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LEVEL DENSITY FLUCTUATIONS IN THE 1D HEISENBERG MODEL[1]

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Spectral statistics are applied to study level density fluctuations in the $S = 1/2$ quantum spin chains on a finite lattice under periodic boundary conditions. The use of $P(s)$ and Δ_3 statistical measures for selecting integrable cases of spin exchange interaction is discussed.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR and Universita di Padova, Italy.

О флуктуациях плотности распределения уровней в одномерной модели Гейзенберга

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В работе изучаются статистические свойства флуктуаций плотности уровней квантовых систем спинов 1/2 на конечной решетке. Обсуждается возможность применения $P(s)$ и Δ_3-распределений для исследования вопроса об интегрируемости этих систем для различных форм обменного взаимодействия.

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1. Introduction

The problem of finding integrable models is of current interest in studies of various classical and quantal many-body systems. It is generally believed [1] that the most distinct sign of complete integrability is the existence of an appropriate set $\{I_\alpha\}$ of integrals of motion in involution which can be used for dividing the whole phase space into subspaces with simple dynamics. Apart from certain trivial examples, this procedure is extremely complicated for quantum integrable systems since no quantum analog of classical Liouville theorem has yet been proved.

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When a certain physical model is considered, other criteria are usually required to discover whether it is integrable or not due to the lack of general analytical methods of constructing the integrals $\{I_\alpha\}$ or proof of their absence. The formulation of these criteria based on numerical methods of investigation is relatively clear in classical mechanics [2]. Indeed, many nonintegrable classical systems show chaotic behavior marked by instability under variations of initial data and exponential divergence of nearby trajectories whereas the motion of integrable systems is always confined to invariant tori [3].

In quantum mechanics one cannot apply the classical concepts and methods directly since the notion of trajectory is absent. Nevertheless, many efforts have been made to establish the features of quantum systems which reflect the qualitative difference in the behavior of their classical counterparts [4—6]. Many schematic models [7—9] have shown that this difference reveals itself in the properties of fluctuations in eigenvalue sequences. The spectral statistics for the systems with underlying chaotic behavior agree with the predictions of random matrix theory; by contrast, quantum analogs of classically integrable systems display the characteristics of Poisson distribution.

This important observation leads us to hope that we may select the cases of integrable quantum models or find arguments against integrability by analyzing their discrete spectra.

In this note we attempt to investigate the quantum Heisenberg chains of $S = 1/2$ spins on a finite 1D lattice by using two kinds of statistics, the nearest-neighbor spacing distribution $P(s)$ and the measure of spectral rigidity $\Delta_3(L)$. Unlike previous studies [7—9], there is no classical counterpart of these systems at a fixed value of the spin. Hence they also enable us to check the universality of quantum criterium mentioned above which has a sufficiently strong analytic support only in the semiclassical limit [10].

However, as discussed in great detail in reference [11] there are some deviations for large values of L, in particular for $\Delta_3(L)$. These are related to a breakdown of universal when L becomes larger than a certain correlation length L_{max}. A semiclassical theory which accounts for these non-universal departures has been developed by Berry [11], on the basis of Gutzwiller's periodic orbit theory [12]. It not only gives the same results as the statistical theories for $L \ll L_{max}$, but also predicts the correct asymptotic behaviour for $L \gg L_{max}$, where random matrix theories fail. For the spectral rigidity $\Delta_3(L)$ the semiclassical theory predicts asymptotic saturation both in the regular and in the chaotic region.

2. The Integrability Prolbem for the 1D Heisenberg Model

The magnetic properties of solids have long been studied by using the lattice hamiltonian [13]

$$H_s = \sum_{<j,l>}^{N} h(j-l)\left[\vec{s}_j \vec{s}_l - \frac{1}{4}\right], \tag{1}$$

where $\vec{s}_j = \frac{1}{2}\vec{\sigma}_j$ is 2x2 matrix of the spin operator located at a site j, the sum runs over all pairs of sites $<j,l>$ and the strength of spin interaction is given by exchange integrals $\{h(j)\}$. The set $\{h(j)\}$ is usually chosen in such a way as to satisfy periodic boundary conditions and quantities like free energy should be calculated first for finite systems of N spins. The results of interest for physical applications are obtained in the thermodynamical limit as $N \to \infty$.

The operators can be treated as 2^N x 2^N hermitian matrices with a complicated structure defined by $\{h(j)\}$. The investigation of the possibilities of their analytical diagonalization began with H.Bethe's seminal paper [14] devoted to the eigenproblem for hamiltonian (1) in the case of nearest-neighbor spin interaction,

$$h(j) = J\left[\delta_{|j|,1} + \delta_{|j|,N-1}\right]. \tag{2}$$

The solution can be descibed as follows. Let $|0>$ be a ferromagnetic ground state with all spins aligned along z-axis,

$$|0> = \bigotimes_{j=1}^{N} \begin{pmatrix}1\\0\end{pmatrix}_j .$$

The whole space of the spin lattice states with the dimension 2^N is easily divided into subspaces $\{\Omega_M\}$ with basis vectors $|n_1 \ldots n_M>$ of the form

$$|n_1 \ldots n_M> = \left(\prod_{l=1}^{M} s^-_{n_l}\right) |0>, \tag{3}$$

where $s^-_k = s_{kx} - is_{ky}$ turns kth spin down and $1 \le n_1 < n_2 \ldots < n_M \le N$.. The matrix of (1) is block diagonal since exchange interaction conserves the number of overturned spins M. The eigenstates are constructed as linear superpositions of (3),

$$\left|\psi\right\rangle = \sum_{n_1<n_2\ldots<n_M} \psi\left(n_1\ldots n_M\right)\left|n_1\ldots n_M\right\rangle . \tag{4}$$

According to Bethe's empirical guess, the functions $\psi\left(n_1\ldots n_M\right)$ are given for the exchange (2) by symmetrized combinations of plane waves $\left\{\exp\left(i\sum_{j=1}^{M} k_j n_j\right)\right\}$. It shows that in this particular case there is no diffraction in the scattering of M simplest spin excitations. More than thirty years later it was interpreted as the presence of hidden symmetry. The commutative ring of N functionally independent operators, which includes the hamiltonian, was found within the framework of the transfer matrix method [15].

In the last few years much attention has been paid to the generalization of the Bethe result to cases of more complicated exchange. As has been claimed in [16], integrability might also take place for interaction of nearest and next-nearest spins given by

$$h(j) = J\left[\delta_{|j|,1} + \delta_{|j|,N-1} + \lambda\left(\delta_{|j|,2} + \delta_{|j|,N-2}\right)\right] \tag{5}$$

at arbitrary values of the coupling λ. The arguments of the author of ref. [16], however, would seem to be quite insufficient. They were based only on the treatment of two spin waves analogously to usual two-particles scattering. The corresponding S matrix is, of course, scalar and obeys Yang — Baxter equations [15] but it does not guarantee the absence of diffraction if the number of interacting spin waves exceeds two. So far no explicit solution has been found even in the $M = 3$ sector at a certain nonzero value of λ, neither has it been possible to construct examples of integrals of motion. The instability of properties of the ground state under variations of λ found numerically in [17] would tend rather to indicate the nonintegrability of the model.

Another way to overcome the restriction to nearest-neighbor exchange (2) is connected with the remarkable analogy between $\psi\left(n_1\ldots n_M\right)$ in (4) for the Bethe case and wave functions of the M-particle problem on a continuous line with pair interaction $V(x) \sim \delta(x)$ [18]. There are several integrable many-particle systems of that type [19] and the most general ones correspond to the two-body elliptic potential $V(x) \sim \wp_{\omega_1,\ \omega_2}(x)$, where $\wp_{\omega_1,\ \omega_2}$ is the Weierstrass elliptic function with two periods ω_1 and $i\omega_2$ $\left(\omega_1, \omega_2 \in \mathrm{R}\right)$,

$$\wp_{\omega_1,\ \omega_2}(x) = \left(\frac{\pi}{\omega_2}\right)^2 \left\{ -\frac{1}{3} + \sum_{m=-\infty}^{\infty} \left[\sinh\left(\pi\,\frac{x - m\,\omega_1}{\omega_2}\right)\right]^{-2} - \right.$$

$$\left. - 2\sum_{m=0}^{\infty} \left[\sinh\left(\pi\,\frac{m\,\omega_1}{\omega_2}\right)\right]^{-2} \right\}. \qquad (6)$$

It has been proposed that precisely the same form of spin exchange leads to integrable models on a 1D lattice if the real period of the $\wp$ function coincides with the number of lattice sites [20],

$$h(j) = J\,\wp_{N,\,\omega_2}(j)\,. \qquad (7)$$

As $\omega_2 \to 0$, it gives the nearest-neighbor exchange (2) after proper renormalization of the coupling J. The complete commutative ring of integrals of motion has not yet been constructed, but there are some examples of these operators,

$$I_3(\alpha) = \sum_{j\neq k\neq l}^{N} f_{jk} f_{kl} f_{lj} \left(\mathbf{s}_j \times \mathbf{s}_k \times \mathbf{s}_l\right),$$

$$I_4(\alpha) = \sum_{j\neq k\neq l\neq m}^{N} \left[f_{jl} f_{lk} f_{km} f_{mj} + f_{jm} f_{mk} f_{kl} f_{lj}\right] \left(\mathbf{s}_j \mathbf{s}_k\right)\left(\mathbf{s}_l \mathbf{s}_m\right) +$$

$$+ 2\sum_{j\neq k}^{N} \left(f_{jk} f_{kj}\right)^2 \left(\mathbf{s}_j \mathbf{s}_k\right),$$

where $f_{jl}(\alpha) = \dfrac{\sigma(j - l + \alpha)}{\sigma(j - l)} \exp\left[-\left(j - l\right)\zeta(\alpha)\right]$, α is an arbitrary parameter and the Weierstrass functions $\zeta(x)$, $\sigma(x)$ are expressed through $\wp(x)$ as

$$\zeta(x) = x^{-1} + \int_0^x \left[x^{-2} - \wp(x)\right] dx, \quad \sigma(x) = x \exp\left[\int_0^x \left(\zeta(x) - x^{-1}\right) dx\right].$$

Although non-diffractive behavior has been established for the scattering of an arbitrary number of spin waves on a infinite lattice, the rigorous proof of the integrability of the model (7) in the most important case of finite N and ω_2 has not yet been found.

To conclude this section, it is worth noting that a statement such as «the quantum system is integrable» can be confirmed, at least in principle, by direct analytic construction of integrals of motion. The contrary statement evidently needs other criterium for its verification. If the concept of «quantum chaos» is to some extent universal, it is natural to expect that discrete spectra of nonintegrable cases of (1) might display the peculiarities of random matrix fluctuations. The possibility of applying this criterium is studied in the best section for all three previously discussed forms of exchange interaction.

3. The Procedures and Results of Calculations

The dimension of matrices corresponding to (1) grows exponentially with the number of interacting spins. To avoid the enormous consumption of computer time and obtain a reasonable number of levels for statistical analysis, we chose for numerical procedures the $M = 6$ sector of the model on the lattice with 12 sites. The total number of basis vectors (3) in the case is $C^6_{12} = 924$. The action of the hamiltonian (1) on these vectors is given by

$$H_s \left| n_1 ... n_M \right\rangle = \left[\sum_{j \neq k}^{M} h\left(n_j - n_k\right) - M \sum_{j=1}^{N-1} h(j) \right] \left| n_1 ... n_M \right\rangle + \\ + \sum_{k \neq n_1 ... n_M}^{N} \sum_{s=1}^{M} h\left(n_s - k\right) \left| n_1 ... n_{s-1}\, k n_{s+1} ... n_M \right\rangle . \qquad (8)$$

The matrices with elements determined by (8) have been diagonalized numerically by a standard routine [22]. Most of their eigenvalues are double degenerated due to left-right symmetry in spreading spin excitations over

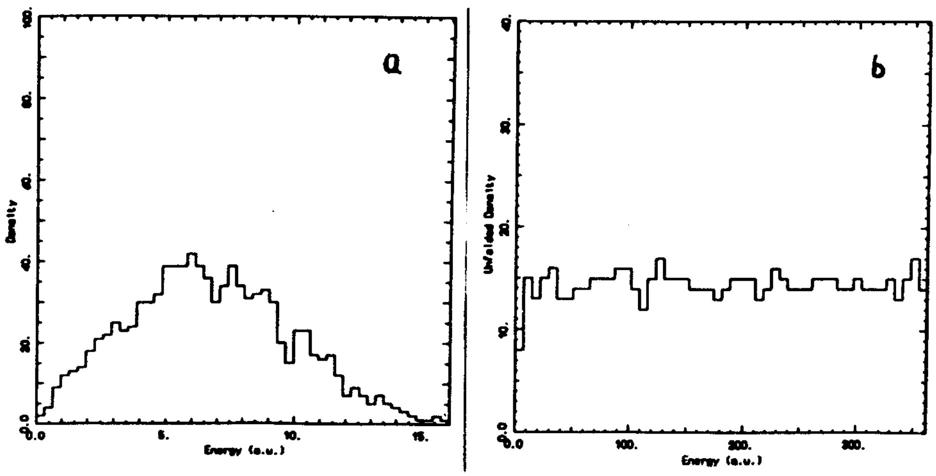

Fig.1. The density of levels: (a) before (b) after the unfolding procedure for nearest-neighbor exchange (2)

the lattice. In fact, it is easy to show that if $|\psi\rangle$ is an eigenvector of the hamiltonian (1) of the type (4) with some $\{\psi(n_1...n_M)\}$, then $|\psi\rangle = \sum_{1 \le n_1...n_M \le N} \psi(\tilde{n}_1...\tilde{n}_M) \times |n_1...n_M\rangle$ $(\tilde{n}_j = N + 1 - n_j)$ also obeys the eigenvalue condition with the same energy. This kind of symmetry can be used, in principle, to reduce the dimension of matrices accompanied, however, by a complication of their structure. An equivalent procedure for obtaining the spectra with removed symmetry consists of eliminating one element of each pair of coinciding eigenvalues obtained by diagonalization of the hamiltonians using a total set of basis states (3).

The level densities are approximately of the Gaussian form (Fig.1a) for all three forms of spin interaction used in our calculations. By performing the unfolding procedure descibed in detail in ref. [21], each spectrum has been mapped into one with the quasiuniform level density (Fig.1b).

The nearest-neighbor spacings were calculated and histogrammed in units of mean spacing so as to show the $P(s)$ distribution for $s \le 4$

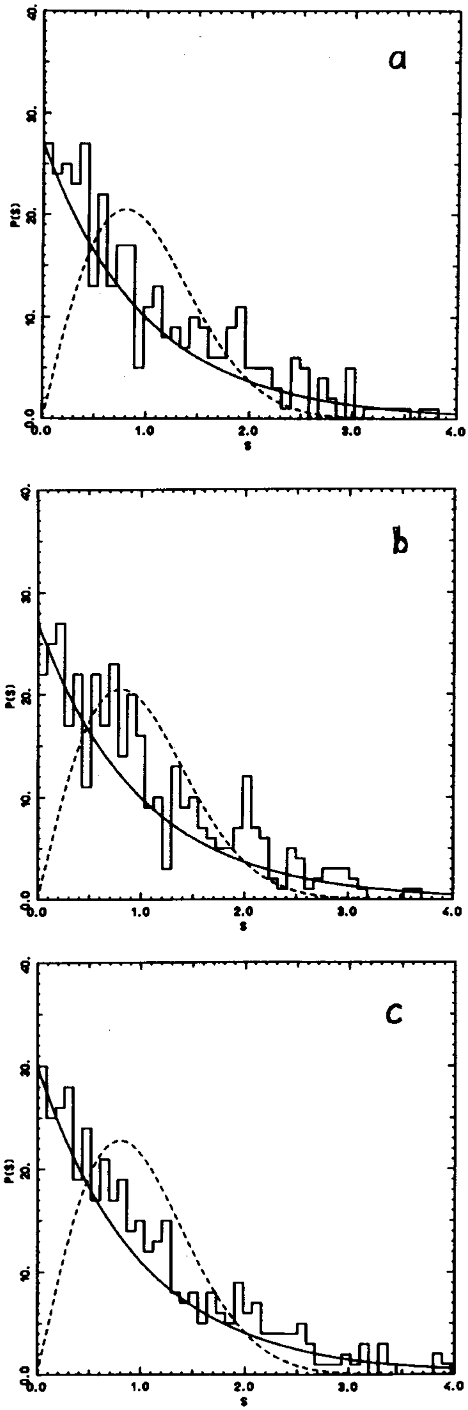

Fig.2. The histograms of nearest-neighbor level spacings $P(s)$: (a) the Bethe case (2); (b) the elliptic exchange (7), $\omega_2 = \pi$ (c) the case of nearest and next-nearest spin interaction (6) at $\lambda = -1$. The solid lines correspond to the Poisson distribution normalized by the first bins.

(Fig.2). As can be seen, there are large fluctuations around the Poissonian line, $P(s) = A\exp(-s)$, A being determined by the first bin, for both integrable cases (a—b). In the last example (2c), where the coupling was chosen so as to magnify the role of next-nearest-neighbor exchange, the data exceed the Poisson distribution normalized analogously. The best exponential fit which would probably show some lack of events near $s = 0$ was not performed. It is clear, however, that the data are not consistent either with the Wigner distribution given by the random matrix theory since there is no indication of the strong level repulsion.

The results concerning the second statistical measure $\Delta_3(L)$ (the best fit of the spectral staircase function by a straight line on a fixed interval) are plotted in Fig.3. The error bars were obtained by varying the positions of the ends of the interval on which the spectral rigidity was calculated.

In cases (a—b) the data display behavior intermediate between the Poisson distribution $\frac{1}{15}L$ and GOE predictions (Fig.3a—b). Within the interval $6 \le L \le 11$ the $\Delta_3(L)$ values of the integrable cases are closer to the Poisson line than to the GOE one. In the whole range of $L \ge 6$ they

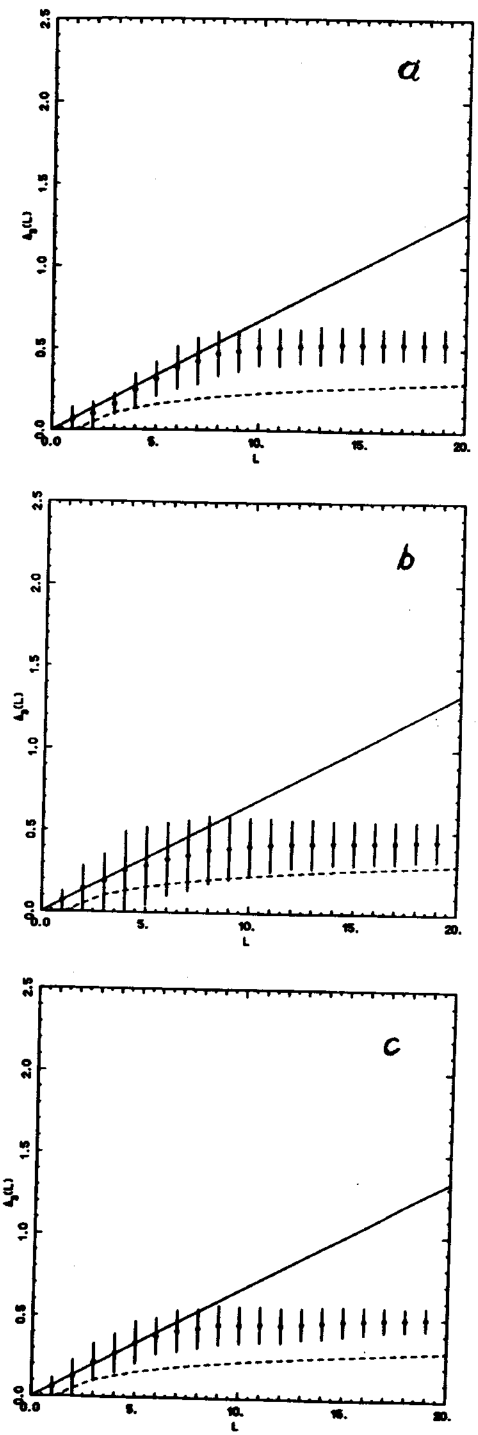

Fig.3. The spectral rigidity $\Delta_3(L)$ for the same three cases as in Fig.2. The solid and dashed lines show the Poisson and GOE distributions

exceed systematically the corresponding values for the interaction of the form (5) at $\lambda = -1$ (Fig.3c). The latter show a tendency to be more consistent with GOE than with the Poisson form of the $\Delta_3(L)$ measure.

4. Discussion

The reasons for the ambiguity of the results listed and briefly discussed above seem to be twofold. First, the systems of $S = 1/2$ spins are of an extreme quantal nature. A certain classical analog, of course, can be constructed in the limit $S \to \infty$ by replacing quantum operators $\{S\langle S^2\rangle^{-1/2}\}$ by the vectors on unit sphere as was done in [23] for two-spin system but the treatment of higher spins may lead to the loss of integrability. Second, even in classical mechanics there are examples demonstrating the ambiguities of numerical analysis. More than ten years ago the authors of ref. [24], after studying Poincare sections in a very wide range of energies, claimed that the transition from the exponential Toda to Morse pair potential conserves integrability in a three-particle problem on a line. There has so far not been any analytic support for such a claim.

The intermediate character of the $P(s)$ and $\Delta_3(L)$ behavior was reported earlier in the paper [8] devoted to a simple mechanical system with two degrees of freedom. It was also found in the study of quantum billiards on the pseudosphere by using a much more extensive set of levels [25].

In conclusion, we should mention that our results do not indicate a sharp transition from the «regular» to «chaotic» regime under variations of the form of exchange interaction in a spin lattice model. The tendency to the GOE statistics can be seen in the case (4) at $\lambda = -1$ which seems to be nonintegrable. Perhaps the whole integrability problem for this type of model cannot be completely disentangled by statistical analysis of level sequences.

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