

Statistical properties of spectra of the Heisenberg Hamiltonian

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Spectra of several types of finite Heisenberg lattices have been studied using methods of statistical spectroscopy. In particular, spectral density distributions, discrete spectra generated from the spectral density distribution moments, and the distributions of spacings between the neighboring energy levels have been analyzed. The densities have been shown to be nearly Gaussian and the spectra generated from their several-moment Gram-Charlier approximations are in a good agreement with the exact ones, except for several extreme energy levels. Spacings between the neighboring levels exhibit clustering of the energy levels stronger than that given by the Poisson distribution, showing an essential influence of the point-group symmetries of the lattices. [S0163-1829(99)11303-1]

I. INTRODUCTION

The most common approach to studies of the spectrum of a Hamiltonian defined in a finite-dimensional model space is based on a diagonalization of the corresponding matrix and a subsequent analysis of the eigenvalues. Another approach, often referred to as *statistical spectroscopy*,¹⁻³ focuses on properties of the entire spectrum rather than of the individual energy levels. The set of energy levels is treated as a statistical ensemble. The statistical description, on one hand, brings some new information about structure of the spectrum and, on the other, is applicable in the cases when the traditional approach is prohibitively inefficient (as, for example, when the number of the energy levels of interest is very large). Statistical theories of spectra have been developed starting from several, rather diverse, motivations. Their origin may be traced back to the early works of Bethe.⁴ During decades they were mainly applied in nuclear physics where not exactly known character of the interparticle interactions supplied the main motivation for using the language of statistics and stimulated the development of the so called *random matrix theory*.^{2,5} It was noticed that very useful information about some global properties of spectra may be derived by applying methods of statistical spectroscopy to systems for which the Hamiltonian matrix does not contain any randomness. This gave a motivation to the development of the statistical theory of atomic spectra.⁶⁻¹¹ Statistical studies of molecular spectra were initiated by Haller *et al.*¹² They were mainly concentrated on understanding relationships between classical chaotic systems and their quantum analogs.¹³⁻¹⁷ However they also were applied to a determination of the effects of molecular complexity on the structure of vibrational spectra¹⁸ or to studies of the relations between the dynamical symmetries and spacings of the neighboring vibrational levels.¹⁶ Another application of statistical spec-

troscopy is directed towards a determination of the envelopes of spectral bands in complex atomic²² and molecular^{23,24} spectra.

Usually the information about the global character of spectra is derived from a knowledge of the spectral density distribution moments, closely related to the traces of powers of the Hamiltonian matrix^{2,3,19}. Spectral density distribution moments are invariant with respect to the unitary transformations of the basis in the model space. Therefore they are independent of the selection of a specific basis and can be determined *a priori*, without any N -particle matrix element evaluation.¹⁹ The results always correspond to the complete N -particle model space. In spectroscopy most interesting applications are connected with deriving detailed properties of spectra (e.g., the Hamiltonian eigenvalues) from the spectral density distributions, i.e., from the corresponding moments^{9,20,21,25}. Their development may result in new methods of approximating the eigenvalues by quantities whose evaluation is not limited by dimensions of the matrices. This approach is relatively common in predicting structure of the nuclear spectra,^{2,3} however, only some pilot studies have been performed in the case of many-electron systems.^{9,10,21,25}

In this paper statistical properties of spectra of the Heisenberg Hamiltonian are studied. The spectra have been found to be Gaussian-like and are well approximated by several-term Gram-Charlier expansions.²⁶ The exact spectra (obtained by diagonalizations of the Hamiltonian matrices) are compared with the ones derived from the moment-generated spectral density distributions. This approximation gives a very good description of the spectrum in its central part, however, as one should expect, deteriorates at the extremes. Relations between the exact and the moment-generated spectra are analyzed for several kinds of the lattices as a function of the number of moments. It has been observed that the

quality of the statistical description improves with an increase of the dimension of the problem and with a lowering of the symmetry of the lattice.

II. THE HEISENBERG HAMILTONIAN

The Heisenberg Hamiltonian for an N -electron system, or rather for a system of N spins, may be written as²⁷⁻²⁹

$$\hat{H} = \sum_{i < j}^N J_{ij} \left(\frac{1}{2} + 2\hat{s}_i \hat{s}_j \right), \quad (1)$$

where J_{ij} are the exchange parameters and \hat{s}_i is the one-electron spin operator of the i th electron. The Hamiltonian is defined in a complete antisymmetric and spin-adapted space of covalent structures corresponding to a single electronic configuration in which all the orbitals are singly occupied. The dimension of this model space is equal to²⁷

$$f(S, N) = \frac{2S+1}{N+1} \binom{N+1}{N/2-S}, \quad (2)$$

where S is the quantum number corresponding to the total spin operator \hat{S}^2 .

Spectral density distribution moments are defined as

$$\mu_q = \frac{1}{f(S, N)} \text{Tr} \hat{H}^q. \quad (3)$$

They may be expressed in the form²⁵

$$\mu_q = \sum_i^{l(q)} T_q(i) R_q(i), \quad (4)$$

where $l(1)=1, l(2)=3, l(3)=8, \dots$. The elements $T_q(i)$ are linear combinations of the normalized irreducible characters of S_N (which may be expressed as rational functions of N and S), and the elements $R_q(i)$ are combinations of products of the exchange parameters. Explicit formulas are given in Refs. 19, 25, 30. The coefficients $R_q(i)$ carry all the information about the topology of the molecule. They describe specific features of the molecule and may be determined from knowledge of the molecular graph. They are referred to as the *topological invariants* of the molecule. The coefficients $T_q(i)$ express the way in which these specific features propagate when N and S change. Therefore they are called *propagation coefficients*.²

III. STATISTICAL DESCRIPTION OF THE SPECTRUM

Let us consider a discrete spectrum $E_1 \leq E_2 \leq \dots \leq E_D$ with the eigenvalues treated as a statistical ensemble. The density of the energy level distribution is described by the following frequency function:

$$\rho(E) = \frac{1}{D} \sum_{i=1}^D \delta(E - E_i). \quad (5)$$

It is normalized

$$\int_{-\infty}^{\infty} \rho(E) dE = 1 \quad (6)$$

and its q th moment is equal to

$$\mu_q[\rho] = \int_{-\infty}^{\infty} E^q \rho(E) dE. \quad (7)$$

Using Eq. (5) we get

$$\mu_q[\rho] = \frac{1}{D} \sum_{i=1}^D E_i^q. \quad (8)$$

Particularly, for the Heisenberg Hamiltonian the moments may be expressed as in Eq. (4).

The normalized moments are defined as

$$\tilde{\mu}_q[\rho] = \int_{-\infty}^{\infty} \left(\frac{E - \mu_1}{\sigma} \right)^q \rho(E) dE = \sigma \int_{-\infty}^{\infty} E^q \rho(\sigma E + \mu_1) dE, \quad (9)$$

where $\sigma = \sqrt{\mu_2 - \mu_1^2}$ is the dispersion or the width of the spectrum. In particular, $\tilde{\mu}_1 = 0$ and $\tilde{\mu}_2 = 1$. The departure of a given distribution from the Gaussian one is frequently measured by the values of two parameters: the skewness $\gamma_1 = \tilde{\mu}_3$ and the excess $\gamma_2 = \tilde{\mu}_4 - 3$ (for the Gaussian distribution $\gamma_1 = \gamma_2 = 0$).

According to the so called *principle of moments*²⁶ we expect that two distribution functions containing some adjustable parameters may be brought to an approximate identity by selecting the parameters so that several lowest moments of these distributions become equal. Then, if p moments of the exact distribution ρ are known, we may approximate this distribution by a p -parameter trial function $\bar{\rho}_p$. These parameters have to be determined so that the lowest p moments calculated using $\bar{\rho}_p$ are equal to the exact ones. The convergence pattern of this approximation strongly depends upon the choice of the trial function.^{23,24} Most commonly the frequency function is approximated by the Gram-Charlier expansion^{9,20,21,26} (identified hereafter by a superscript G):

$$\bar{\rho}_\infty^G(E) = \sum_{j=0}^{\infty} c_j' H_j(E) \alpha'(E), \quad (10)$$

where $H_j(E)$ are the Hermite polynomials,

$$\alpha'(E) = \frac{1}{\sqrt{2\pi}} \exp(-E^2/2) \quad (11)$$

and

$$c_q' = \frac{1}{q!} \left[\mu_q^G - \frac{q^{[2]}}{2!} \mu_{q-2}^G + \frac{q^{[4]}}{2^2 2!} \mu_{q-4}^G - \dots \right] \quad (12)$$

with

$$q^{[n]} = q(q-1)(q-2) \dots (q-n+1).$$

The q th moment of the Gram-Charlier distribution is

$$\mu_q^G \equiv \mu_q[\bar{\rho}_\infty^G] = \int_{-\infty}^{\infty} E^q \bar{\rho}_\infty^G(E) dE. \quad (13)$$

The second-, third-, and fourth-moment Gram-Charlier expansions transformed so that their first and second moments are equal, respectively, to 0 and to 1 are given by the following equations:²⁶

$$\begin{aligned}\bar{\rho}_2^G(E) &= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}E^2\right), \\ \bar{\rho}_3^G(E) &= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}E^2\right) \left[1 + \frac{\tilde{\mu}_3}{6}(E^3 - 3E)\right], \\ \bar{\rho}_4^G(E) &= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}E^2\right) \left[1 + \frac{\tilde{\mu}_3}{6}(E^3 - 3E) + \frac{1}{24}(\tilde{\mu}_4 - 3)(E^4 - 6E^2 + 3)\right].\end{aligned}$$

If we assume that

$$\tilde{\mu}_q[\rho] = \tilde{\mu}_q[\bar{\rho}_p^G] \quad (14)$$

for $q=1,2,\dots,p$, then the Gram-Charlier expansion $\bar{\rho}_p^G$ constitutes a p -moment approximation to the exact frequency function.

The normalized distribution function corresponding to the frequency function $\bar{\rho}_p$ is defined as

$$\bar{F}_p(E) = \int_{-\infty}^E \bar{\rho}_p(x) dx. \quad (15)$$

According to Ratcliff²⁰ the discrete energy values may be derived from $\bar{F}_p(E)$ as a set of values E_i which satisfy the relation

$$\bar{F}_p(E_i) = \frac{1}{D} \left(i - \frac{1}{2}\right) \quad (16)$$

for $i=1,2,\dots,D$. A comparison of the real energy levels and those derived from the spectral density distribution moments leads to notions of the secular eigenvalue density and of fluctuations.^{2,3,20} The secular density is defined by a small number of moments. Usually three or four moments are sufficient to obtain a correct secular density.^{2,21} If the secular density is accurate enough, then the fluctuations are small, energy independent, and nonsensitive to increasing the number of moments used to describe the spectrum.

Another quantity characterizing statistical behavior of a spectrum is the distribution of the adjacent level spacings.^{2,5,6,17,21} The energy level spacings are defined as

$$d_j = E_{j+1} - E_j. \quad (17)$$

Their mean value

$$\bar{d} = \frac{1}{D-1} \sum_{j=1}^{D-1} d_j \quad (18)$$

is referred to as the mean level spacing. The normalized level spacings are given by

$$x_j = \frac{d_j}{\bar{d}}. \quad (19)$$

As it is known (see, e.g., Ref. 17), the distribution of normalized spacings between uncorrelated (randomly sprinkled over an interval) energy levels is Poissonian:

$$\bar{\mathcal{P}}^0(x) = \exp(-x). \quad (20)$$

This distribution is peaked at $x=0$. Then, if the distribution of the adjacent level spacings is Poissonian, the energy levels have a tendency to cluster. If the Hamiltonian matrix is composed of several blocks corresponding to different symmetry species, the eigenvalues associated with different symmetries are not correlated and degeneracies or near degeneracies are frequent. In this case the level spacing distribution is Poisson-like. The level spacings behave entirely differently if all the energy levels correspond to the same symmetry (to the same set of values of all constants of the motion). Due to the “level repulsion,” the probability of degeneracies is very small and the nearest-neighbor spacing distribution is approximately of the Wigner type

$$\bar{\mathcal{P}}^W(x) = \frac{\pi}{2} x \exp\left(-\frac{\pi}{4}x^2\right). \quad (21)$$

A very important observation allows us to link the form of the distribution of the adjacent level spacings in a quantum system with either periodic or chaotic behavior of its classical counterpart: the Poisson-type distributions appear in classically periodic (integrable) systems while the Wigner-like distributions characterize classically chaotic systems.^{17,31} A more general distribution containing the Wigner and the Poisson ones as special cases has been introduced by Berry and Robnik.³² In order to describe the behavior of the level spacings in spectra of the Heisenberg lattices, we introduce another, more general, distribution function:

$$\bar{\mathcal{P}}^D(x) = A x^\alpha \exp\{-x^\beta\}, \quad x \geq 0, \quad (22)$$

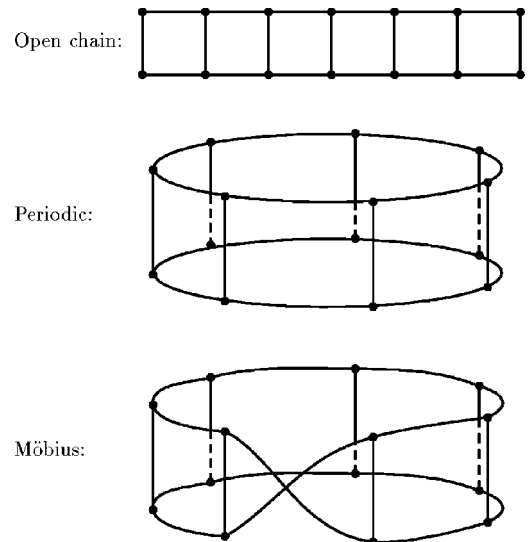


FIG. 1. Types of Heisenberg ladders.

TABLE I. The first two moments of spectral density distributions.

q	L	$S=0$		$S=1$	
		Open	Periodic	Open	Periodic
1	6	5.818	6.545	6.303	7.091
2	6	46.424	56.727	51.448	63.151
1	7	7.308	8.077	7.725	8.538
2	7	68.301	81.503	73.827	88.301
1	8	8.800	9.600	9.167	10.000
2	8	94.646	110.769	100.564	117.846

where A is the normalization constant while α and β are adjustable parameters. The distribution moments corresponding to $\bar{\mathcal{P}}^D(x)$ are equal to

$$\mu_q[\bar{\mathcal{P}}^D] = \int_0^\infty \bar{\mathcal{P}}^D(x) x^q dx = \Gamma\left(\frac{\alpha+q+1}{\beta}\right) \Gamma\left(\frac{\alpha+1}{\beta}\right)^{-1}. \quad (23)$$

The constants defining this distribution function may be evaluated using the method of moments, i.e., imposing the condition that $\mu_q[\bar{\mathcal{P}}^D]$, for $q=1,2$, are equal to the corresponding moments of the exact distribution.

IV. RESULTS AND DISCUSSION

Calculations have been performed on $S=0$ and on $S=1$ states of two-dimensional isotropic $2 \times L$ Heisenberg lattices with $L=6$ up to $L=8$ (i.e., with $N=12$ up to $N=16$). The

TABLE II. Standard deviations between spectra of open and periodic (O-P), open and Möbius (O-M), and periodic and Möbius (P-M) Heisenberg lattices calculated using unnormalized (Δ^{LS}) spectra and the normalized ones (δ^{LS}).

L, S	D	Δ^{LS}			δ^{LS}		
		O-P	O-M	P-M	O-P	O-M	P-M
6,0	132	0.7801	0.7842	0.3135	0.0597	0.0637	0.0841
6,1	297	0.8159	0.8151	0.1751	0.0382	0.0368	0.0488
7,0	429	0.7979	0.7966	0.1777	0.0309	0.0286	0.0441
7,1	1001	0.8317	0.8321	0.0854	0.0167	0.0178	0.0218

exchange parameter has been put equal to 1 for the nearest neighbors and 0 otherwise. Three types of boundary conditions have been chosen: an open ladder (designated hereafter O), a periodic ladder (designated P), and a Möbius-type chain (designated M)—see Fig. 1. Note that all open ladders are nonfrustrated, whereas the periodic and the Möbius ones are frustrated for L odd and even, respectively. The dimensions of the Hamiltonian matrices for singlets are 132 (if $N=12$) up to 1430 (if $N=16$) and for triplets 297 (if $N=12$) up to 3432 (if $N=16$). The exact spectra have been obtained by solving the full eigenvalue problem using the *symmetric group approach* implemented to treat the Heisenberg Hamiltonian eigenequation.^{33,34}

The spectral density distribution moments may be evaluated using the method derived in Ref. 25. In particular, the first moment is equal to

$$\mu_1 = \frac{X+L(L-2)}{L(2L-1)}(3L-a), \quad (24)$$

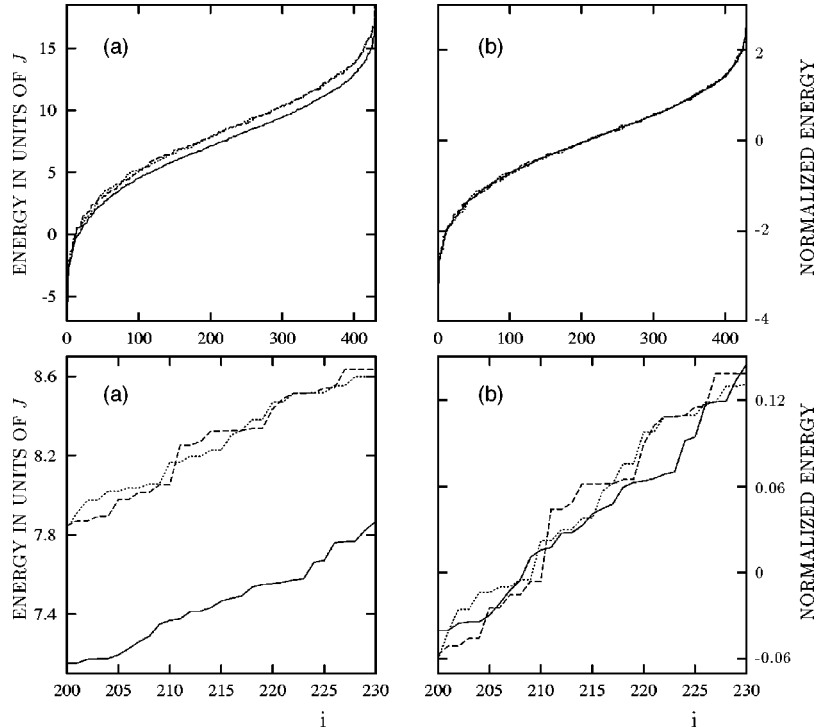


FIG. 2. Unnormalized (a) and normalized (b) spectra (consecutive energy levels E_i plotted versus $i=1,2,\dots,D$) of the Heisenberg Hamiltonians describing the open (solid line), periodic (dashed line), and Möbius (dotted line) ladders for $N=14$ and $S=0$. The unnormalized energy is measured in units of the exchange parameter J ; the normalized energy is measured with respect to μ_1 in units of σ . In the second-row figures magnifications of parts of the spectra are displayed.

TABLE III. The normalized moments $\tilde{\mu}_q[\rho]$.

q	$N = 12, S = 0$			$N = 14, S = 0$		
	Open	Periodic	Möbius	Open	Periodic	Möbius
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
3	-0.2620	-0.2525	-0.2525	-0.2377	-0.2291	-0.2291
4	2.8465	2.8049	2.8049	2.8565	2.8339	2.8339
5	-2.3584	-2.2536	-2.2536	-2.1379	-2.0491	-2.0491
6	13.7157	13.1967	12.9066	13.4876	13.1389	13.1389
7	-21.4516	-20.7972	-19.0952	-19.6378	-18.4070	-18.5961
8	92.4592	88.4496	80.0287	90.9729	85.3752	86.8885
9	-202.9063	-199.0681	-165.2016	-198.2364	-177.4582	-186.5217
10	751.4143	722.8082	592.7546	788.0126	699.3857	743.5555

where $X = S(S+1)$ and

$$a = \begin{cases} 2 & \text{for open ladder,} \\ 0 & \text{for periodic and Möbius lattices.} \end{cases}$$

Asymptotically, for $N \gg 1$

$$\mu_1^P - \mu_1^O \approx 1 + \frac{X}{L^2}, \quad (25)$$

where the superscripts P and O refer, respectively, to the periodic and open ladders. The corresponding expressions for higher moments are given by rather lengthy polynomials in L and X . For $N \gg 1$,

$$\mu_2^P - \mu_2^O \approx 3L \left(1 + \frac{X}{L^2} \right)^2. \quad (26)$$

Then, for given L and S , the average energy and the width of the spectrum of a periodic ladder are larger than those of an open one. The numerical values of the first two moments for the cases studied in this paper are collected in Table I. For the periodic and for the Möbius-type lattices the first moments are the same. In fact, one can easily demonstrate using results of Ref. 25 that the first $L-1$ moments of the periodic ladder and of the Möbius-type chain are the same. Therefore one should expect that also the corresponding spectra are similar and that the similarity increases with an increasing L . In order to study this subject in more detail we evaluated the standard deviations Δ_{A-B}^{LS} between spectra of lattices A and B , where $A, B = O, P, M$:

$$\Delta_{A-B}^{LS} = \sqrt{\frac{1}{D} \sum_{n=1}^D (E_n^A - E_n^B)^2}, \quad (27)$$

where E_n^A/E_n^B stands for the n th energy level in the spectrum of the lattice A/B composed of L segments, i.e., $N = 2L$ spins coupled to the total spin S . The values of Δ are displayed in Table II. As one can see,

$$\Delta_{P-M} \ll \Delta_{O-P} \approx \Delta_{O-M} \quad (28)$$

and

$$\Delta_{P-M}^{7S} \ll \Delta_{P-M}^{6S}, \quad (29)$$

in full agreement with these expectations. This feature of the spectra may be seen even better in Fig. 2(a), where the consecutive energy levels E_n are plotted versus n . Since $\mu_q^P = \mu_q^M$ for $q = 1, 2, \dots, L-1$, the differences between spectra of the periodic and Möbius-type lattices are due to the high ($q \geq L$) moments only. Therefore these differences may be taken as a measure of the upper limit of the accuracy which can be achieved within a low-moment approximation in generation of spectra from the spectral density distributions.

The distribution of the energy level density may be reasonably well approximated by a Gaussian distribution (the density is small at the ends of the spectrum and reaches a single maximum in the middle). In order to compare the “beyond Gaussian” contributions to different spectra, it is convenient to normalize the spectra so that $\mu_1 = 0$ and $\mu_2 = 1$ [it is equivalent to shifting the origin of the energy scale to the average energy and measuring energy in units of the dispersion, cf. Eq. (9)]. The standard deviations between the normalized spectra associated with lattices A and B , denoted δ_{A-B}^{LS} , are displayed in Table II. The normalized spectra are plotted in Fig. 2(b). The results are rather surprising: in most cases, contrary to the expectations based on a naive application of the principle of moments, the difference between the energy level densities of the M - and the P -type lattices are larger than the corresponding differences between the spectral densities of either M and O or P and O type lattices. In fact, differences between all three spectra are very small; they fall within limits of accuracy of a statistical description.

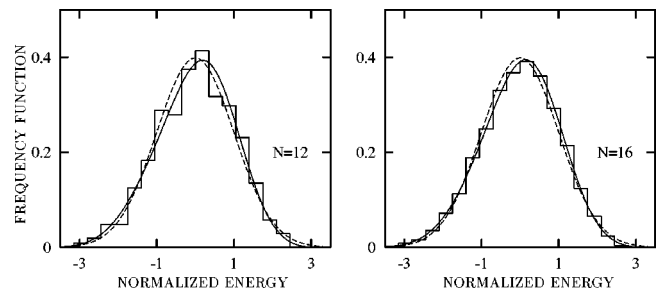


FIG. 3. Exact density distributions of the triplet energy levels of the open-chain Heisenberg Hamiltonians (histograms) compared with the corresponding second- and fifth-moment Gram-Charlier expansions (dashed lines and solid lines, respectively). The energy is measured with respect to μ_1 in units of σ .

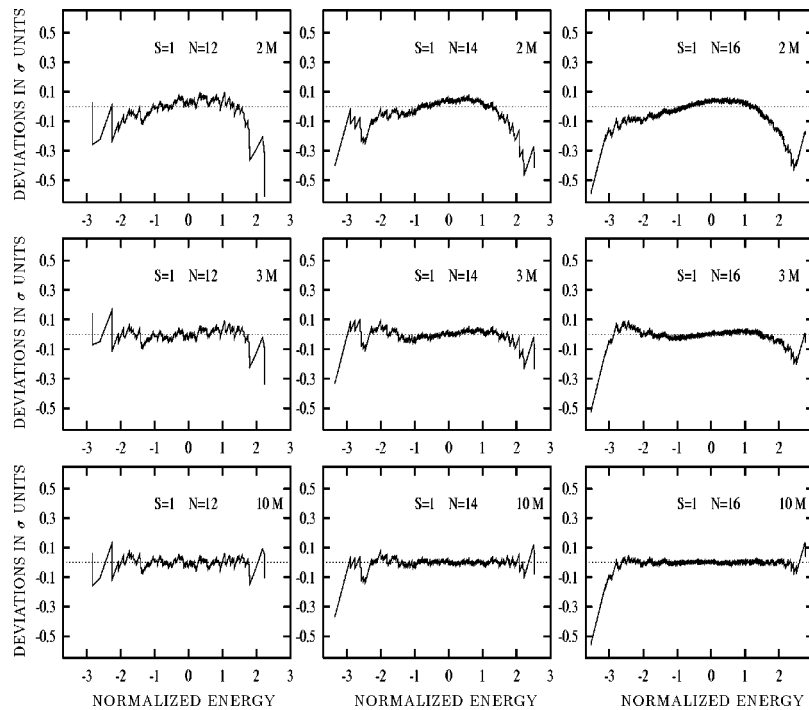


FIG. 4. Differences between the exact energy levels and the energy levels derived from second-, third-, and tenth-moment (designated as 2 M, 3 M, and 10 M, respectively) Gram-Charlier expansions as functions of the normalized energy for the Möbius case. All spectra are normalized so that $\mu_1=0$ and $\mu_2=1$.

The spectral density distribution moments of the normalized spectra are collected in Table III. The values of the corresponding moments for all the cases displayed are similar. We conclude that the exact equality of the higher moments in the case of the periodic and Möbius lattices is not essential for the structure of the corresponding spectra. One may say that the density distributions of the normalized spectra of all three kinds of lattices are not distinguishable on the grounds of statistical spectroscopy.

The histograms of the exact spectral density distributions are compared with the second- and fifth-moment Gram-Charlier approximations in Fig. 3. The Gauss-like shape and increasing accuracy of the approximation with an increase of the lattice size is visible. The approximately Gaussian char-

acter of the distributions seen in the plots is confirmed by an analysis of the data in Table III. The spectral density is nearly symmetric relative to the mean. The skewness parameter γ_1 is small: it varies between -0.26 and -0.23 . The odd moments are all negative. This means that the spectrum extends more towards the small eigenvalues than towards the large ones. The “symmetric part” of the distribution is nearly Gaussian: the moments of the normalized Gauss distribution for $q=4,6,8,10$ are, respectively, equal to $3,15,105,945$, i.e., they are quite close to the corresponding values in Table III and the excess parameter γ_2 varies between -0.20 and -0.15 .

The quality of the moment-generated spectra is analyzed in Figs. 4 and 5. In Fig. 4 differences between the exact

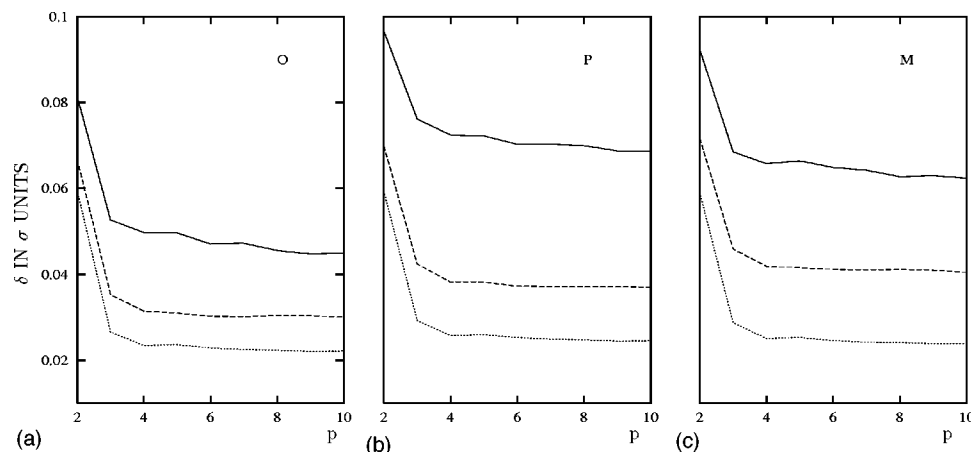


FIG. 5. Standard deviations δ (in units of σ) between the exact and the moment generated singlet spectra as functions of the number of moments p in the corresponding Gram-Charlier expansions for $N=12$ (solid lines), $N=14$ (dashed lines), and $N=16$ (dotted lines). Designations (a) O, (b) P, and (c) M refer, respectively, to the open, periodic, and Möbius-type lattices.

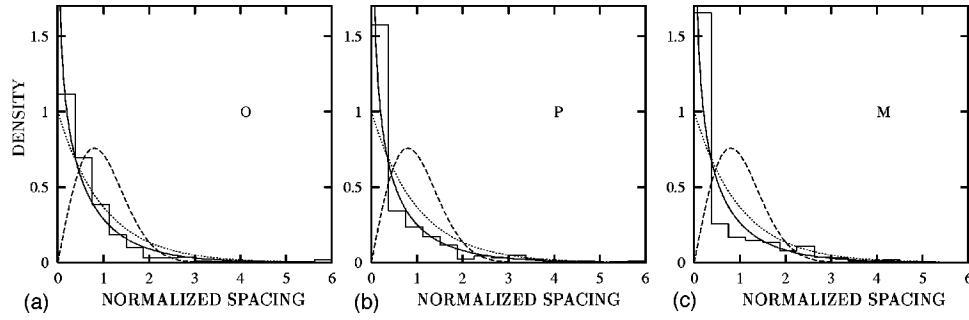


FIG. 6. Nearest-neighbor spacing histograms $\mathcal{P}(x)$ as functions of the normalized spacing x (measured in units of the mean level spacing) in the singlet spectra of $N=14$ (a) open (O), (b) periodic (P), and (c) Möbius (M) lattices compared with $\bar{\mathcal{P}}^D(x)$ (solid line), Poisson (dotted line), and Wigner (dashed line) distribution functions.

energy levels and the ones derived according to Eq. (16) from the smooth (Gram-Charlier) density distribution function are displayed. In Fig. 5 standard deviations between the moment generated spectra and the exact ones are plotted versus the number of moments used to generate the smooth density distributions. As one can see, the quality of the moment-generated spectra dramatically improves when the number of moments increases from 2 to 4. However, with a further increase of the number of moments the quality of the corresponding spectra remains approximately constant. The same behavior of moment generated spectra was discovered earlier in the nuclear spectra² and in the eigenvalues of the Pariser-Parr-Pople Hamiltonian for many-electron systems.²¹ The present result confirms the assumption about a universal character of this behavior of spectra of systems interacting with binary forces.

Figs. 4 and 5 exhibit several properties of the moment-generated spectra of the Heisenberg Hamiltonian.

(i) Quality of the moment-generated spectra is very good in their central parts but strongly deteriorates towards the extremes. This behavior must be attributed to the form of the Gram-Charlier expansion which extends from $+\infty$ to $-\infty$ and does not reflect the fact that a spectrum of an operator represented in a finite-dimensional model space extends over a finite range.²⁵

(ii) The quality of the smoothed spectrum (also in the limit of a large number of moments) improves when the dimension of the lattice increases. This result indicates that for very large lattices, when a diagonalization of the energy matrix is not possible, the moment generated spectra may give a reasonable approximation to the exact ones.

(iii) The higher the symmetry, the lower is the quality of the moment-generated spectrum. This is because the higher the symmetry, the more frequent are clusters of the energy levels in the corresponding spectra. The moment-generated spectra, by construction, do not contain any clusters of the energy levels (unless the density distribution function is highly irregular).

Similar properties were also found in spectra of many-electron systems modeled by the Pariser-Parr-Pople Hamiltonian,²¹ in atomic spectra,⁷ and in nuclear spectra.² Therefore one may assume that they are universal, independent of specific features of the Hamiltonian.

Another measure of the frequency of clusters of the energy levels in spectra is given by the distributions of spacings between neighboring levels. The corresponding histo-

grams for $S=0, N=14$ spectra are displayed in Fig. 6. In all cases the histograms resemble the Poisson rather than the Wigner-type distribution. This behavior should be expected: in all cases the lattices possess some “hidden” constants of the motion related to the spatial symmetries. However, the number of the symmetry operators is much smaller in the case of the open chain than in the cases of the periodic and of the Möbius lattices. Therefore the maximum at $x=0$ is considerably lower in spectrum of the open chain than in spectra of either periodic or Möbius lattices. The maxima of the distributions for small spacings are considerably larger than 1. This means that the tendency of the energy levels to cluster is much stronger than that described by the Poisson distribution. The parameters α and β of distribution $\bar{\mathcal{P}}^D$ defined in Eq. (22) have been obtained using the method of moments and are collected in Table IV. They behave in a regular way as functions of L . Also differences between distributions of spacings between neighboring eigenvalues of the Hamiltonians corresponding to the open ladders and to the periodic or Möbius lattices are clearly seen: $\alpha^O > \alpha^P \approx \alpha^M$ and $\beta^O > \beta^P \approx \beta^M$.

V. CONCLUSIONS

Spectra of the Heisenberg Hamiltonian describing finite lattices exhibit statistical properties similar to those discovered earlier in the nuclear spectra and in spectra of model Hamiltonians modeling many-electron systems.^{2,21} To a good approximation the spectral density distributions are Gaussian. The spectra, in their central parts, may be very well approximated by several-moment Gram-Charlier expansions, however, at the limits (the lowest and the highest eigenvalues) the statistical description is poor. The quality of

TABLE IV. Parameters defining distributions of the neighboring energy levels (in all cases $S=0$).

	L	Open	Periodic	Möbius
α	6	-0.155	-0.254	-0.372
	7	-0.280	-0.381	-0.347
	8	-0.252	-0.374	-0.388
β	6	1.04	0.93	0.83
	7	0.97	0.91	0.94
	8	1.07	0.93	0.94

the statistical description improves with an increase of the number of nodes in the lattice and with the decrease of the spatial symmetry.

The principle of moments has to be used with a great caution. Its application in the case of the lattices considered in this paper may lead to wrong conclusions: spectra of the lattices for which a considerable number of the lowest moments is the same, may differ more from each other than spectra of lattices for which all moments are different.

Distributions of spacings between the neighboring levels,

though they are peaked at 0 and monotonously decrease with increasing spacing, are essentially not Poissonian. They are rather well approximated by an exponential distribution function assuming much larger values for $x \rightarrow 0$ than the Poisson distribution.

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