Classical statistical mechanics of a few-body interacting spin model

Fausto Borgonovi[1,2,3,*] and F. M. Izrailev[4]
[1]*Department of Physics, University of Maryland, College Park, Maryland 20742*
[2]*Istituto Nazionale di Fisica della Materia, Unità di Milano, Via Celoria 16, 22100 Milano, Italy*
[3]*Istituto Nazionale di Fisica Nucleare, Unità di Pavia, Via Bassi 6, 27100 Pavia, Italy*
[4]*Instituto de Física, Universidad Autónoma de Puebla, Apartado Postal J-48, 72570 Puebla, Mexico*
(Received 10 November 1999)

We study the emergence of Boltzmann's law for the ''single-particle energy distribution'' in a closed system of interacting classical spins. It is shown that for a large number of particles Boltzmann's law may occur, even if the interaction is very strong. Specific attention is paid to classical analogs of the average shape of quantum eigenstates and ''local density of states,'' which are very important in quantum chaology. Analytical predictions are then compared with numerical data.

PACS number(s): 05.45.−a

I. INTRODUCTION

Chaotic properties of few-degrees-of-freedom systems have attracted much attention during the last years. The knowledge and classification of chaotic dynamical systems is now extremely accurate, if compared with the state of the art at the beginning of the century. On the other hand, conventional statistical mechanics was born long before the chaology of dynamical systems. It is well known that, in contrast to chaotic dynamical systems with few degrees of freedom, for the onset of statistical equilibrium in systems with an infinitely large number of particles neither nonlinearity nor interaction between particles is needed. Indeed, in such systems the thermodynamic limit (infinite number of particles $N\rightarrow\infty$) leads to the statistical behavior of a system since any weak interaction (with an environment or between particles) gives rise to mixing properties and onset of chaos.

Although statistical mechanics has undoubtedly obtained results in many different fields, fundamental questions about statistical descriptions of systems with finite number of particles are still open [1]. It is clear that in such systems the interparticle interaction is crucial; however, its role in producing chaos or ergodicity is still not understood. Due to computing difficulties and lack of theoretical studies, many-body chaotic systems have been scarcely investigated, and little is known about them.

Recently, an approach to quantum isolated systems with a finite number of interacting particles was developed [2–6]. The goal of this approach was a direct relation between the average shape of exact eigenstates (F function), and the distribution of occupation numbers n_s of single-particle levels. This relation shows that there is no need to know the eigenstates exactly; instead, if these eigenstates are chaotic (random superposition of a very large number of components of basis states), the F function absorbs the statistical effects of interaction between particles and determines the form of the n_s distribution. The approach was mainly developed for a model with completely random two-body interaction between a finite number of Fermi particles; however, it can be also applied to dynamical models with chaotic behavior.

One of the few dynamical models studied with the use of this approach was a system of two interacting spins [7,8]. The most interesting result obtained numerically in Ref. [7] is that the distribution of occupation numbers (even for two interacting particles) in the chaotic region can be described in the form of the standard Bose-Einstein (BE) distribution (only symmetric states have been considered which results in the BE statistics). It was shown that the statistical effects of the interaction lead to an increase of temperature which is related to the BE distribution. Also, it was discovered that the canonical distribution is recovered if one randomizes the *nonzero elements* of the interaction V, keeping the dynamical constraints of the model. This means that random interaction plays the role of a heat bath, and allows one to use statistical and thermodynamical descriptions for isolated systems.

In order to extend the approach of Refs. [2–6] to classical dynamical systems with a large number of particles, we introduce the model of N interacting spins in one dimension. Due to the well-defined classical limit, it is first of interest to explore similar problems in the classical counterpart. The problem of a quantum-classical correspondence for chaotic systems with a large number of interacting particles seems to us extremely important in view of many physical applications. In this paper we mainly concentrate on the occurrence of Boltzmann's law, and on the classical counterparts of the quantum local density of states and the shapes of the eigenfunctions. The investigation of the analogous Fermi-Dirac or Bose-Einstein statistics in a quantized version of such a model is reserved for future work [9].

Our investigation is complementary to the approach based on the so-called *dynamical* temperature [10–12], introduced for the study of the statistical properties of few-degrees-of-freedom classical models with chaotic behavior. Specifically, our interest is in the notion of *statistical* temperature associated with Boltzmann's distribution (if any) for single-particle energy. The relation between statistical and dynamical temperatures represents an open and interesting question.

II. MODEL OF INTERACTING SPINS

Our purpose is to investigate a few-body dynamical system from a statistical mechanics point of view. Following

*On leave of absence from the Dipartimento di Matematica e Fisica, Università Cattolica, Via Trieste 17, I-25121 Brescia, Italy.

previous works on the two-particle spin problem [8,7], we consider the Hamiltonian

$$H=B\sum_{i=1}^{N} S_i^z+J\sum_{i=1}^{N} \vec{S}_i\cdot\vec{S}_{i+1}, \tag{1}$$

which is known as the one-dimensional Heisenberg model in a magnetic field; see, for instance, Ref. [13]. Here $\vec{S}_i$ are spin vectors, and, for the sake of definiteness, we take periodic boundary conditions $\vec{S}_1=\vec{S}_{N+1}$. The classical version is a solvable model from the statistical point of view (namely, when the number of particles $N\to\infty$; see Ref. [14]).

Instead, here we are interested in a dynamical approach, in particular for a small number of particles, when the usual statistical approach is at least questionable. In what follows, we shall consider a more simple version of the classical Heisenberg model, which is described by the Hamiltonian

$$H=H_0+V=B\sum_{i=1}^{N} S_i^z+J\sum_{i=1}^{N} S_i^y S_{i+1}^y, \tag{2}$$

where $N>2$ is the number of spins in the chain. We do this in order to simplify analytical calculations. The equations of motion can be written in the usual way,

$$\frac{d\vec{S}}{dt}=\{H,\vec{S}\}, \tag{3}$$

where $\{,\}$ are Poisson brackets (see Refs. [15,16] for similar dynamical models). Constants of motion are the energy E and the magnitude of the angular momenta $|\vec{S}_i|=s$ (the latter is assumed to be the same for each spin). Without loss of generality, we can put $s=1$.

Contrary to the common viewpoint (spin Hamiltonian plus a magnetic field as a perturbation) we consider the ''magnetic'' part as an unperturbed Hamiltonian. Indeed, we are interested in models which can generally be expressed as a sum of single-particle Hamiltonians, this feature not being shared by the perturbation V. Therefore, the Heisenberg kernel ($J\Sigma\vec{S}_i\vec{S}_{i+1}$) will be considered as a perturbation between nearest-neighbor spins.

The unperturbed Hamiltonian is integrable, and the solution of the unperturbed equations of motion can be written down at a glance. It should be pointed out that the perturbation itself is not chaotic. Indeed, it can be verified numerically that two close trajectories diverge only linearly in time when $B=0$. This means that the maximal Lyapunov exponent is zero for any choice of the initial conditions. On the other hand, the same Lyapunov analysis shows that the total Hamiltonian, for generic values of the coupling J and for energy values in the middle of the band ($E\sim 0$), is chaotic. Maximal Lyapunov exponents, as a function of time for different J and B values and fixed energy E , are shown in Fig. 1.

As one can see, the Lyapunov exponents approach zero when B decreases, or J increases. On the other hand, for fixed J, and B different from zero, the region where the maximal Lyapunov exponent approaches zero is close to the edge of the energy spectrum (see Fig. 2). Maximal Lyapunov exponents have been calculated using the standard recipe [17].

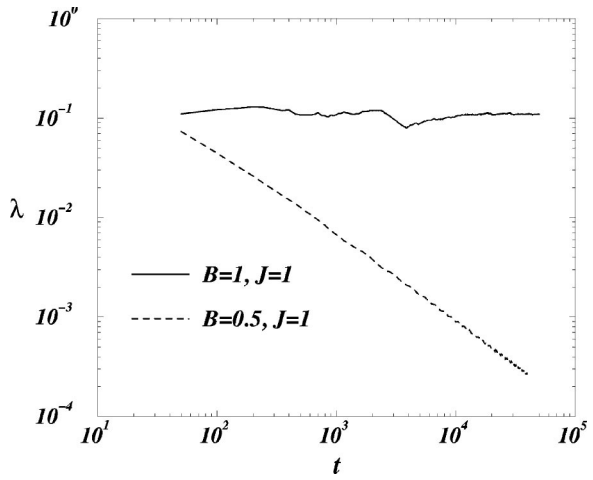

FIG. 1. Maximal Lyapunov exponents as a function of time for $E=-2$ and $J=1$ and $B=0.5$ and 1, as indicated in the picture. The system has $N=4$ spins.

Besides integrability, the unperturbed Hamiltonian H_0, in the limit $N\to\infty$, has good statistical properties which we exploit in Sec. III. It is indeed interesting to compare our results with those obtained with the standard statistical approach.

III. IDEAL GAS OF SPINS

This particular choice of the model, being extremely simple, allows an analytical treatment of the case $N\to\infty$ in both unperturbed and perturbed cases. Let us first analyze the unperturbed Hamiltonian H_0. This should be thought of as a model of a very weakly interacting system. In what follows, without loss of generality, we assume $B=1$. The microcanonical ensemble represents the most natural way to analyze an isolated system of N spins. One goal is to find the thermodynamical temperature as it depend on the energy E. Another is to study the single-particle energy distribution and

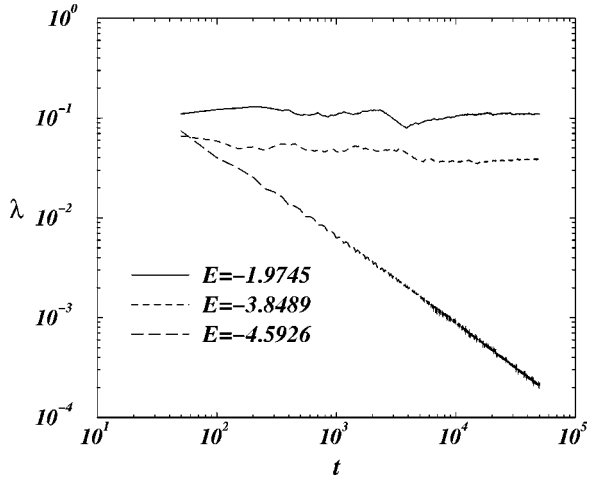

FIG. 2. (a) Maximal Lyapunov exponents as a function of time for $J=1$, $B=1$, and different energy E as indicated in the text. Simulations have been made with four spins.

the conditions under which it can be assimilated to the Boltzmann distribution.

The temperature $T=\beta^{-1}$ ($k_B=1$ hereafter) can be defined via the microcanonical ensemble

$$\beta_{mc}=\frac{dS}{dE}, \tag{4}$$

where S is the entropy. For a sufficiently large number of particles this can in turn be defined as $S=\log\rho(E)$. Here $\rho(E)$ can be defined through the phase space volume [18]. If the motion of N spins is ergodic, each of them covers uniformly the unit three-dimensional (3D) sphere. Therefore, each component of $\vec{S}$ has a uniform probability density function in the interval $[-1,1]$ [19]; that is,

$$p(h)=\frac{\partial P(S_i^z\leqslant h)}{\partial h}=\begin{cases}1/2 & \text{when } -1\leqslant h\leqslant 1\\ 0 & \text{elsewhere,}\end{cases} \tag{5}$$

and the same for the other components S_i^y and S_i^x. Here the quantity $P(x\leqslant a)$ gives the probability that the continuous random variable x has values less than a. In the same way, the density of states can be evaluated as a probability:

$$\rho_0(E_0,N)=\frac{\partial P\left(\sum_{i=1}^{N} S_i^z\leqslant E_0\right)}{\partial E_0}. \tag{6}$$

The distribution of the sum of N independent random variables can be obtained using the central limit theorem (when $N\to\infty$)

$$\rho_0(E_0,N)\simeq\frac{1}{\sigma_0\sqrt{2\pi}}\exp\left(-\frac{E_0^2}{2\sigma_0^2}\right), \tag{7}$$

where

$$\sigma_0^2=\frac{N}{3}. \tag{8}$$

As a result, from Eq. (4) one obtains an unusual *microcanonical relation* for the energy vs inverse temperature [14]:

$$\beta_{mc}=-\frac{3E_0}{N}. \tag{9}$$

In principal, the energy E_0 ranges from $E_{\min}<0$ to $E_{\max}=-E_{\min}>0$; therefore, in this model negative temperatures are also possible. One should note that typical physical systems have densities of states increasing with energy, thus giving positive temperature. For this reason, in what follows, we consider only positive temperatures which correspond to the left (part of the symmetric) energy spectrum, $E_0<0$.

It is important to note that the density of states can also be obtained for finite system of particles without invoking central limit theorems. This can be done by a direct integration over the phase space volume,

$$\begin{aligned}\rho_0(E_0,N)&=\int_{-\infty}^{+\infty}dS_1^z\,p(S_1^z)\cdots\\ &\quad\times\int_{-\infty}^{+\infty}dS_N^z\,p(S_N^z)\,\delta\left(\sum_{i=1}^{N}S_i^z-E_0\right)\\ &=\int_{-\infty}^{+\infty}\frac{1}{2\pi}d\lambda\;e^{-i\lambda E_0}\left[\int_{-1}^{1}dx\,\frac{1}{2}e^{i\lambda x}\right]^N\\ &=\frac{N}{2^N}\sum_{k=0}^{M}(-1)^k\frac{(N+E_0-2k)^{N-1}}{k!(N-k)!},\end{aligned} \tag{10}$$

where M is the integer part of $(E_0+N)/2$.

Let us now concentrate on the ''single-particle energy distribution'' (*SPE distribution*) defined as:

$$n_0(h|E_0)=N\frac{\partial P\left(S_1^z\leqslant h\left|\sum_{i=1}^{N}S_i^z=E_0\right.\right)}{\partial h}, \tag{11}$$

where $P(x\leqslant a|y=b)$ is the conditional probability.

This quantity is the classical analog of the quantum *distribution of occupation numbers*, which gives the number of particles occupying a single-particle level with energy E_0. Correspondingly, the above classical distribution determines the probability that *any* of N spins has the energy E_0. From this definition, it is clear that the SPE distribution [Eq. (11)] is normalized to the total number of particles, and it defines the mean energy of *all* particles, or, the same, the mean total energy of the system. In this way, one can treat an isolated model in the same way as the model in contact with a heat bath (see details in Refs. [8,6]).

It is well known that for $N\to\infty$ the single-particle energy should be distributed according to Boltzmann's law. Under suitable conditions this holds true in this model, too. Indeed, one obtains

$$\begin{aligned}n_0(h|E_0)&=N\frac{p\left(S_1^z=h,\sum_{i=1}^{N}S_i^z=E_0\right)}{\rho_0(E_0,N)}\\ &=N\frac{p\left(S_1^z=h,\sum_{i=2}^{N}S_i^z=E_0-h\right)}{\rho_0(E_0,N)}\\ &=N\frac{p(S_1^z=h)\,p\left(\sum_{i=1}^{N-1}S_i^z=E_0\right)}{\rho_0(E_0,N)}\\ &=N\frac{\rho_0(h,1)\rho_0(E_0-h,N-1)}{\rho_0(E_0,N)},\end{aligned} \tag{12}$$

where the last equality is due to the independence of S_i^z. The quantity $p(S_1^z=h,\Sigma_{i=1}^{N-1}S_i^z=E_0)$ defines the joint probability density function.

Substituting expression (7) into the above relation, it is easy to obtain (in the limit of a very large $N\gg 1$)

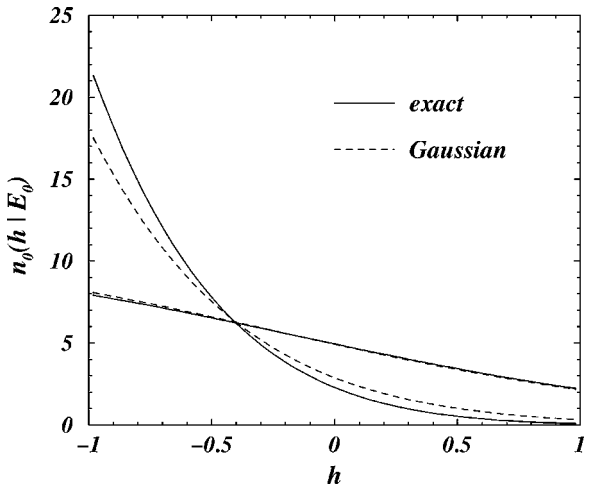

FIG. 3. Single-particle energy distribution for $N=10$ and $J=0$. Full lines represent the exact distribution [Eq. (12)] obtained from the exact unperturbed density of states [Eq. (10)]. Dashed lines are the correspondent infinite approximations [Eq. (13)] with a proper normalization. Upper curves are for $E_0=-6$, lower ones for $E_0=-2$.

$$n_0(h|E_0) \simeq \exp\left(-\frac{3E_0^2}{2N(N-1)} - \frac{3h^2}{2(N-1)} + \frac{3E_0 h}{N-1} \right), \tag{13}$$

where $E_0<0$.

Obviously, a correspondent expression for any number of particles can be obtained, using the exact value of the unperturbed density of states Eq. (10). In Fig. 3 we show the infinite (Gaussian) approximation ($N\to\infty$) and the exact one, computed for two different energy values. As one can see, while in the middle of the spectrum the distributions are almost the same, close to the band edges they are remarkably different. The Gaussian, or infinite approximation, works very well even for a small number of particles as soon as the energy E_0 is not close to the edges of the band (the interval $[-N,N]$ for noninteracting spins). Indeed, the Gaussian density of states has infinitely long tails, while the exact one is sharply defined within $[-N,N]$. On the other hand, while the support of the density function scales as N, its variance depends on $\sqrt{N}$. It follows that the region close to the edges becomes less and less important as N becomes large.

Let us briefly comment on Eq. (13). Although it has been obtained for a large number of particles, it nevertheless shows that, generally speaking, the single-particle energy distribution for finite weakly interacting systems *is not necessarily described by an exponential law*. One can see that the latter occurs in a very strong limit $N\to\infty$, provided that $|E_0| \gg |h|$,

$$n_0(h|E_0) \simeq \exp(-\beta_0 h), \tag{14}$$

where the temperature $T_0=\beta_0^{-1}$ is defined via

$$\beta_0 = -\frac{3E_0}{N-1} = \beta_{mc} + O(1/N), \tag{15}$$

and $E_0<0$. One should stress that, apart from the limit $N\to\infty$, the exponential distribution arises when the second condition $E_0 \gg |h| \sim 1$ is fulfilled. Physically this means that the total energy must be larger than the typical single-particle energy, a condition naturally satisfied for a thermodynamical system.

Another important relation can be obtained from Eq. (12). Specifically, taking the derivatives of both sides of Eq. (14) over h, and exchanging the derivative on the right-hand side, one obtains

$$-\frac{d}{dh}\log n_0(h|E_0) = \frac{d}{dE_0}\log \rho_0(E_0-h, N-1), \tag{16}$$

One can see that in the limit $N\to\infty$ and $|E_0| \gg |h|$, the right-hand side coincides with the microcanonical definition of the temperature, while the left-hand side shows that the only possible exponential distribution should have a microcanonical temperature.

We have thus found that in the noninteracting system, when the number of particles becomes sufficiently large and the total energy of the system is larger than the typical single-particle energy, the *microcanonical temperature* [Eq. (9)], defined by the density of states, coincides with the *statistical temperature* defined directly from the SPE distribution [Eq. (11)], which is the standard Boltzmann law. One can then assume that if the interaction is sufficiently small, in order not to change the previous results dramatically, but enough to produce ergodicity (from the equations of motion), Boltzmann's law again results from taking a sufficiently large but finite number of particles.

Let us stress that in order to obtain these results, the motion has been assumed to be fully ergodic on the unit 3D sphere. Rigorously speaking, this can be true, from the dynamical point of view, only in the presence of interaction $J\neq 0$. Indeed for $J=0$ the motion is foliated onto regular tori, and no ergodicity at all is allowed. Thus this ideal spin model has been worked out following the traditional statistical mechanics picture, where the interaction is assumed to be sufficiently weak in order to apply noninteracting results, but sufficiently strong in order to obtain ergodicity.

IV. MANY INTERACTING SPINS

A. Density of states

1. Infinitely strong interaction

Before switching to the interacting case, let us compute the density of states in the presence of an infinitely strong interaction (namely, formally setting $B=0$). In this case the density of states can be written as follows:

$$\rho_V(E,N) = \frac{\partial P(V\leqslant E)}{\partial E} = \frac{P\left(J\sum_{i=1}^{N} S_i^y S_{i+1}^y \leqslant E \right)}{\partial E}. \tag{17}$$

The central limit theorem can also be applied in this case, keeping in mind that the normalized probability distribution of the product $z=xy$ of two uniformly distributed random variables x,y in the interval $(-1,1)$ is given by [20]

$$\rho_V(E/J,1) = -(1/2J)\log(|E/J|), \tag{18}$$

so that the variance is $\langle z^2 \rangle = 1/9$. Equation (17) then becomes (in the large N limit)

$$\rho_V(E,N) \simeq \frac{1}{\sigma_V^2 \sqrt{2\pi}} \exp\left(-\frac{E^2}{2\sigma_V^2} \right), \tag{19}$$

with

$$\sigma_V^2 = \frac{NJ^2}{9}. \tag{20}$$

Note that, even in this case, an explicit integral equation can be obtained for finite systems. Following the same steps as in Eq. (10), one obtains

$$\rho_V(E,N) = \int_{-\infty}^{+\infty} d\lambda \, e^{-i\lambda E} \left[\frac{s(\lambda)}{\lambda} \right]^N, \tag{21}$$

where $s(\lambda)$ is the sine-integral function defined by

$$s(\lambda) = \int_0^{\lambda} dx \frac{\sin x}{x}.$$

2. General case

In the same way the density of states in the presence of both the interaction and the ''kinetic'' term can be computed by assuming that H_0 and V are independent. Indeed, let us define

$$P(H_0 + V \leqslant E) = \int_{-\infty}^{E} dE' \rho(E'). \tag{22}$$

On the other hand, if H_0 and V are independent, their joint probability density function can be written as

$$\rho_{H_0,V}(E_0,E) = \rho_0(E_0)\rho_V(E). \tag{23}$$

The probability density function of the sum of two independent random variables is thus given by [20].

$$\rho(E) = \int_{-\infty}^{+\infty} dE' \rho_0(E - E')\rho_V(E'). \tag{24}$$

Substituting Eqs. (7) and (17), and performing simple Gaussian integrals, one obtains

$$\rho(E,N) \simeq \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{E^2}{2\sigma^2} \right), \tag{25}$$

where the variance

$$\sigma^2 = \frac{N}{3v}, \qquad v = \frac{1}{1 + J^2/3}, \tag{26}$$

should be compared with Eq. (20).

In Eq. (25) there are two different approximations. The first one is the Gaussian form for the density of states, which is valid when $N \to \infty$. The second is the independence of the (random) terms H_0 and V which, of course, cannot be true in general. For instance, a configuration with all spins aligned along the z axis, for which $E_0 = N$, implies $V = 0$. However, if the motion is ergodic and the energy is not too close to the band edges, the second assumption can be considered as a good approximation.

B. Classical analogs of quantum eigenstates and the LDOS

Another important relation can be obtained linking the two quantities, the *shape of the ''eigenfunctions''* (SE) and the *local density of states* (LDOS), whose concepts were motivated by quantum mechanics (see, for example, Refs. [3,21,8,6]). The latter quantity, the LDOS, also known in nuclear physics as the *strength function*, is very important when describing the spread of the energy initially concentrated in a specific unperturbed state. The classical analogs of these functions were introduced in Ref. [22], and recently applied to dynamical models in Refs. [8,21]. The very point is that in the limit of $N \to \infty$ these two quantities can be explicitly found, and a relation between them can be established.

In the case of ergodic motion the classical analog of the SE can be defined as

$$W_E(E_0) = \frac{\partial P(H_0 \leqslant E_0 | H_0 + V = E)}{\partial E_0}. \tag{27}$$

Correspondingly, the classical analog of the LDOS is

$$w_{E_0}(E) = \frac{\partial P(H_0 + V \leqslant E | H_0 = E_0)}{\partial E}. \tag{28}$$

It is very important that both the SE and LDOS can be computed more efficiently [22] using the equations of motion. For the SE one has to choose a chaotic trajectory at some fixed energy E, compute the $H_0(t)$ trajectory, and sample the values of the unperturbed Hamiltonian H_0 along this trajectory at some fixed time intervals. This procedure gives us the ergodic distribution inside the *energy shell* constructed by a projection of the phase space of H onto H_0 (see details in Refs. [8,21]). In the same way, the classical LDOS can be numerically computed taking a bunch of (regular) trajectories of the unperturbed Hamiltonian $H_0 = E_0$, and computing the correspondent spread of $H(t)$ along these unperturbed trajectories. The sample of the values of the total Hamiltonian $H(t)$, taken at given intervals of time, results in the classical LDOS. Let us stress that even in the case of ergodic motion of the total Hamiltonian H, when only one single trajectory is needed in order to obtain the SE, an ensemble of trajectories of H_0 is necessary in order to obtain a reliable result for the LDOS. This is a consequence of the integrability of H_0.

Alternatively one can choose, as indicated by definitions (27) and (28), many different initial conditions on the same energy surface, and sum over them. It is clear that the two procedures (dynamical and taking the average over the phase volume) should give the same result in the case of ergodic motion.

An important identity can be easily proven from relations (27) and (28). Let us write

$$P(H_0+V\leqslant E,H_0\leqslant E_0)$$
$$=\int_{-\infty}^{E_0} dE_0'\,P(H_0+V\leqslant E,H_0=E_0')$$
$$\times\int_{-\infty}^{E_0} dE_0'\,P(H_0+V\leqslant E|H_0=E_0')\rho_0(E_0'), \tag{29}$$

from which one can obtain the classical SE,

$$w_{E_0}(E)\rho_0(E_0)=\frac{\partial^2 P(H_0+V\leqslant E,H_0\leqslant E_0)}{\partial E\,\partial E_0}. \tag{30}$$

In the same way one can obtain the classical LDOS,

$$W_E(E_0)\rho(E)=\frac{\partial^2 P(H_0\leqslant E_0,H_0+V\leqslant E)}{\partial E_0\partial E}. \tag{31}$$

From the above, the following relation emerges:

$$w_{E_0}(E)\rho_0(E_0)=W_E(E_0)\rho(E). \tag{32}$$

Let us stress that the previous identity does not depend on the Gaussian approximation, and that it takes dynamical correlations into account as well. This simple relation between the classical SE and LDOS is very important in different applications. Remarkably, only unperturbed and perturbed densities of states $\rho_0(E)$ and $\rho(E)$ enter into this relation. This allows one to relate the shape of eigenstates to that of the LDOS in the corresponding quantum model, in a deep semiclassical region. In fact, a knowledge of these two functions leads to a semiclassical approach, according to which it is easy to detect quantum effects of localization; see details in Refs. [3,6].

It should be stressed that the classical SE and LDOS, in essence, are ergodic measures for energy shells defined by the projection of H_0 onto H (and vice versa) in the energy representation.

Functions $W_E(E_0)$ and $w_{E_0}(E)$ can be considered as kernel operators transforming unperturbed quantities into total ones, and vice versa. For instance, by integrating Eq. (32) one has

$$\rho(E)=\int dE_0\,w_{E_0}(E)\rho_0(E_0), \tag{33}$$

and the converse,

$$\rho_0(E_0)=\int dE\,W_E(E_0)\rho(E). \tag{34}$$

In a certain way w and W each can be considered the inverse of the other. It is also easy to check that when $J\to 0$ then $W_E(E_0)=w_{E_0}(E)=\delta(E-E_0)$.

Assuming the Gaussian approximation for the densities of states, and using Eq. (32), we can easily obtain an analytical expression for the classical SE,

$$W_E(E_0)=\frac{1}{\sigma_W\sqrt{2\pi}}\exp\left[-\frac{(E_0-E_c)^2}{2\sigma_W^2}\right], \tag{35}$$

where

$$\sigma_W^2=\frac{NJ^2}{9}v \tag{36}$$

is the variance, and $E_c=vE$ is the center of the SE.

In order to obtain the LDOS distribution, one can use relation (32), from which one obtains

$$w_{E_0}(E)=\frac{1}{\sigma_w\sqrt{2\pi}}\exp\left[-\frac{(E_0-E)^2}{2\sigma_w^2}\right], \tag{37}$$

where

$$\sigma_w^2=\frac{NJ^2}{9}. \tag{38}$$

It is interesting to note that the above distribution, in the Gaussian approximation, coincides with Eq. (19):

$$w_{E_0}(E)=\rho_V(E-E_0). \tag{39}$$

This relation can be also obtained independently, using the assumption of the independence of H_0 from V.

One can see that although the two Gaussians are different, for a weak interaction $J\ll 1$, and then $v\sim 1$, they appear to be close to one another. This fact is of a general nature, and occurs in other models; see Refs. [22,21,7].

On the other hand, this result shows that, strictly speaking, even in the case of ergodic motion, one should not expect the SE and LDOS to be the same. As found above, the relation between the SE and LDOS is given by Eq. (32). One can obtain a very useful relation for the variances of the SE and LDOS (valid in the Gaussian approximation only),

$$\frac{\sigma_w^2}{\sigma_W^2}=\frac{\sigma_0^2}{\sigma^2}. \tag{40}$$

We would like to stress again that both the SE and LDOS have a proper meaning only in the case of ergodic motion. In other cases they depend strongly on initial conditions and on the energy, thus not allowing one to use any statistical approach.

C. Distribution of single-particle energies and different temperatures

For $N\gg 1$, the microcanonical temperature $T_{mc}=\beta^{-1}$ can be defined from the total density of states [Eq. (25)],

$$\beta_{mc}=\frac{\partial\log(\rho)}{\partial E}=-\frac{3E}{N}v, \tag{41}$$

with $v=1/(1+J^2/3)$. In fact, Eq. (41) determines the *thermodynamical temperature*, since it establishes the relation between the temperature and total energy of a system. Now we are going to find the *statistical temperature* associated with the SPE distribution. First of all, let us note that, if the variables H_0 and V are independent, the following approximate relation can be obtained:

$$n(h|E)=\frac{dP(S_1^z\leqslant h|H_0+V=E)}{dh}$$

$$=\int dE_0\, n_0(h|E_0)W_E(E_0). \tag{42}$$

Substituting Eqs. (13) and (35) into Eq. (42), one obtains

$$n(h|E)\simeq\exp\left(-\frac{3E_c^2}{2N(N-v)}-\frac{3vh^2}{2(N-v)}+\frac{3E_ch}{N-v}\right), \tag{43}$$

where $E_c=vE$. Note that when $J=0$, then $v=1$, and Eq. (13) is recovered.

One can see that in the limits $|E|\gg|h|\sim 1$ and $N\gg v$ the SPE distribution can be approximated by the exponential dependence

$$n(h|E)\sim e^{-\beta(E)h}, \tag{44}$$

where

$$\beta(E)=-\frac{3E}{N}v=\beta_{mc}. \tag{45}$$

The last equality, claiming that the statistical temperature coincides with the thermodynamical one, is by no means trivial. On the one hand, the presence of strong interaction suggests some statistical equilibrium property, thus leading to microcanonical predictions. On the other hand, we do not know if the single-particle description is valid since the interaction is strong. Even in the case when mean field approach would be possible (in such a way that part of the interaction actually becomes a single-particle energy), the single-particle distribution would depend on the mean field, and there are no reasons to expect, *a priori*, that the Boltzmann distribution occurs with the same temperature as given by the microcanonical ensemble.

Another way to find the statistical temperature which corresponds to the SPE distribution is as follows. First we note that, in the presence of interaction, one has

$$\int dh\, hn(h|E)=\overline{E}\neq E; \tag{46}$$

this is different from the noninteracting case, for the latter the obvious relation holds;

$$\int dh\, hn_0(h|E_0)=E_0. \tag{47}$$

Note that the SPE distribution in Eq. (46) depends on the interaction; however, the ''mean value'' of the energy of all particles does not correspond to the energy of a system. This very fact allows one to relate statistical effects of the interaction to an increase of the total energy (in application to quantum systems, this approach was considered in Refs. [3,4,6]).

Specifically, in order to find the SPE distribution $n(h|E)$ from Eq. (46), one needs to know the *renormalized energy* $\overline{E}$. One can see that the Boltzmann distribution gives a correct result for an isolated system, if we take into account the shift of the energy $\Delta_E=\overline{E}-E$ which is due to the interaction between particles. In a sense, the (statistical) effects of the interaction are absorbed by the increase of the energy of a system, compared to the case of noninteracting particles. Therefore, pseudorandom interaction may be treated as an internal heat bath, thus giving rise to a statistical equilibrium.

The shift Δ_E can be found by assuming the absence of correlations between H_0 and V in a way described above. One can show that

$$\overline{E}=\int dE_0E_0\, W_E(E_0)=E_c, \tag{48}$$

where $E_c=vE$ is the center of the classical SE, and the last equality occurs in a strong limit $N\gg 1$ using Eq. (35). Therefore, the shift is given by the relation

$$\Delta_E=\overline{E}-E=-\frac{\sigma_w^2}{\sigma_0^2}E=-\frac{J^2}{3}E. \tag{49}$$

It is important that the shift is defined by the width σ_w of the LDOS and by the width of the unperturbed density. One should note that in a quantum representation, the variance σ_w^2 is defined by the sum of squared off-diagonal matrix elements. Therefore, this energy shift can be found without diagonalization of huge quantum Hamiltonian matrices. Using this shift, one can find the temperature from Eq. (46) by assuming the Boltzmann dependence for $n(h)$.

Another way to obtain the temperature is via the unperturbed density of states evaluated at the renormalized energy $\overline{E}$:

$$\beta_r=\left.\frac{d\log\rho_0}{dE_0}\right|_{E_0=\overline{E}}=-\frac{3\overline{E}}{N}. \tag{50}$$

Using the relation between $\overline{E}$ and E, one obtains

$$\beta_r=-\frac{3\overline{E}}{N}=-\frac{3E}{N}v=\beta_{mc}. \tag{51}$$

Once again, we should remember that, apart from the limit $N\gg 1$, the above relation is valid when neglecting the correlations between H_0 and V. However, the smaller the number of particles, the larger the energy region where (dynamical) correlations will be important.

It is now interesting to find the increase of temperature $\Delta T=T-T_0$ due to the interaction, in comparison with the temperature $T_0=\beta_0^{-1}$ of the system with noninteracting spins:

$$\frac{\Delta T}{T_0}=\frac{\sigma_w^2}{\sigma_0^2}=\frac{J^2}{3}. \tag{52}$$

One can see that the relative increase of temperature is given in terms of the variance of the LDOS and the width of the unperturbed density only [also see Eq. (49)]. This fact seems to be generic; see the discussion in Refs. [3,6].

A more accurate relation for the definition of temperature via the SPE distribution, without the assumption of the

Gaussian form of the density of states, can be obtained as follows. In close analogy to Eq. (16) one can write

$$n(\epsilon|E)=\frac{\partial P(S_1^z\leqslant\epsilon|H=E)}{\partial\epsilon}$$

$$=\frac{1}{\rho(E,N)}\frac{\partial P(S_1^z\leqslant\epsilon,H=E)}{\partial\epsilon}. \tag{53}$$

On the other hand, defining $x_i=S_i^z$, and $y_i=JS_i^yS_{i+1}^y$ it follows that

$$P(x_1\leqslant\epsilon,H=E)$$

$$=\int_{-\infty}^{\epsilon}d\epsilon' P\left(x_1=\epsilon',x_1+y_1+\sum_{i=2}^{N}x_i+y_i=E\right)$$

$$=\int_{-\infty}^{\epsilon}d\epsilon' P\left(x_1=\epsilon',y_1+\sum_{i=2}^{N}x_i+y_i=E-\epsilon'\right)$$

$$=\int dh\int^{\epsilon}d\epsilon' P\left(x_1=\epsilon',y_1=h,\sum_{i=2}^{N}x_i\right.$$

$$\left.+y_i=E-\epsilon'-h\right). \tag{54}$$

Owing to the independence of the three random variables, the joint probability density can be factorized, and one obtains

$$n(\epsilon|E)\rho(E,N)=\rho_0(\epsilon,1)\int dh\,\rho_V(h,1)\rho(E-\epsilon-h,N-1). \tag{55}$$

Now defining now the ''interacting'' density of states

$$Z_\epsilon(E)=\int dh\,\rho_V(h,1)\rho(E-\epsilon-h,N-1), \tag{56}$$

one obtains a relation similar to Eq. (16):

$$-\frac{\partial}{\partial\epsilon}\log n(\epsilon|E)=\frac{\partial}{\partial E}\log Z_\epsilon(E). \tag{57}$$

Equation (57) states that if correlations can be neglected, then a renormalized density of states must be introduced in order to obtain the ''correct'' temperature as obtained from the single-particle energy distribution. On the other hand, it is clear that in the limit $N\to\infty$, and $|E|\gg 1$, we have $Z_\epsilon(E)\sim\rho(E)$ and the usual definition is recovered. It is now interesting to apply our estimates to a system with a not very large number of spins.

V. NUMERICAL DATA

A. Large number of spins

Let us first consider the model with $N=100$ spins. On the one hand, this situation is far from the thermodynamic limit; on the other hand, the number of particles is quite large, and one can expect a good correspondence with analytical results obtained in Sec. IV. In Fig. 4 two SPE distributions are plotted for different values of the total energy E. In both cases, the trajectories have been found to be chaotic with positive maximal Lyapunov exponents. For comparison, the analytical expression [see Eq. (43)], obtained in the Gaussian approximation, is shown. As one can see, the agreement is fairly good. On the other hand, a direct comparison of the microcanonical temperature β_{mc} with the approximated temperature, obtained by fitting the SPE distribution by an exponent, gives different answers; see Fig. 5. In this figure, crosses represent the fitted inverse temperatures as a function of the total energy, while the dashed curve is the microcanonical relation between the inverse temperature and the energy. In order to smooth fluctuations, the derivative has been calculated performing local averages in small energy win-

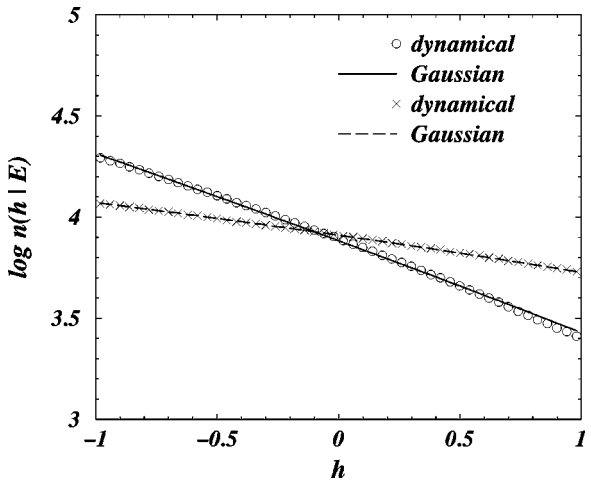

FIG. 4. Single-particle energy distributions for $N=100$ and large interaction $J=1$, for different energy values. One single trajectory has been iterated for a given energy, up to a time $t=10^6$. Numerical data should be compared with the analytical expression [Eq. (43)] obtained from the Gaussian approximation for the density of states. Circles stand for $E=-19$, crosses for $E=-7$.

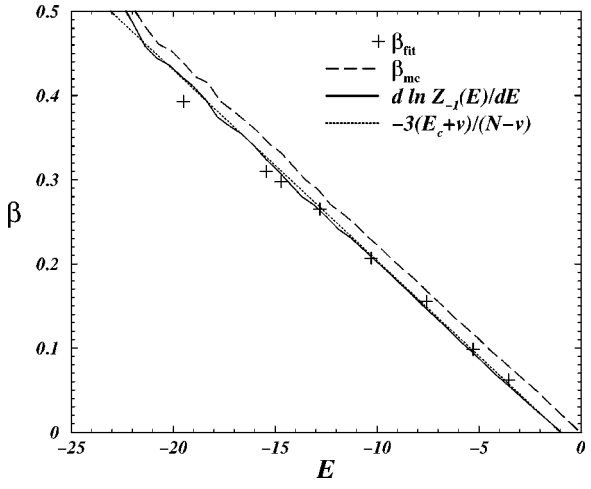

FIG. 5. Inverse temperatures vs total energy for $N=100$ and $J=1$. Crosses are the extracted β_{fit} from the best fit of the SPE distributions $n(h|E)$ to the exponential dependence. Typical examples of these distributions are given in Fig. 4. The dashed line is the microcanonical relation [Eq. (41)] found numerically from the density of states $\rho(E)$. The full line is the theoretical prediction, obtained from Eq. (57) with $\epsilon=-1$. The dotted line is the Gaussian approximation (see the text).

dows. A small, but systematic, difference between the statistical and microcanonical temperatures is clearly seen.

A much better agreement can be achieved by directly using (instead of the total density of states) the renormalized density [Eq. (56)]. The corresponding result is presented by the full line. One can see quite good correspondence to numerical data for the statistical temperature. This result means that Eq. (56) is more accurate than the usual statistical definition [Eq. (41)].

One can also introduce the effective (statistical) temperature by making use of Eq. (43), keeping all terms in the exponent. The temperature can be defined as a slope of $\ln n(h|E)$ at the bottom of the energy spectrum,

$$\beta_{fit}=\frac{d\ln n(h|E)}{dh}=\frac{3E_c}{N-v}-\frac{3vh}{N-v}=\frac{3v(E-h)}{N-v}, \quad (58)$$

with $h\rightarrow -1$. The corresponding result is shown in Fig. 5 by the dotted line. One can see that this dependence practically coincides with both the fit to the actual distribution $n(h|E)$ (crosses) and with the temperature determined by Eq. (56) (full line). This means that these two approximations correctly take into account both the dynamical correlations and the finite number of particles.

We can conclude that, in spite of the relatively small number of particles, if compared with the usual thermodynamical systems of 10^{23} particles, our model of $N=100$ interacting spins can be approximately described by a standard statistical approach which ignores dynamical correlations between particles. Indeed, the difference between the microcanonical temperature and the approximate temperature, found by the fit of the SPE distribution close to the edge of the energy spectrum, is quite small, and may be neglected in some cases. However, even for a relatively large number of spins, $N=100\gg 1$, a clear influence of dynamical correlations and finite number of particles remains. However, one should stress that in spite of a clear manifestation of the influence of dynamical correlations and finite number of particles, the SPE distribution $n(h|E)$ for low energies can be effectively described by the standard Boltzmann distribution, though with a renormalized temperature.

B. Chaos versus ergodicity

It is reasonable to think that a statistically stable distribution would require a certain degree of chaoticity. But chaos itself, as indicated, for instance, by the positivity of the maximal Lyapunov exponent, is not enough in order to obtain equipartition among different degrees of freedom (see the general discussion of this very important problem in Ref. [23]). We have found such cases for a small number of particles and an energy close to the center of the spectrum.

It is instructive to work out a specific example. Let us consider a system of $N=4$ spins. For $J=B=1$ and energy $E_*=-1.9745$, the single-particle energy distribution is very different from the phase average distribution (obtained with many different initial conditions in a small energy window close to E_*); see Fig. 6. Nevertheless, the Lyapunov exponent is positive for many initial conditions inside the same energy window.

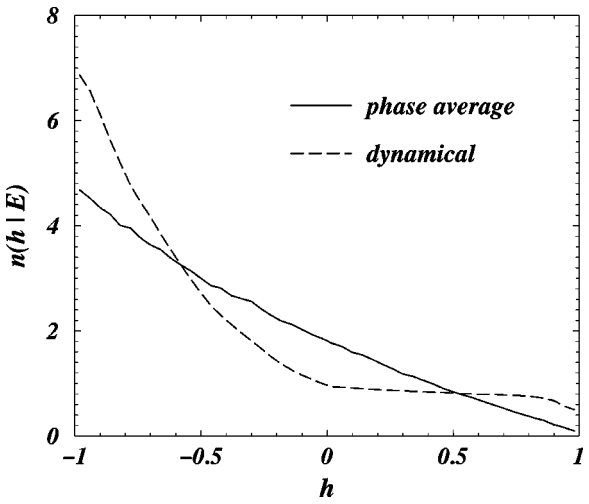

FIG. 6. Single-particle energy distribution for $N=4$ and $J=1$. The dashed line is obtained dynamically, by integrating the equations of motion for a single trajectory with energy $E_*=-1.9745$ up to the time $t=10^7$. The full line is the phase average distribution obtained for 10^6 different initial conditions in the energy range $[-1.98,-1.97]$.

This lack of ergodicity is also reflected in the lack of equipartition. Indeed, defining the average unperturbed single-particle energy as

$$\langle S_i^z\rangle=\lim_{T\rightarrow\infty}\int_0^T dt\, S_i^z(t), \quad (59)$$

we obtain that, typically, for trajectories with energy E close to E_*, neighbor spins do not share the same energy (lack of equipartition). In Table I, we show the average kinetic energy per spin for a dynamical trajectory with the energy E_* (second column), to be compared with the average kinetic energy per spin as obtained from the phase average distribution (right column) within the energy range $\Delta E=[-1.98, -1.97]$.

C. Ergodicity versus dynamical correlations

In this section we deal with systems having a small number of spins (let us say, on the order of ten). In contrast to the case considered in Sec. IV, we select only those energy values which correspond to both a positive Lyapunov exponent and to equipartition among different spins; this means, in particular, that ''dynamical'' and ''statistical'' distributions (the former obtained by integration of equations of motion for one trajectory, the latter by choosing many different initial conditions onto the energy surface and performing a phase average) are close to one another.

TABLE I. Average kinetic energy per spin.

Spin label i	$\langle S_i^z(E_*)\rangle$	$\langle S_i^z(\Delta E)\rangle$
1	−0.7248	−0.3783
2	−0.1387	−0.3788
3	−0.7248	−0.3788
4	−0.1388	−0.3801

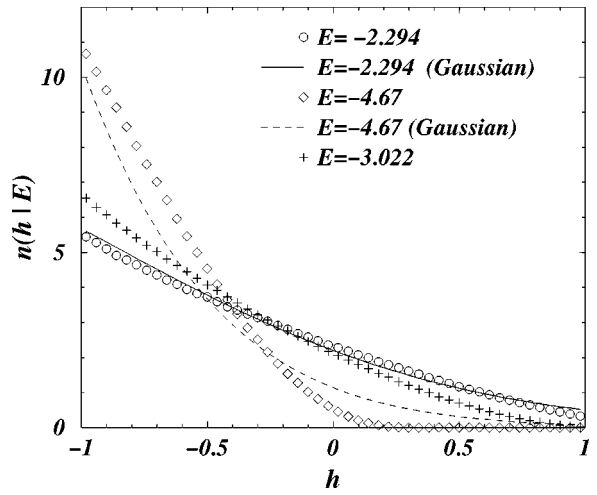

FIG. 7. Single-particle energy distribution $n(h|E)$ for $N=5$, with interaction $J=1$ as a function of the single-particle energy h. Different symbols indicate different energy values E, as shown in the window. For a few sets of symbols the Gaussian approximation, as given by Eq. (43), is also shown.

Let us focus on two different samples of $N=5$ and 10 interacting spins with strong and chaotic interactions ($J=1$). In Figs. 7 and 8 we show the SPE distribution for different energies, together with the correspondent Gaussian approximations [Eq. (43)].

The first important point is a remarkable deviation from the Gaussian approximation, at least for energy values E close to the band edge. This simply means that the approximations involved in order to obtain Eq. (43) are no longer valid. One of these approximations was to consider a Gaussian shape for the SE in Eq. (42). According to additional data, effective SE's (statistical or dynamical, they are very close to each other) for the same energy value show remarkable deviations from the Gaussian. Nonetheless, the substitution of the ''true'' SE in Eq. (42) does not affect $n(h|E)$ considerably. This amounts to saying that Eq. (42) itself does not constitute a good approximation for energy values close to the edges.

Indeed, due to the small number of spins, and to the relatively large energy shared by each spin particle, they are strongly correlated, and most of the uncorrelation assumptions (between H_0 and V, for example) made in the previous sections are no longer valid.

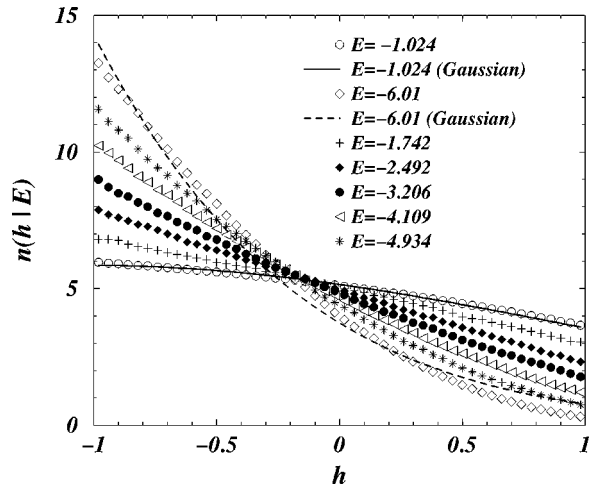

FIG. 8. The same for $N=10$.

To be more precise, it can be shown that Eq. (42) can be considered as the ''diagonal'' approximation of the exact relation

$$n(h|E)=\int dE_0\, W_E(E_0) n_E(h|E_0), \tag{60}$$

where

$$n_E(h|E_0)=P(S_1^z=h|H_0=E_0, H=E). \tag{61}$$

In the limit when H and H_0 are independent one recovers Eq. (42), since $n_E(h|E_0)=n_0(h|E_0)$. The study of the correlation kernel [Eq. (61)] beyond the diagonal approximation will be reserved for future investigations.

On the other hand, in the middle of the energy band $|E| \sim 0$ there is a rough agreement with the Gaussian approximation (see Fig. 7). Indeed, for such energy values, there is no preferred direction of the spin (the energy shared by each single spin is relatively small), and Eq. (42) still represents a good approximation. However, the bad point is that, close to the center of the band, the Gaussian approximation for $n(h|E)$ is far from an exponential [in fact, it is close to a Gaussian, see Eq. (43)]. Indeed, let us remember that one of the conditions for obtaining the Boltzmann distribution was $|E| \gg 1$, which is of course not satisfied at the center of the energy spectrum.

Even if not completely satisfactory from the theoretical point of view, but in close analogy with the case of $N=100$ spins, one could define a temperature as (minus) the slope of the fitting straight line to $\log n(h|E)$. Operatively we observe that in the region to the left of their intersection point ($h \sim -0.6$ for $N=5$ and $h \sim -0.7$ for $N=10$), distributions with different energy values have a behavior closer to that of an exponential. Therefore, it is natural to fit the numerical $n(h|E)$ with an exponential only to the left of the intersection point. Let us call β_{fit} the inverse temperature obtained in this way.

Needless to say, when compared with both the statistical and microcanonical temperatures, one can see important deviations. In Figs. 9 and 10 we plot the obtained β_{fit} as a function of the energy E, together with other definitions of temperature for $N=5$ and 10.

As one can see, none of the previous definitions seems to fit the numerical values. This is not surprising, in spite of the fact that only an approximate exponential behavior has been found. We do not have any approximate theory able to describe such temperature differences when the number of spins is small. Strictly speaking, one recognizes the importance of the classical SE in the description of the behavior of single-particle distribution, but it becomes technically complicated to go beyond the diagonal approximation, which is correct only when the number of particles is sufficiently large and the energy is not too close to the ''many-body ground state'' (bottom of the energy spectrum).

The following approximate phenomenological scaling relation has been found numerically:

$$\beta_s=-\frac{3\langle E\rangle}{N}-\frac{(1+\alpha)J^2}{N}, \tag{62}$$

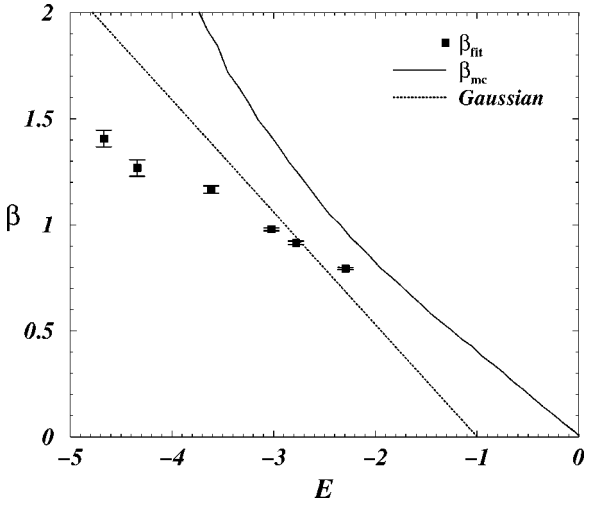

FIG. 9. Comparison between different definitions of temperature for $N=5$. Symbols represent the numerically extracted β_{fit}, while different curves refer to different definitions of temperature, the microcanonical approximation (full line), and the Gaussian approximation (dotted line). Since the latter also turns out to be dependent on h, we computed it at $h=-1$.

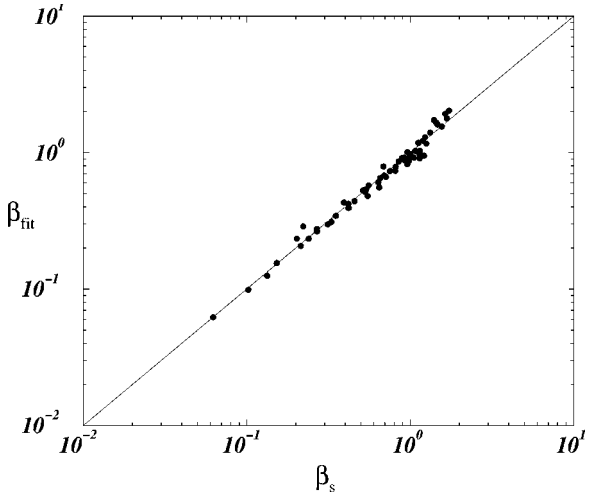

FIG. 11. β_{fit} obtained by fitting the single-particle energy distribution in the negative part of the single-particle spectrum, vs the proposed phenomenological scaling β_s. Full circles represent the numerical data for $N=4$, 5, 10, 20, and 100 and $J=0.1$, 0.5, and 1, and different energy. The full line is the scaling relation.

where $\alpha=0.7$ is the fitting parameter and $\langle E\rangle = \int dh\, hn(h|E)$. In Fig. 11 for different N, J, and energy E, we show the numerical data and the scaling relation [Eq. (62)].

For the time being, we have no theoretical explanation for this scaling relation. It should be stressed that, in the limit $N\to\infty$ and sufficiently large energy $\langle E\rangle$ the second term on the left-hand side of Eq. (62) is negligible with respect to the first one, and Eq. (51) is recovered. We point out that it is not possible to take $J\gg 1$ in this model, since it becomes integrable, and most of the previous results are necessarily wrong.

The disagreement between the microcanonical temperatures and the statistical one for a small number of particles has few important theoretical implications. First, we note that they are obtained in two completely different ways. While the single-particle distribution reflects a property of the constant energy surface $H=E$, the microcanonical definition requires a derivative *across* the energy surface. In principle, the knowledge of the correlation kernel [Eq. (61)] would solve the problem completely. But this in turn requires a knowledge of the (infinite) intersections among the $H=E$ and $H_0=E_0$ surfaces.

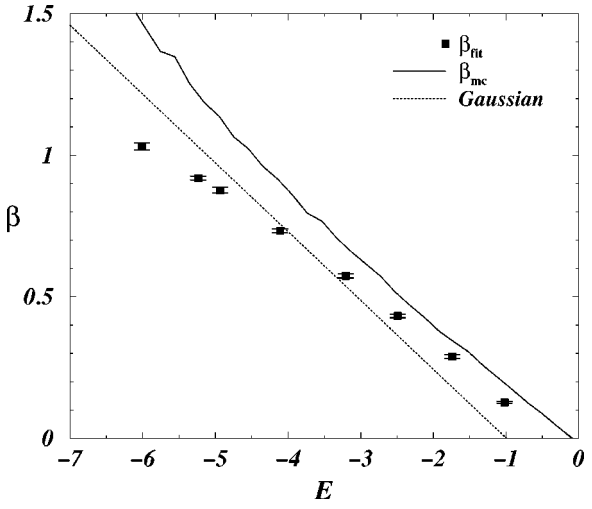

FIG. 10. The same for $N=10$ spins.

VI. CONCLUDING REMARKS

In this paper we have studied the emergence of Boltzmann's law for the single-particle energy distribution $n(h|E)$ in a isolated dynamical model of a finite number of interacting spins. In the limit of a very large number of spins, this model allows for an analytical treatment. We have shown that in this strong limit, Boltzmann's distribution, indeed, occurs with an effective *statistical* temperature which coincides with that defined by the standard *microcanonical temperature*. The latter is defined via the total density of states. Since our analytical proof is also valid for a strong spin interaction, it is far from trivial. Indeed, it is not *a priori* clear that the SPE distribution, which pertains to a noninteracting property, follows the Boltzmann distribution with the temperature determined via the total density of states.

The above result has been obtained in an approach which is very similar to that recently suggested in the study of the so-called *two-body random interaction model* [2–4]. According to this approach, the distribution of occupation numbers for single-particle levels in a quantum many-body system is directly related to the average shape of chaotic eigenstates in the basis of the unperturbed Hamiltonian (the latter can be considered as the mean-field part of a system). This means, in fact, that there is no need to know exact eigenstates of huge Hamiltonian matrices which take into account two-body interaction between particles. This is due to the chaotic nature of eigenstates, which results from the (assumed) randomness of the two-body matrix elements.

An important point of the above approach is that in some cases the average shape of eigenstates can be found analytically from off-diagonal matrix elements of the total Hamiltonian H_0; see Refs. [3,5]. The same happens to another important quantity, the *strength function*, which in solid state

physics is also known as the *local density of states* (LDOS). These two quantities are related to each other; however, so far this relation is not well studied. Numerical data for different models, both disordered [3] and dynamical [21,8], have shown that for not very strong interaction, these two quantities are very close to one another. Knowledge of the LDOS is very important in many applications. Indeed it provides information on how energy, initially concentrated in a specific unperturbed state, spreads over all other states due to the interaction between particles. The inverse width of the LDOS is, in fact, the effective time of this spread.

Until recently, the above two quantities were discussed only in the context of quantum systems. On the other hand, in Ref. [22] it was noted that both LDOS and SE have very clear classical analogs. The study of the *classical* LDOS and SE were begun in Refs. [21,8], and the first results showed that the average shape of quantum eigenstates (and the same for the LDOS) for chaotic eigenstates coincides fairly well with the classical counterpart. For this reason, when studying the occurrence of Boltzmann distribution in our model of interacting spins, we have also paid attention to the classical LDOS and SE.

Our results in what concerns classical SE and LDOS have shown a nice correspondence with the main findings for a quantum model with random two-body interaction [3,4,6]. In particular, in our classical model we have proved the basic expressions for an increase of both total energy [Eq. (49)] and temperature [Eq. (52)] due to statistical effects, which in a quantum model were derived directly from the shape of exact eigenstates in the unperturbed energy basis. Moreover, additional relations [Eqs. (32) and (40)] have been found which may also be important in quantum systems.

Numerical data for our model have confirmed the main theoretical predictions for a large number of particles, $N=100$. However, it was also found that in spite of a relatively large N, one can detect clear deviations for the statistical temperature related to the SPE distribution. Detailed analysis shows that these deviations are mainly due to dynamical effects of correlations originating from a finite number of particles. As shown, analytical results can be interpreted as a ''diagonal'' approximation, neglecting correlations between the total Hamiltonian and the unperturbed Hamiltonian. One should stress that corrections to the thermodynamical expressions are not only on the order of $1/N$, as commonly assumed in the literature, but depend on the interaction strength as well.

Drastic deviations from the thermodynamical approach have been found for two interacting spins ($N=10$ and 5). Both the thermodynamical temperature defined from the microcanonical relations, and the statistical temperature found analytically for a very large N, are very different from the approximate temperature. The latter has been determined numerically from the Boltzmann dependence of the SPE distribution, used as a fitting expression for low energies of the system. A phenomenological expression has been found from the analysis of the data, but without a proper analytical explanation. These problems, as well as the development of a *semiquantal* approach for which a quantum distribution of occupation numbers is computed with the use of a classical analog of the shape of the eigenstates, will be a subject of future investigations.

ACKNOWLEDGMENTS

F.B. would like to thank the Department of Physics of the University of Maryland at College Park, the Department of Physics at the University of Puebla, and the ''Cientro Internacional de Ciencias'' at Cuernavaca where part of this work was done. Useful discussions with R. E. Prange, I. Guarneri, G. Casati, and V. Flambaum are also acknowledged. F.M.I. gratefully acknowledges financial support from CONACyT (Mexico), Grant Nos. 26163-E and 28626-E. F.B. acknowledges financial support from INFM and INFN (IS MI41).

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