Maximum-entropy approach to critical phenomena in ground states of finite systems

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A scheme for detecting signatures of phase transitions associated with pure quantum states, from the knowledge of a limited set of expectation values, is introduced. An accurate prediction of critical regions in ground states of systems with a finite number of particles is obtained.

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I. INTRODUCTION

The investigation of critical phenomena constitutes one of the most active and exciting areas of scientific endeavor. Although most concomitant work is related to the thermodynamic limit [1], this kind of study can also be of interest in the case of ground states of finite systems, offering rewarding insights into the intricacies of the many-body problem [2, 3]. Indeed, the very concept of phase transition is both valid and useful even for a relatively small number of particles, as discussed by Gilmore, Feng and others [4–8]. The work of Kümmel [9] is especially significant in this respect. He recommended the term "shape transitions" for finite systems.

Without referring specifically to phase transitions, one would surely be most interested in studying the physics of a given system in those regions of an (appropriately defined) space of control parameters where the pertinent wave function exhibits significant changes. From a practical point of view, the question then arises as to what extent it is possible to make predictions, based on a limited amount of *a priori* information, about the location of those regions.

The aim of the present work is to provide some tentative answers to this question within the context of pure quantum states by recourse to recent developments [10–12] based on information theory [13–18]. The possibility of reconstructing the ground state (GS) of a given system on the basis of a limited amount of information has been discussed in Refs. [10–12], within the context of a special version of the maximum-entropy principle (MEP). An appropriately defined pseudoentropy (or quantal entropy) was seen to constitute a useful tool for discussing some aspects of the many-body problem. We shall here discuss the relationship between this pseudoentropy and critical regions. On this basis, we shall show that the knowledge of a few GS expectation values may suffice *to infer* the location of those regions referred to above where the interesting physics takes place. At the same time we shall be able to obtain a criterion for defining critical regions in finite systems.

The paper is organized as follows. The pertinent formalism is developed in Sec. II and is illustrated in Sec. III in two exactly solvable many-body models, which exhibit different critical behavior. Finally, some conclusions are drawn in Sec. IV.

II. FORMALISM

A. Maximum-entropy scheme

The state of a quantum system is fully determined by the knowledge of the corresponding statistical operator $\hat{\rho}$. However, in most practical cases only a set of expectation values O_i of n observables $\hat{O}_i$ is available:

$$O_i \equiv \langle \hat{O}_i \rangle = \mathrm{Tr}\hat{\rho}\hat{O}_i . \tag{2.1}$$

Unless the operators $\hat{O}_i$ constitute a complete set, this information does not suffice to univocally determine $\hat{\rho}$. According to the standard prescription of information theory, the least-biased $\hat{\rho}$ compatible with the available data is that which maximizes the entropy (we set the Boltzmann constant $k_B = 1$)

$$S = -\mathrm{Tr}\hat{\rho}\ln\hat{\rho} \tag{2.2}$$

subject to the constraints (2.1). This leads to the well-known result [13, 14]

$$\hat{\rho} = \exp\left(-\lambda_0 - \sum_{i=1}^{n}\lambda_i\hat{O}_i\right), \tag{2.3}$$

where the λ_i ($i = 1, \ldots, n$) are Lagrange parameters to be determined by satisfying Eq. (2.1), and

$$\lambda_0 = \ln\mathrm{Tr}\exp\left(-\sum_{i=1}^{n}\lambda_i\hat{O}_i\right) \tag{2.4}$$

is the normalization constant (which can also be considered as an additional Lagrange parameter associated with the identity operator $\hat{O}_0 \equiv \hat{I}$, with the constraint $\langle\hat{O}_0\rangle = 1$), satisfying

$$\frac{\partial\lambda_0}{\partial\lambda_i} = -O_i, \quad i = 1, \ldots, n. \tag{2.5}$$

The ensuing maximum entropy acquires the form [13, 14]

$$S = \lambda_0 + \sum_{i=1}^{n}\lambda_i O_i \tag{2.6}$$

and fulfills the relationships

$$\frac{\partial S}{\partial O_i} = \lambda_i, \quad i = 1, \ldots, n. \tag{2.7}$$

If the state of the system depends upon some control parameters, a fact which will obviously be reflected in the available information, we can associate phase transitions or critical phenomena with those regions of the parameter space where (2.6) exhibits appreciable changes. This will be the central idea of this work. Actually, in thermodynamics (which corresponds, within the previous scheme, to the case where just the mean values of the Hamiltonian $\hat{H}$ and eventually a reduced set of observables commuting with $\hat{H}$ are available [14]) phase transitions can be associated, for infinite systems, with those points in the space of control parameters where the thermodynamic entropy exhibits indeed a singularity of a certain type [4]. For finite systems, no such singularities will actually occur, but remnants of these will survive as regions where the entropy exhibits a significant variation. We remark that in all these situations, the entropy which is studied is that associated with an incomplete description given by just a few relevant observables.

B. Application to pure states

The goal of the present work is to apply these ideas to the study and detection of transitions in ground states of finite quantum systems. For a pure state $|\psi\rangle$, the exact statistical operator reduces to $\hat{\rho}_{\text{ex}} = |\psi\rangle\langle\psi|$, with zero entropy. However, in the case of an *incomplete* description based on a reduced set of observables, the corresponding entropy (2.6), associated with the inferred density (2.3), will not vanish in general and measures the missing information needed to completely specify the state [10–12]. This is the entropy we shall examine for detecting shape transitions in these systems.

We shall consider, for this purpose, the most simple and tractable case where the observables $\hat{O}_i$ conform a mutually *commuting* set. Let us examine in this case the relationship between the inferred and exact statistical operators. For an Abelian set of operators $\hat{O}_i$ there exists a common basis spanned by vectors $|j\rangle$, $j = 1, \ldots, L$, in which they possess a diagonal representation

$$\langle j'|\hat{\rho}|j\rangle = \delta_{jj'} p_j, \qquad p_j = \exp\left(-\lambda_0 - \sum_{i=1}^{n} \lambda_i O_i(j)\right), \tag{2.8}$$

where $O_i(j) = \langle j|\hat{O}_i|j\rangle$. The entropy (2.6) becomes thus

$$S = -\sum_j p_j \ln p_j . \tag{2.9}$$

In the present Abelian context, the available information can be regarded as "complete" if the operators $\hat{O}_i$ form a complete basis for the expansion of any other *commuting* operator. In this case, the inferred $\hat{\rho}$ will possess *exact diagonal elements* in order to predict the exact mean value of any diagonal operator. Therefore, if the exact state $|\psi\rangle$ is expanded in the common basis as

$$|\psi\rangle = \sum_j C_{\text{ex}}(j)|j\rangle, \tag{2.10}$$

then $p_j = |C_{\text{ex}}(j)|^2$, since the quantities p_j and $|C_{\text{ex}}(j)|$ are in this situation univocally determined by the constraints (2.1) [10]. The entropy (2.9) coincides in this case with the *quantal entropy* of the exact state,

$$S_{\text{ex}} = -\sum_j |C_{\text{ex}}(j)|^2 \ln[|C_{\text{ex}}(j)|^2], \tag{2.11}$$

defined in Ref. [10], relative to the *common basis* determined by the operators $\hat{O}_i$. This quantal entropy measures the lack of information associated with the probability distribution of the state $|\psi\rangle$ over this basis. For incomplete diagonal information, the inferred entropy (2.9) will be an upper bound to the exact quantal entropy (2.11).

We should remark that in the case of incomplete descriptions, the common basis employed in the previous expressions is not, however, unique, unless the eigenvalues of the operators $\hat{O}_i$ suffice to univocally label the basis vectors. The states $|j\rangle$ can actually be labeled as $|k, l_k\rangle$, where k stands for a set of K labels, $K \leq n$, determined by the eigenvalues of the operators $\hat{O}_i$, whereas l_k stands for the additional set of labels necessary to uniquely identify the state. We shall define the multiplicity d_k as the dimension of the subspace characterized by a given value of k, i.e., $1 \leq l_k \leq d_k$, which is obviously independent of the choice of basis.

Evidently, the inferred probabilities (2.8) do not depend upon l_k, and can thus be labeled directly as p_k. Therefore, we can rewrite the inferred entropy as

$$S = -\sum_k p'_k \ln(p'_k/d_k), \tag{2.12}$$

where

$$p'_k = d_k \exp\left(-\lambda_0 - \sum_{i=1}^{n} \lambda_i O_i(k)\right), \tag{2.13}$$

with $O_i(k) = \langle k, l_k|\hat{O}_i|k, l_k\rangle$. The multiplicity d_k can thus be interpreted as a measure or prior probability [14] of the "states" $|k\rangle$, ignoring the label l_k.

C. Determination of critical regions

We are in a position now, within this framework, to tackle the central point of the present work, i.e., the study of the behavior of ground states with respect to certain control parameters, which we shall take as simple parameters of the Hamiltonian. In particular, we shall consider a system described by a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}(z_\alpha), \tag{2.14}$$

where $\hat{H}_0$ is the unperturbed part and z_α, $\alpha = 1, \ldots, r$ are parameters which determine the strength of the different interaction terms.

The quantal entropy (2.11) depends on the choice of basis. Following our definition of control parameters, we shall consider for our purpose the set of eigenstates of $\hat{H}_0$ (unperturbed basis) as the proper basis for detecting signatures of phase transitions, and shall take as available data the expectation values of a set of relevant operators which commute with the unperturbed Hamiltonian. The ensuing exact quantal entropy (2.11) in this basis will vanish for the unperturbed system (assuming a nondegenerate ground state), but as the interaction is switched on, it will acquire a finite value, reflecting the evolution from weak- to strong-coupling regimes.

As will be shown in subsequent sections, a very accurate prediction of the exact quantal entropy in the unperturbed basis can in general be achieved with just a few expectation values of relevant operators. Therefore, those intervals in the space of control parameters where the inferred entropy (2.9) exhibits a strong variation will indicate regions where the exact distribution over the common basis undergoes a significant qualitative change. This can be interpreted as a "transition" between different regimes, and we shall associate transitions in finite systems with those intervals where the greatest variations take place. As the system approaches a thermodynamic (or classical) limit, these variations may increase in magnitude, indicating a "real" transition in case they evolve into discontinuities of a certain kind. However, as far as finite systems are concerned, the magnitude of this variation is what determines the "intensity" of the transition, independent of the behavior in the thermodynamic limit. This last fact is not taken into account when one employs the conventional theoretical tools devised to attack this sort of problem (such as mean-field-based methods), as they usually reflect, more or less directly, the behavior in the classical or thermodynamic limit.

Our available information is given thus by the set of expectation values $\{O_i, i = 1, \ldots, n\}$ which depend upon the parameters z_α. For a particular parameter z_α, critical points can be identified with maxima of $|\partial S/\partial z_\alpha|$, with [see (2.7)]

$$\frac{\partial S}{\partial z_\alpha} = \sum_{i=1}^{n} \lambda_i \frac{\partial O_i}{\partial z_\alpha}, \tag{2.15}$$

where we have assumed that the operators $\hat{O}_i$ do not depend explicitly on z_α [O_i denotes the expectation value (2.1)]. The location of critical z_α in finite systems is thus obtained from the necessary condition

$$0 = \frac{\partial^2 S}{\partial z_\alpha^2} = \sum_{i=1}^{n} \left(\lambda_i \frac{\partial^2 O_i}{\partial z_\alpha^2} - \sum_{j=1}^{n} (A^{-1})_{ij} \frac{\partial O_j}{\partial z_\alpha} \frac{\partial O_i}{\partial z_\alpha} \right), \tag{2.16}$$

where A_{ij} denotes the covariance matrix

$$A_{ij} = -\frac{\partial O_i}{\partial \lambda_j} = \langle \hat{O}_i \hat{O}_j \rangle - O_i O_j \tag{2.17}$$

(the condition for uniqueness of $\hat{\rho}$ is that the matrix A be regular [14]). Thus, transitional regions for the shape of the distribution of the state $|\psi\rangle$ over the common unperturbed basis are associated with the neighborhood of those values of z_α satisfying the necessary condition (2.16). We remark that we need in principle only the knowledge of the mean values O_i (either from experiment or from approximate or exact calculations) for a sufficiently large set of values of z_α to numerically determine the corresponding derivative (2.15).

III. APPLICATION

A. Description of the models

1. U(n) model

This model [19, 5] is also known as the extended Lipkin-Meshkov-Glick (LMG) model [20] and consists of N fermions distributed within n single particle (SP) levels denoted 2Ω-fold degenerate denoted by $|p, i\rangle$, $p = 1, \ldots, 2\Omega$, $i = 1, \ldots, n$, which interact through a monopole interaction. The corresponding Hamiltonian reads

$$\hat{H} = \sum_{i=1}^{n} \varepsilon_i \hat{G}_{ii} + \tfrac{1}{2} \sum_{i<j}^{n} V_{ij} \, (\hat{G}_{ij}^2 + \hat{G}_{ji}^2), \tag{3.1}$$

where the first term will be taken as the unperturbed Hamiltonian, with $\varepsilon_i \leq \varepsilon_j$ for $i < j$. The collective operators

$$\hat{G}_{ij} = \sum_{p=1}^{2\Omega} c_{pi}^{\dagger} c_{pj}, \tag{3.2}$$

where $c_{pi}^{\dagger}$ and c_{pj} denote the usual fermion creation and annihilation operators, satisfy a U(n) algebra under commutation.

The ground state of the Hamiltonian (3.1) belongs to the completely symmetric representation of $U(n)$, $(N, 0, \ldots, 0)$ [11], and is an eigenstate of the n parities $\hat{P}_i = \exp(i\pi \hat{G}_{ii})$, with eigenvalue $+1$. It can thus be expanded as

$$|\psi_0\rangle = \sum_{n,\text{even}} C(n_2, \ldots, n_n) \, |n_2, \ldots, n_n\rangle, \tag{3.3}$$

where the states [11]

$$|n_2, \ldots, n_n\rangle = (n_1!/N!)^{1/2} \prod_{i\geq 2} (n_i!)^{-1/2} \hat{G}_{i1}^{n_i} |0\rangle,$$

$$0 \leq \sum_{i\geq 2} n_i \leq N \tag{3.4}$$

constitute the complete orthonormal unperturbed basis of dimension $d = \binom{N+n-1}{n-1}$ within the symmetric representation (in other irreducible representations, additional labels are required to completely identify a state). The quantities n_i denote the number of particles in the ith level, and $|0\rangle$ the unperturbed ground state.

Within the Hartree-Fock (HF) picture, this model exhibits second-order ground-state shape transitions [5] as the coupling parameters vary. The HF solutions depend just on the scaled coupling parameters

$$v_{ij} = V_{ij} \, (N - 1), \tag{3.5}$$

being independent of N for fixed v_{ij}, in which case the intensive energy is finite in the thermodynamic limit. In the particular case $v_{ij} = -v(1-\delta_{ij})$, $v > 0$, this approach predicts $n-1$ transitions at the critical values [21, 22]

$$v_c^{(i)} = i\varepsilon_i - \sum_{j=1}^{i} \varepsilon_j, \quad i = 2, \ldots, n. \tag{3.6}$$

For $v > v_c^{(i)}$, the ith level begins to be occupied. HF yields the exact intensive expectation values of the collective operators in the thermodynamic limit ($N \to \infty$) [4, 5], which represents the classical limit in this context. Accordingly, the HF phase transitions represent real transitions of the system only in this limit.

2. AFP model

This model consists of N interacting fermions distributed over two 2Ω-fold-degenerate SP levels ($n = 2$ in the above given model), which are described by a monopolar Lipkin-type Hamiltonian with the addition of a one-body interaction term

$$\hat{H} = \varepsilon \hat{J}_z + v\hat{J}_x - \frac{v}{N}\hat{J}_x^2, \tag{3.7}$$

where, using the notation of Sec. III A 1,

$$\hat{J}_z = \tfrac{1}{2}(\hat{G}_{22} - \hat{G}_{11}), \quad \hat{J}_x = \tfrac{1}{2}(\hat{J}_+ + \hat{J}_-), \tag{3.8}$$

with $\hat{J}_+ = \hat{G}_{21} = \hat{J}_-^\dagger$, are the usual quasispin operators satisfying an SU(2) algebra. Expression (3.7) is a slightly modified version of the Abecasis-Faessler-Plastino (AFP) Hamiltonian [23] which has been proposed by Gilmore and Feng in Ref. [24]. The original AFP Hamiltonian

$$\hat{H}_{\rm AFP} = \varepsilon \hat{J}_z + \tfrac{1}{2}v(\hat{J}^2 - \hat{J}_x^2 + \hat{J}_x) \tag{3.9}$$

can be seen to be a special case of (3.7) by dropping the term $\frac{1}{2}v\hat{J}^2$, which simply adds a constant energy to all states in the ground-state manifold. The factor $1/N$ in the coupling term has been introduced for thermodynamical reasons [24] in order to obtain a *finite* intensive energy in the classical limit.

The original AFP model was considered to exhibit a ground-state shape instability [25] associated with an absolute minimum of the second derivative of the ground-state energy E. It was however demonstrated later [24] that the Hamiltonian (3.7) does not undergo any phase transition in the thermodynamic limit, the rapid variation in $\partial^2 E/\partial v^2$ being entirely attributed to the nonthermodynamic scaling. Accordingly, the HF solution of this model (being, as in the previous case, exact in the thermodynamic limit) exhibits no transition.

Expressions (3.3) and (3.4) of the previous subsection, for $n = 2$, are valid for the ground state of the present model, except that the sum over n_2 runs now over both even and odd values, since the Hamiltonian (3.7) does not commute now with the (two-level) parity operator $\hat{P} = \exp(i\pi\hat{J}_z)$.

B. Maximum-entropy approach

We are particularly interested in the behavior of the ground state for *finite values* of N as a function of the interaction parameters V_{ij}, which are now taken to be the control parameters z_α. According to Sec. II C, we shall investigate the entropy associated with an incomplete set of expectation values of operators commuting with $\hat{H}_0$, which we shall choose here as functions of the collective operators (3.2).

We shall consider two different sets of accessible states: (a) the full space of dimension n^N, which includes all pertinent irreducible representations (we exclude paired states characterized by $n_p > 1$, with $n_p = \sum_i c_{pi}^\dagger c_{pi}$), and (b) the completely symmetric representation spanned by the states (3.4). Case (a) corresponds to no *a priori* information, whereas in (b) one assumes that the observer knows with certainty that the state to be inferred lies within the symmetric subspace. In addition to this, we shall suppose in both cases that in the $U(n)$ model the parity of the state is known, so that traces will be restricted to the corresponding eigenspace.

In the case of the $U(n)$ model, we shall consider the description constructed on the basis of the information given by expectation values of one-body operators $\hat{G}_{ii}$ as well as two-body operators $\hat{G}_{ii}\hat{G}_{jj}$ representing the information about the diagonal elements of the SP density matrix and the corresponding fluctuation or covariance matrix $A_{ij} = \langle \hat{G}_{ii}\hat{G}_{jj}\rangle - \langle \hat{G}_{ii}\rangle\langle \hat{G}_{jj}\rangle$. Since $\sum_{i=1}^{n}\langle \hat{G}_{ii}\rangle = N$, there are only $n-1$ one-body and $n(n-1)/2$ two-body independent mean values.

The eigenvalues of any set of operators of this kind will just be functions of the labels n_i, and hence they completely identify a many-body state within the symmetric representation. However, this does not hold within the full accessible space. In this case, the multiplicity factor d_k is

$$d_{n_2,\ldots,n_n} = \frac{N!}{n_1!\ldots n_n!}, \tag{3.10}$$

which counts the total number of states with n_i particles in the ith level. For symmetric space calculations, we should set $d_{n_2,\ldots,n_n} = 1$.

The corresponding statistical operator is

$$\hat{\rho} = \exp\left(-\lambda_0 - \sum_{i\geq 2}\lambda_i \hat{G}_{ii} - \sum_{i\geq j\geq 2}\lambda_{ij}\hat{G}_{ii}\hat{G}_{jj}\right), \tag{3.11}$$

where

$$\lambda_0 = \ln \sum_{n_2,\ldots,n_n} d_{n_2,\ldots,n_n} \times \exp\left(-\sum_{i\geq 2}\lambda_i n_i - \sum_{i\geq j\geq 2}\lambda_{ij}n_i n_j\right) \tag{3.12}$$

and the Lagrange parameters are determined from the available data by

$$\frac{\partial\lambda_0}{\partial\lambda_i} = -\langle \hat{G}_{ii}\rangle, \quad \frac{\partial\lambda_0}{\partial\lambda_{ij}} = -\langle \hat{G}_{ii}\hat{G}_{jj}\rangle. \tag{3.13}$$

The inferred entropy is

$$S = \lambda_0 + \sum_{i\geq 2} \lambda_i \langle \hat{G}_{ii} \rangle + \sum_{i\geq j \geq 2} \lambda_{ij} \langle \hat{G}_{ii} \hat{G}_{jj} \rangle. \quad (3.14)$$

In the one-body case ($\lambda_{ij} = 0$) in the full space, (3.14) can be explicitly expressed as $S = -\sum_i \langle \hat{G}_{ii} \rangle \ln(\langle \hat{G}_{ii} \rangle / N)$, after analytically solving (3.13) for λ_i.

For the ground state, the available information will obviously saturate (i.e., become complete in the sense of Sec. II B) when $\binom{N+n-1}{n-1}$ independent expectation values of commuting collective operators are given. In this situation the inferred entropy will coincide with the exact quantal entropy of the ground state (2.11), which can be written, using the expansion (3.3) as

$$S_{\rm ex} = - \sum_{n_i \text{even}} |C(n_2, \ldots, n_n)|^2 \times \ln(|C(n_2, \ldots, n_n)|^2 / d_{n_2, \ldots, n_n}). \quad (3.15)$$

Thus, the exact coefficients represent the limit of the effective probabilities (2.13). It should be stressed that as $N \to \infty$, the entropy (3.15) becomes of order N in the full space, and is therefore suitable for thermodynamic scaling. On the other hand, in the symmetric representation the entropy is of order $\ln(N)$.

In order to compare the derivative of the inferred entropy (3.14) with the exact result, it is necessary to compute $\partial S_{ex} / \partial z_\alpha$. This step can be done by adding as many expectaction values as necessary for saturation in (3.14) or, otherwise, by calculating the quantities

$$\frac{\partial C(n_2, \ldots, n_n)}{\partial z_\alpha} = \left\langle n_2, \ldots, n_n \left| \frac{\partial}{\partial z_\alpha} \right| \psi_0 \right\rangle, \quad (3.16)$$

which can be obtained by deriving the exact eigenvalue equation, resulting in

$$\frac{\partial}{\partial z_\alpha} |\psi_0\rangle = \sum_{k \neq 0} (E_0 - E_k)^{-1} \left\langle \psi_k \left| \frac{\partial \hat{H}}{\partial z_\alpha} \right| \psi_0 \right\rangle |\psi_k\rangle, \quad (3.17)$$

where $\hat{H} |\psi_k\rangle = E_k |\psi_k\rangle$. Expression (3.17) is generally valid for a nondegenerate ground state (we have omitted an arbitrary component $i\gamma|\psi_0\rangle$, γ real, in (3.17), which does not influence the derivative of $|C(n_2, \ldots, n_n)|$).

As in the previous case, for the AFP Hamiltonian we shall consider the description based on the information of commuting one- and two-body mean values, represented here by $\langle \hat{J}_z \rangle$ and $\langle \hat{J}_z^2 \rangle$. The ensuing density is

$$\hat{\rho} = \exp(-\lambda_0 - \lambda_1 \hat{J}_z - \lambda_2 \hat{J}_z^2). \quad (3.18)$$

Remaining details are similar to those of the previous model for the case $n = 2$, without parity projection.

C. Results

1. U(n) model

Numerical calculations have been performed for the two- and three-level versions of this model ($n = 2$ and 3), assuming $\varepsilon_i = (i-1)\varepsilon$ and a common coupling constant $V_{ij} = -v(1 - \delta_{ij})/(N-1)$. In this case, within the HF picture, the ground state undergoes a single transition for $n = 2$ at $v_c/\varepsilon = 1$, and for $n = 3$, two transitions at $v_c^{(2)}/\varepsilon = 1$ and $v_c^{(3)}/\varepsilon = 3$. Accordingly, as control parameters we shall choose the scaled coupling parameter v. Figures 1 and 2 depict the derivative of the inferred entropy [expression (2.15)] together with the exact one, for fixed N, within the symmetric representation (results in the full space are similar).

It can be seen that the inference with one-body mean values gives a good qualitative description of the entropy, whereas that including two-body information overlaps with the exact results within the scale of the figures. In both cases, the derivative of the entropy clearly exhibits maxima located in the vicinity of the HF critical points, indicating transitional regions of finite width. As N increases, the locations of all maxima approach the HF values, evolving into singularities [actually, if the entropy is constructed with one-body HF mean values, which are exact in the thermodynamic limit, the entropy derivative becomes infinite at both critical points (for $v \to v_c^{(i)+}$)].

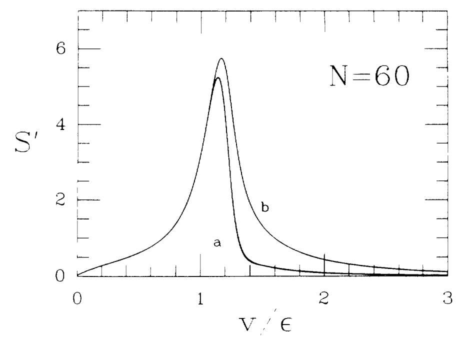

FIG. 1. Exact and inferred values of the entropy derivative $S' = \partial S / \partial v$ (in units of k_B/ε in all figures), for the ground state of the Lipkin U(2) model as a function of the (dimensionless) scaled coupling parameter. Curve (a) corresponds to exact results together with the inferred value employing expectation values of one- and two-body operators ($\langle \hat{J}_z \rangle$ and $\langle \hat{J}_z^2 \rangle$ in the present model), undistinguishable in the scale of the figure, whereas curve (b) to the one-body inference (employing $\langle \hat{J}_z \rangle$). Results correspond to calculations in the completely symmetric representation. N denotes the number of particles present.

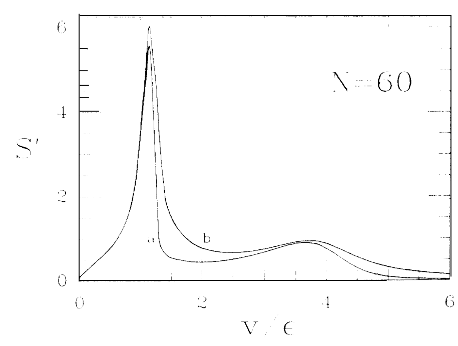

FIG. 2. Same details of Fig. 1 for the ground state of the U(3) model.

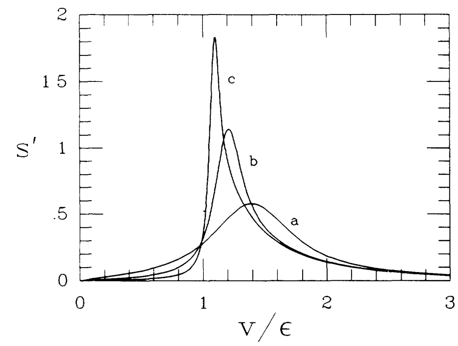

FIG. 3. The exact intensive entropy derivative $s' = N^{-1}\partial S/\partial v$, calculated in the full space, for the ground state of the U(2) model and for different values of N. Curve (a) corresponds to $N = 20$, (b) to $N = 60$, and (c) to $N = 200$.

Nevertheless, we remark that for finite N, the critical regions may be slightly displaced from the HF values (see the second maximum in Fig. 2) and may become much less noticeable. In the three-level case, as the number of particles decreases, the second maximum may even disappear, being absorbed into a single wide transitional region. This is due to the fact that for a small number of particles the third SP level begins to be occupied almost simultaneously with the second one (see Ref. [11] for more details), so that it is no longer possible to clearly distinguish two transitions.

The features of the behavior of the intensive derivative of the exact quantal entropy $N^{-1}\partial S_{\rm ex}/\partial v$ for different particle numbers can be seen in Fig. 3 for the case $n = 2$. The entropy has been evaluated now in the full space. For all N, we are able to clearly distinguish two different regimes characterized by negligible variations of the quantal entropy, separated by the critical region located around $v/\varepsilon = 1$. As N increases, the critical region becomes narrower and approaches the HF value $v/\varepsilon = 1$, whereas the maximum increases in magnitude, thus describing the most abrupt changes of the ground-state distribution. Results in the symmetric space are qualitatively similar.

We would like to remark that the amount and type of information required for an accurate inference depends on the regions separated by the maxima of the entropy derivative. For instance, in the U(2) situation, it can be seen that for $v/\varepsilon < 1$, two-body information is actually irrelevant for the entropy evaluation. The fluctuation matrix A_{ij} becomes important in the critical region, whereas for high values of v/ε, one-body information is no longer relevant, and the inference with just two-body mean values yields accurate results.

2. AFP model

Results of numerical calculations for the ground state of the AFP model are shown in Figs. 4 and 5, assuming $\varepsilon = 1$ and $v > 0$, which we shall take as the control parameter. The derivatives of the inferred and exact quantal entropies are depicted in Fig. 4 for fixed N within the symmetric representation. Similar results hold in full space calculations. A clear maximum can be appreciated both in the exact and inferred treatments, indicating a transition between weak- and strong-coupled regimes, similar to that of the previous U(2) model.

The intensive entropy derivative is depicted in Fig. 5. It is seen that even though both models exhibit very similar features for small particle numbers, they behave in a strikingly different way as N increases, as the entropy remains smooth for all values of N and no transitional point is expected to be found in the thermodynamic limit.

IV. CONCLUSIONS

Our goal was to establish a criterion to predefine critical regions in ground states of finite systems within the framework of information theory. The scheme is based on the variation experienced by the inferred entropy associated with a reduced set of commuting observables upon changes of the corresponding control parameters. These variations reflect the qualitative changes occurring in the ground-state distribution over the common basis defined by the commuting observables and, accordingly, transitional regions are associated with those regions of maximum variation.

In the examples considered, it is seen that just with

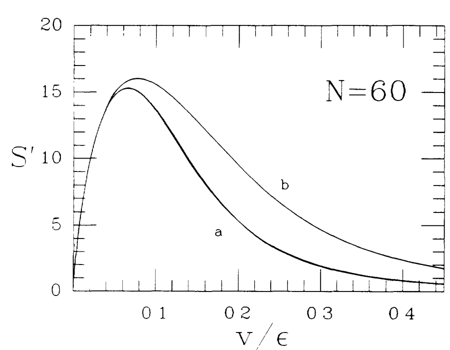

FIG. 4. Exact and inferred values of $S' = \partial S/\partial v$ for the ground state of the AFP model. Remaining details as in Fig. 1.

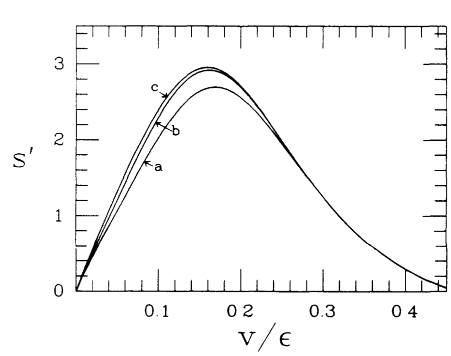

FIG. 5. The exact intensive entropy derivative for the ground state of the AFP model, for $N = 20$ (a), $N = 60$ (b), and $N = 200$ (c), calculated in the full space.

the expectation values of a few relevant observables commuting with the unperturbed Hamiltonian, the critical regions can be clearly determined with the present prescription. Within this context, the ensuing exact critical regions can be identified with those regions where the entropy associated with a complete set of abelian operators exhibits the most significant variations. This entropy, equal to the quantal entropy of Refs. [10–12], measures the exact lack of information related with the distribution of the pertinent quantum state over the common basis, and differs from the usual thermodynamical entropy. When the size of the system increases, the critical regions determined by our method become narrower and approach critical points in case the system possesses a real transition in the thermodynamic limit. Otherwise, no discontinuities ensue.

Thus, we conclude that by means of a suitable extension of thermodynamic concepts within the generalized statistical framework of information theory, it is possible both to consistently define transitions in ground states of finite systems and, at the same time, to infer the location of these critical regions with a reduced amount of information.

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