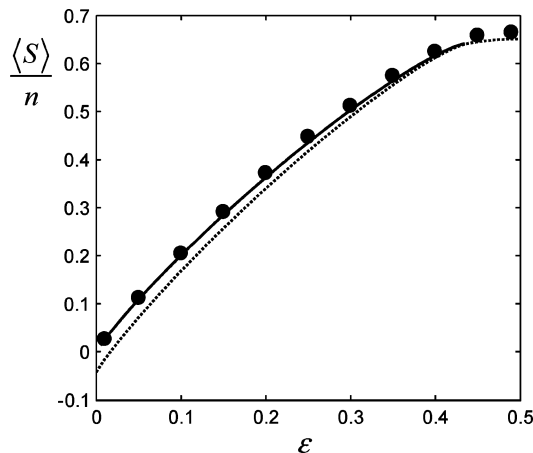


**Figure 7.** FEEE average entropy per spin as a function of the expectation energy per spin for a system composed of $n = 10$ spins. The figure displays the average values obtained from Monte Carlo sampling (circles), the average according to the Wootters approximation of the distribution of eq 34 (dotted line), and the average according to the second approximate form of the FEEE eq 42 (continuous line).

the approximate distribution of eq 34, the FEEE average entropy reads

$$\langle S \rangle = -\sum_{k=1}^{N} \int_0^\infty d\eta_k w_{\text{FEEE}}(\eta_k)\eta_k \ln \eta_k =$$

$$\sum_{k=1}^{N} \frac{\ln(\lambda + \mu E_k)}{\lambda + \mu E_k} - (1 - \gamma) \qquad (37)$$

which should be considered as an implicit function of the expectation energy (or its value per spin $\varepsilon = E/n$) because of the constraints of eq 36 for the parameters $\lambda$ and $\mu$.

However, the comparison between the average entropy calculated according to eq 37 and the average value obtained by the numerical sampling of the FEEE distribution of the entropy for a 10 spin system points out a discrepancy. This is clearly shown in Figure 7, where the averages of the entropy per spin obtained from the Monte Carlo sampling of the FEEE distribution for different values of the expectation energy per spin $\varepsilon = E/n$ are represented by circles, while the average entropy calculated according to eq 37 is represented by the dotted line. The difference between the results of the two procedures increases as the energy decreases. In particular, eq 37 predicts a negative entropy for low values of the energy per spin $\varepsilon$, a value which can never be recovered from the definition of eq 21 for the entropy, whatever the set of populations.

In order to understand the origin of these discrepancies, one should compare the exact population distributions as obtained from the Monte Carlo procedure with the approximate ones previously derived. We have verified that the exponential distribution given in eq 34 is a good approximation for all of the populations, except for the ground-state population $P_1$. As an example, Figure 3 shows the good agreement recovered for the distributions on the populations $P_2$ and $P_{43}$ in a particular situation. On the contrary, no agreement is found for the distribution on $P_1$ because, as shown in Figure 4, in this case, the Monte Carlo procedure leads to a distribution with a maximum which obviously cannot be recovered from the exponential form of eq 34.

In order to obtain a better approximation, we should take into account the peculiarity of the distribution on the ground-

state population. The basic idea is to use again the procedure of minimization of the information functional of eq 28 but with a specific restriction on the space of the allowed function for the distribution on the first variable $\eta_1$. Then, we introduce a new probability distribution, denoted as $W_{\text{FEEE,II}}(\eta)$, where the functional dependence on $\hat{\eta} = (\eta_2, ..., \eta_N)$ has to be determined from the minimization of the information functional of eq 28, while for the first variable $\eta_1$ (associated with the ground-state population $P_1$), we impose a well-defined functional form $G_a(\eta_1)$ even if parametrically dependent on a set of constants $a = (a_1, a_2, ...)$. Thus, the overall probability density is written as

$$W_{\text{FEEE,II}}(\eta) = G_a(\eta_1)\hat{W}_{\text{FEEE,II}}(\hat{\eta}) \tag{38}$$

where $\hat{W}_{\text{FEEE,II}}(\hat{\eta})$ describes the functional dependence on $\hat{\eta}$. For the functional dependence on the first variable, because of the bell-shaped profiles suggested by the results of Monte Carlo calculations and reported in Figure 4, we choose a normalized Gaussian function

$$G_a(\eta_1) = \sqrt{\frac{a_2}{\pi}} e^{-(\eta_1 - a_1)^2 a_2} \tag{39}$$

specified according to the two parameters $a = (a_1, a_2)$ for the center and the inverse squared width of the distribution. As a matter of fact, truly Gaussian distributions are recovered from the Monte Carlo calculations when sufficiently low energy per spin is considered, as one can perceive from Figure 4.

The procedure employed to determine the distribution of eq 38, which minimizes the information functional of eq 28, is described in detail in Appendix B, and here, we report only the final result. For the functional dependence on the variables $\hat{\eta}$, an exponential form is recovered like in the previous approximation of eq 34

$$\hat{W}_{\text{FEEE,II}}(\hat{\eta}) = \frac{N-1}{E} \prod_{k=2}^{N} E_k \exp\{-(N-1)E_k\eta_k/E\} \tag{40}$$

while for the Gaussian distribution of eq 39, the following relation is derived for its center

$$a_1 = 1 - \frac{E}{N-1} \sum_{k=2}^{N} \frac{1}{E_k} \tag{41}$$

and a vanishing value for its width (i.e., $1/a_2 = 0$) which corresponds to a Dirac delta profile. In conclusion, the resulting probability density is specified as

$$W_{\text{FEEE,II}}(\eta) = \delta(\eta_1 - a_1)\hat{W}_{\text{FEEE,II}}(\hat{\eta}) \tag{42}$$

This second form of the approximate distribution is practically equivalent to the previous one for all of the populations except the first one, which is distributed like a Dirac delta at its average value $\langle\eta_1\rangle = a_1$. Such a distribution can be employed to evaluate the average entropy

$$\langle S \rangle = -\sum_{k=1}^{N} \langle\eta_k\rangle \ln\langle\eta_k\rangle - (1-\gamma)(1 - \langle\eta_1\rangle) \tag{43}$$

It can be rewritten as an explicit function of the scaled expectation energy $e = E/N$

$$\langle S \rangle = -(1 - eS_0)\ln(1 - eS_0) - eS_0 \ln e + eF_0 - (1-\gamma)eS_0 \tag{44}$$

where the quantities $S_0 = \sum_{k=2}^{N} 1/E_k$ and $F_0 = \sum_{k=2}^{N} (\ln E_k)/E_k$ are characteristic properties of the energy spectrum of the considered system. In Figure 6, such an average entropy per spin is represented as a continuous line, and a good agreement is found in the comparison with the numerical sampling of the exact distribution. In particular, the unphysical negative values of entropy are avoided.

However, Monte Carlo results point out that the distribution on $P_1$ has a finite width. Of course this represents a shortcoming of such an approximation which could be overcome by introducing more complex profiles for $G_a(\eta_1)$, but at the price of a much more cumbersome procedure. On the other hand, we think that there is not strictly a necessity of these further developments, as long as the approximate distribution of eq 42 leads to accurate enough values for the average entropy.

## 5. Conclusions

In order to identify the methodologies suitable to statistically characterize quantum pure states, we have presented an analysis of the probability distributions which emerge from the geometry of the Hilbert space. In particular, by using a parametrization of the wave function in terms of populations and phases, we have explicitly derived the distributions of these variables associated with the random pure state ensemble (RPSE) and with the fixed expectation energy ensemble (FEEE). While the phase variables are statistically independent and uniformly distributed, the ensemble probability densities on the populations are defined in high-dimensional domains with a nontrivial topology because the populations are not statistically independent for the presence of the constraints. On the one hand, we have characterized such distributions through numerical sampling by using Monte Carlo techniques. On the other hand analytical approximations valid in the large $N$ limit have been developed and compared with the numerical results. These methods allow one to study the marginal distributions of single populations, as well as those of any function of interest. We have focused on the Shannon entropy associated with the pure state of the whole system in the energy representation. An interesting point which emerges from the study of the ensemble distribution in the chosen model system composed of $n$ spins of 1/2 is the following; while the probability distribution of the populations itself is the broadest one compatible with the constraints of the considered ensemble, the ensemble distributions of the observable entropy are, on the contrary, very peaked functions, and this allows its characterization through their typical values. Within the statistical framework presented here, the typicality of the entropy is evidence which does not depend on the nature of the system; rather, it is a simple consequence of the high dimensionality of the phase space together with the structure of the observed function which is defined as a sum of many terms. For this reason, the tools developed here can be used to calculate and analyze the typical values of a wide class of observables, including the expectation value of a generic

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operator or the elements of the reduced density matrix of a subsystem. The connection between the behavior of such typical values and the relevant constraints which define the ensembles are interesting issues which will be considered elsewhere.

## Appendix

**A. Metric Tensors and Volume Elements in the Ensemble Representative Spaces.** Let us first consider the space $\mathbb{R}^{2N}$ and perform the change of representation from the Euclidean coordinates $x \equiv (\text{Re } c, \text{Im } c)$ to the generalized coordinates $y = (P, \alpha)$ determined by populations and phases. The Jacobian matrix of the following transformation

$$x_{2i-1} = \sqrt{P_i} \cos \alpha_i \qquad x_{2i} = \sqrt{P_i} \sin \alpha_i \qquad (45)$$

for $i = 1, 2, ..., N$ is block diagonal and the $i$th block reads

$$\begin{vmatrix} \dfrac{\partial x_{2i-1}}{\partial P_i} & \dfrac{\partial x_{2i-1}}{\partial \alpha_i} \\ \dfrac{\partial x_{2i}}{\partial P_i} & \dfrac{\partial x_{2i}}{\partial \alpha_i} \end{vmatrix} = \begin{pmatrix} (2\sqrt{P_i})^{-1} \cos \alpha_i & -\sqrt{P_i} \sin \alpha_i \\ (2\sqrt{P_i})^{-1} \sin \alpha_i & \sqrt{P_i} \cos \alpha_i \end{pmatrix}$$

$$(46)$$

Therefore, according to eq 9, the metric tensor in the $y = (P, \alpha)$ representation is diagonal, with components

$$g_{P_i P_i} = \frac{1}{4P_i} \qquad g_{\alpha_i \alpha_i} = P_i \qquad (47)$$

from which one derives the volume element in the new set of coordinates

$$dV = \sqrt{|g(P, \alpha)|} dP d\alpha = 2^{-N} dP_1 ... dP_N d\alpha_1 ... d\alpha_N$$

$$(48)$$

By imposing the constraint of eq 13, which can be used to determine the last population as a function of the others considered as independent variables

$$P_N = 1 - \sum_{i=1}^{N-1} P_i \qquad (49)$$

we now derive the geometrical measure for the RPSE described by coordinates $z = (P_1, P_2, ..., P_{N-1}, \alpha_1, \alpha_2, ..., \alpha_N)$. According to the prescription in eq 10, the metric tensor $g_{ij}(z)$ induced in the surface results in being partitioned into two blocks, the block on the phases which is diagonal

$$g_{\alpha_i \alpha_i} = P_i \quad \text{for} \quad i \neq N \qquad g_{\alpha_N \alpha_N} = 1 - \sum_{i=1}^{N-1} P_i$$

$$(50)$$

and the block on the populations

$$g_{P_i P_j} = \frac{1}{4P_i} \delta_{ij} + \frac{1}{4(1 - \sum_{k=1}^{N-1} P_k)} \qquad i, j = 1 \div (N-1)$$

$$(51)$$

In order to calculate the determinant of the metric tensor $g(z) = \det(g_{ij}(z))$, we can employ the following property of determinants. Let us suppose that $A$ is an invertible square matrix and $u$, $v$ are two column vectors; then, it can be verified[48] that

$$\det(A + uv^{\mathrm{T}}) = (1 + v^{\mathrm{T}} A^{-1} u) \det(A) \qquad (52)$$

By identifying $A$ with the diagonal matrix whose entries are $1/(4P_i)$, $v$ with the vector whose elements are all unitary, and the elements of $u$ with the second term on the rhs of eq 51, we find the following contribution for the population block

$$\det(g_{P_i P_j}) = \frac{1}{4^{N-1}} \frac{1}{1 - \sum_k^{N-1} P_k} \prod_{k=1}^{N-1} \frac{1}{P_k} \qquad (53)$$

while the determinant of the diagonal phase block is directly recovered from eq 50.

$$\det(g_{\alpha_i \alpha_j}) = (1 - \sum_k^{N-1} P_k) \prod_{k=1}^{N-1} P_k \qquad (54)$$

Therefore, the overall determinant of the metric tensor is simply

$$g(z) = \det(g_{P_i P_j}) \det(g_{\alpha_i \alpha_j}) = \frac{1}{4^{N-1}} \qquad (55)$$

By taking into account that the surface of the hypersphere in eq 4 is $2\pi^N/(N-1)!$, one finally derives the probability density eq 16 for the RPSE.

The possible states for the FEEE must satisfy the constraints of eqs 13 and 14, which can be employed to determine the last two populations as a function of the remaining ones

$$P_N = f_1(P_1, ..., P_{N-2}) = \frac{E}{E_N - E_{N-1}} -$$

$$\sum_{i=1}^{N-2} \frac{E_i}{E_N - E_{N-1}} P_i + \frac{E_{k'}}{E_N - E_{N-1}} \left( \sum_{i=1}^{N-2} P_i - 1 \right)$$

$$P_{N-1} = f_2(P_1, ..., P_{N-2}) = 1 - \sum_{i=1}^{N-2} P_i - f_1(P_1, ..., P_{N-2})$$

$$(56)$$

and these equations provide the parametric representation of the FEEE hypersurface. Thus, according to eq 10, the metric tensor on the populations is given as

$$g_{P_j P_t} = \frac{1}{4P_j} \delta_{jt} + \frac{1}{4f_1} \frac{\partial f_1}{\partial P_j} \frac{\partial f_1}{\partial P_t} + \frac{1}{4f_2} \frac{\partial f_2}{\partial P_j} \frac{\partial f_2}{\partial P_t} \qquad (57)$$

Again, we can calculate the determinant of this matrix by using a general property of the determinant[48]

$$\det(A + UU^{\dagger}) = \det(I + U^{\dagger}A^{-1}U)\det(A) \qquad (58)$$

where $A$ is a nonsingular square matrix and $U$ is a rectangular matrix with the same number of rows of $A$. By identifying $A$ with the diagonal matrix with entries $A_{ij} = (1/4P_j)\delta_{ij}$ and $U$ with a $(N - 2) \times 2$ matrix with entries $U_{ij} = [1/(4f_j)^{1/2}](\partial f_j/\partial P_i)$, we get

$$\det(g_{P_iP_j}) = ((1 + R_{11})(1 + R_{22}) - R_{12}^2)\prod_{j=1}^{N-2}\frac{1}{4P_j} \qquad (59)$$

with the following coefficients

$$a_j = \frac{E_{N-1} - E_j}{E_N - E_{N-1}} \qquad (60)$$

$$R_{11} = \frac{1}{f_1}\sum_{j=1}^{N-2} P_j a_j^2, \quad R_{22} = \frac{1}{f_2}\sum_{j=1}^{N-2} P_j (1 + a_j)^2,$$

$$R_{12} = \frac{1}{\sqrt{f_2 f_1}}\sum_{j=1}^{N-2} P_j a_j(1 + a_j) \qquad (61)$$

By employing also the determinant of the phase block (eq 54), finally we derive the FEEE volume element

$$dV = \frac{1}{2^{N-2}}\left[\sum_{j=1}^{N-2} P_j(1 + a_j)a_j - \left(\frac{E - E_{N-1}}{E_N - E_{N-1}}\right)^2 + \left(\frac{E - E_{N-1}}{E_N - E_{N-1}}\right)\right]^{1/2} dP_1...dP_{N-2}d\alpha_1...d\alpha_N \qquad (62)$$

from which the FEEE probability density (eq 17) follows directly.

## Appendix

**B. Minimization of the Information Functional.** The information functional eq 28 with the distribution function eq 38 can be written as

$$I[W_{FEEE,II}] = \int d\eta_1 G_a(\eta_1) \ln G_a(\eta_1) + \int d\hat{\eta}\hat{W}(\hat{\eta}) \ln \hat{W}(\hat{\eta}) = I_1(a) + \hat{I}[\hat{W}] \qquad (63)$$

where $\hat{W}(\hat{\eta}) = \hat{W}_{FEEE,II}(\hat{\eta})$. The constraints which have to be satisfied are the normalization of the average populations, eq 27, a fixed value of the average expectation energy, eq 33, and the normalization of the probability density

$$\int d\hat{\eta}\hat{W}(\hat{\eta}) = 1 \qquad (64)$$

By introducing suitable Lagrange multipliers $\lambda$, $\mu$, and $\kappa$, the functional to be minimized reads

$$F([\hat{W}], a) = I_1(a) + \hat{I}[\hat{W}] - \lambda(\sum_k \langle \eta_k \rangle - 1) - \mu(\sum_k \langle \eta_k \rangle E_k - E) - \kappa(\int \hat{W}(\hat{\eta})d\hat{\eta} - 1) = I_1(a) - a_1(\lambda + \mu E_1) + \int \hat{W}(\hat{\eta})d\hat{\eta}[\ln \hat{W}(\hat{\eta}) - \lambda\sum_{k\neq 1}\eta_k - \mu\sum_{k\neq 1}E_k\eta_k - \kappa] + \lambda + \mu E + \kappa \qquad (65)$$

where $F([\hat{W}],a)$ has to be considered as a functional of $\hat{W}(\hat{\eta})$ and an ordinary function of the parameters $a = (a_1, a_2)$. The minimization thus requires setting to zero the following derivatives

$$\frac{\partial F}{\partial a_m} = \frac{\partial}{\partial a_m}[I_1(a) - a_1(\lambda + \mu E_1)] = 0 \qquad \text{for} \quad m = 1, 2 \qquad (66)$$

$$\frac{\delta F}{\delta \hat{W}(\hat{\eta})} = -\ln \hat{W}(\hat{\eta}) - 1 - \lambda\sum_{k\neq 1}\eta_k - \mu\sum_{k\neq 1}E_k\eta_k - \kappa = 0 \qquad (67)$$

From eq 67, one obtains

$$\hat{W}(\hat{\eta}) = \exp[-(1 + \kappa) - \lambda\sum_{k\neq 1}\eta_k - \mu\sum_{k\neq 1}E_k\eta_k] \qquad (68)$$

which, by taking into account the normalization condition of eq 64, can be written in the normalized form

$$\hat{W}(\hat{\eta}) = \prod_{k\neq 1}^{N}(\lambda + \mu E_k)e^{-(\lambda + \mu E_k)\eta_k} \qquad (69)$$

so leading to the following averages

$$\langle \eta_k \rangle = \frac{1}{(\lambda + \mu E_k)} \qquad k \neq 1 \qquad (70)$$

Lagrange multipliers $\lambda$ and $\mu$ are calculated by evaluating according to eq 71 the constraint (eq 27) of population normalization and the constraint (eq 33) of expectation energy

$$a_1 + \sum_{k\neq 1}^{N}\frac{1}{(\lambda + \mu E_k)} = 1 \qquad E_1 a_1 + \sum_{k\neq 1}^{N}\frac{E_k}{(\lambda + \mu E_k)} = E \qquad (71)$$

while parameters $a = (a_1, a_2)$ are calculated from the solution of eq 66. Thus, by using a scale of the energy such that $E_1 = 0$, the equations to be solved for the specification of the parameters $\lambda$, $\mu$, $a_1$, and $a_2$ are

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$$\begin{cases} a_1 + \dfrac{1}{\mu}\displaystyle\sum_{k=2}^{N}\dfrac{1}{z+E_k} = 1 \\[2ex] \dfrac{(N-1)}{\mu} + \dfrac{z}{\mu}\displaystyle\sum_{k=2}^{N}\dfrac{1}{z+E_k} = E \\[2ex] \dfrac{\partial}{\partial a_m}\left[\dfrac{1}{2} - \ln\left(\dfrac{a_2}{\pi}\right) - a_1 z\mu\right] = 0 \qquad \text{for} \quad m = 1,2 \end{cases} \tag{72}$$

where $z = \lambda/\mu$. This system of equations can be solved analytically, deriving the following values for the parameters

$$\lambda = 0 \qquad \mu = \frac{N-1}{E}$$

$$a_1 = 1 - \frac{E}{N-1}\sum_{k \neq 1}^{N}\frac{1}{E_k} \qquad 1/a_2 = 0 \tag{73}$$

which lead to the distribution specified by eqs 42 and 40.

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