Multifractality of eigenfunctions in spin chains

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We investigate different one-dimensional quantum spin-1/2 chain models and by combining analytical and numerical calculations prove that their ground state wave functions in the natural spin basis are multifractals with, in general, non-trivial fractal dimensions.

One-dimensional quantum spin chains are among the oldest and the most investigated fundamental models in physics. Introduced as toy-models of magnetism [1], they quickly became a paradigm of quantum integrable models (see e.g. [2]-[5]). A prototypical example is the XYZ Heisenberg model [1] for $N$ spins-$1/2$ in external fields with periodic boundary conditions

$$
\mathcal{H} = -\sum_{n=1}^{N} \left[ \frac{1 + \gamma}{2} \sigma_n^x \sigma_{n+1}^x + \frac{1 - \gamma}{2} \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z \right] + \lambda \sigma_n^z + \alpha \sigma_n^x
$$

and its various specifications for different values of parameters. $\sigma_n^x,y,z$ are the Pauli matrices at site $n$.

In the natural basis of $z$-components of each spin, $|\vec{\sigma}\rangle = |\sigma_1, \ldots, \sigma_N\rangle$ where $\sigma_j = \pm 1$, any Hamiltonian of $N$ spins-$1/2$ is represented by a $M \times M$ matrix with dimension $M = 2^N$. Many different methods were developed to determine exact spectra of such matrices [2]-[5]. The calculation of eigenfunctions is more involved. A wave function of $N$ spins-$1/2$ in the spin-$z$ basis can be written as

$$
\Psi = \sum_\vec{\sigma} \Psi_\vec{\sigma} |\vec{\sigma}\rangle
$$

where the summation is taken over all $M = 2^N$ configurations with $\sigma_j = \pm 1$. In general, coefficients $\Psi_\vec{\sigma}$ can be found only after the matrix diagonalization which for large $N$ is a hard numerical problem. Even in integrable cases eigenfunctions of spin chains look erratic (cf. figures below) and their structure is not well understood.

The purpose of this letter is to prove that ground state (GS) wave functions for different one-dimensional spin chain models are multifractals in the spin-$z$ basis.

Multifractality is a general notion introduced to characterize strong and irregular fluctuations of various quantities [3]-[5]. For eigenfunctions like in (2) one uses the following definition (see e.g. [3] and references therein).

Let $S_R(q, M)$ be the Rényi entropy for an eigenfunction (2) of a matrix of finite size $M$

$$
S_R(q, M) = -\frac{1}{q-1} \ln \left( \sum_\vec{\sigma} |\Psi_\vec{\sigma}|^{2q} \right)
$$

with normalized coefficients $\Psi_\vec{\sigma}$, $\sum_\vec{\sigma} |\Psi_\vec{\sigma}|^2 = 1$.

Fractal dimensions, $D_q$, are defined from the behaviour of the Rényi entropy (3) in the limit $M \to \infty$

$$
D_q = \lim_{M \to \infty} \frac{S_R(q, M)}{\ln M}.
$$

The case when $D_q$ is a non-linear function of $q$ corresponds to a multifractal irregular behaviour.

Fractal dimensions give a concise description of wave function moments and are important characteristics of eigenfunctions but it seems that they were overlooked in previous studies. For example, the Rényi and Shannon entropies are calculated for GS wave functions of certain spin chains in [10]-[13] but terms linear in $\ln M$ which determine $D_q$ in (4) were regularly ignored and only next-to-the-leading terms have been investigated as it is usual in conformal field theories. To the best of authors’ knowledge only a recent paper [14] briefly mentioned the existence of multifractality in a spin chain model.

The simplest method to find fractal dimensions is the direct numerical calculation of the GS wave function for different number of spins and a subsequent extrapolation of the Rényi entropy for large $M$. Definition (4) is well suited for positive $q$. For many problems (but not for all) fractal dimensions can be calculated also for negative $q$ [15, 16]. Of course, if certain coefficients in (2) are zero due to an exact symmetry, they are not included in the calculation of the Rényi entropy (3) for $q \leq 0$.

In what follows we investigate various specifications of the Heisenberg model (1) and by combining numerical and analytical methods demonstrate that the multifractality of GS is a generic property of all of them. We choose $\gamma \geq 0$ and $\alpha \geq 0$ to ensure off-diagonal terms of Hamiltonian matrices (1) to be non-positive which, by the Perron-Frobenius theorem, implies that coefficients $\Psi_\vec{\sigma}$ in (2) for the GS wave function are non-negative. For many problems (but not for all) fractal dimensions can be calculated also for negative $q$ [15, 16]. Of course, if certain coefficients in (2) are zero due to an exact symmetry, they are not included in the calculation of the Rényi entropy (3) for $q \leq 0$.

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The quantum Ising model in transverse field [17] is a standard model of quantum phase transitions [18]. It corresponds to the Hamiltonian (1) with $\Delta = \alpha = 0$ and $\gamma = 1$. Its spectrum can be found analytically by the Jordan-Wigner transformation [3] and coefficients $|\Psi_\vec{\sigma}|^2$ are given by the determinant of $N \times N$ matrices [3, 11].
Fractal dimensions of GS wave function for this model computed numerically from linear extrapolation of the Rényi entropy with \( N = 3 - 11 \) are presented in Fig. 1 for a few values of transverse field \( \lambda \). The curves of \( D_q \) as a function of \( q \) for all models have the same characteristic form as for other fractal measures \([7]\). In particular, when \( q \to \pm \infty \) they tend to well defined limits \( D_{\pm \infty} \).

Generalizing results of \([11]\), one gets the exact expressions for limiting values \( D_{\pm \infty} \) and for \( D_{1/2} \)

\[
D_{\pm \infty}(\lambda) = \frac{1}{2} - \frac{1}{2\pi} \ln 2 \int_0^\pi \ln \left[ 1 \pm \frac{\lambda - \cos u}{\sqrt{R(\lambda, u)}} \right] du, \quad (5)
\]

\[
D_{1/2}(\lambda) = 1 - D_{\infty}\left( \frac{1}{\lambda} \right), \quad R(\lambda, u) = 1 - 2\lambda \cos u + \lambda^2.
\]

These formulas prove that fractal dimensions of quantum Ising model are non-trivial. In Fig. 2 these exact expressions are plotted together with numerically calculated points for different \( \lambda \). \( D_{\pm \infty} \) are obtained by a fit \( D_{\pm \infty} + a/q + b/q^2 \) for large \( q \) parts of curves similar to Fig. 1. The good agreement between Eqs. (5) and numerics shows that though we obtain fractal dimensions from relatively small number of spins our results are reliable.

The above curves are qualitatively the same for non-critical and critical (that is \( \lambda = 1 \)) quantum Ising model. Nevertheless, as illustrated in the inset of Fig. 2 the sum of \( D_{\infty} \) and \( D_{-\infty} \) has clear singularity in the critical point in accordance with the relation

\[
D_{-\infty}(\lambda) + D_{\infty}(\lambda) = \begin{cases} 
\frac{2}{\ln |\lambda|}, & |\lambda| < 1 \\
\frac{2}{\ln 2} \left( |\lambda| > 1 \right) 
\end{cases} \quad (6)
\]

which follows from \([5]\). It means that criticality can be observed in fractal dimensions of GS.

The XY model is a specification of \([11]\) with \( \Delta = 2 \) and \( \gamma \neq 1 \). Similar to the quantum Ising model this model is also integrable by the Jordan-Wigner transformation \([3, 11]\) but the structure of its GS is more complicated. An interesting special case is \( \lambda = \lambda_f \) where \( \lambda_f = \sqrt{1 - \gamma^2} \).

It is known \([14]\) that at that field the XY model has two exact factorized GS wave functions

\[
\Psi = \prod_{n=1}^{N} (\cos \theta |1\rangle + \sin \theta |-1\rangle), \quad \cos^2 2\theta = \frac{1 - 2\gamma}{1 + 2\gamma}. \quad (7)
\]

For states with definite parity and \( \lambda = \lambda_f \) fractal dimensions are described by a formula

\[
D_q = -\frac{\ln(\cos^2 2\theta + \sin^2 2\theta)}{(q - 1) \ln 2} \quad (8)
\]

The XY model with anisotropy \( \gamma = 1.4 \). Red line: \( \lambda = 1.6 \), black line: \( \lambda = 1 \), blue line: \( \lambda = 0.4 \). Dashed black line shows for comparison the exact fractal dimensions \([5]\) for \( \lambda = 0.8 \) and \( \gamma = 0.6 \). Inset: GS coefficients for \( \lambda = 0.4 \), \( \gamma = 1.4 \) and \( \lambda = 0.8 \), \( \gamma = 0.6 \).
indicated for $\gamma = 0.6$ and $\lambda = 0.8$ by dashed black line in Fig. 3. This example proves that at least at the factorizing field fractal dimensions of the GS wave function do exist and correspond to the well-investigated case of binomial measures 13.

As for $\lambda^2 + \gamma^2 < 1$ there exist many crossings of lowest states with different parity, for numerical calculations (performed as in the Ising model) we choose $\lambda$ and $\gamma$ outside the unit circle, $\lambda^2 + \gamma^2 > 1$. The results are presented in Fig. 4 and are qualitatively similar to the Ising model.

One may argue that the limiting values, $D_{-\infty}$ and $D_{-\alpha}$ as in the quantum Ising model should correspond to configurations with, respectively, all spins up and all spins down, and, consequently, are expressed similar to (5) as

$$D_{\pm}(\lambda, \gamma) = \frac{1}{2} - \frac{1}{2\pi \ln 2} \int_{-\infty}^{\infty} \ln \left[ 1 + \frac{\lambda - \cos u}{\sqrt{R_{\pm}(\lambda, \gamma, u)}} \right] du (9)$$

with $R_{-}(\lambda, \gamma, u) = (\lambda - \cos u)^2 + \gamma^2 \sin^2 u$. But for small $\lambda$ the minimal contribution is instead given by the antiferromagnetic Néel configuration with alternating spins, $\sigma_n = (-1)^n$. Using the asymptotics of the block Toeplitz matrices [20] we get

$$D_{\text{Néel}}(\lambda, \gamma) = \frac{3}{4} - \frac{1}{2\pi \ln 2} \int_{-\infty}^{\pi/2} \ln \left[ 1 - \frac{\lambda^2 + \gamma^2 - (1 + \gamma^2) \cos^2 u}{\sqrt{R_{-}(\lambda, \gamma, u)}} \right] du (10)$$

where $R_{-}(\lambda, \gamma, u) = (\lambda + \cos u)^2 + \gamma^2 \sin^2 u$. This result for $\gamma = 1.4$ is presented in Fig. 3 by the black line. When $D_{\text{Néel}} > D_{-\infty} = D_{\text{Néel}}$, otherwise $D_{-\infty} = D_{-\alpha}$. For $\gamma = 1.4$ these curves intersect at $\lambda \approx 0.4982$ and $D_{-\infty}$ has the form indicated in Fig. 4 by solid blue and black lines. Numerical results agree well with this prediction.

The Ising model in transverse and longitudinal fields is obtained by adding to the quantum Ising model a longitudinal field $\alpha$. For non-zero $\alpha$ the only known integrable case corresponds to $\lambda = 1$ [21]. This model attracts recently wide attention as certain consequences of its integrability have been checked experimentally in the cobalt niobate ferromagnet [22]. In Fig. 5 the fractal dimensions for a few values of both fields are presented.

As a reference we use $\Delta = -\frac{1}{2}$ called combinatorial point. From the Razumov–Stroganov conjecture proved in [25] it follows that at such $\Delta$ and odd $N = 2R + 1$ the following statements are valid: (i) the GS energy is $-3N/4$, (ii) the largest coefficient in the expansion (2) (the one for the Néel configuration) equals

$$\Psi_{\text{max}}^{-1} = \frac{3^{R/2} \cdot 5 \ldots (3R - 1)}{2^R \cdot 1 \cdot 3 \ldots (2R - 1)},$$

(iii) the smallest coefficient corresponding to a half consecutive spins up and other spins down is $\Psi_{\text{min}}^{-1} = \Psi_{\text{max}}^{-1} A_R$, and (iv) $\sum_{\sigma} \Psi_{\sigma} = 3^{R/2}$. Here $A_R$ is the number of alternating sign matrices [26].

These formulas prove that for $\Delta = -\frac{1}{2}$ fractal dimensions $D_{\infty}$ and $D_{1/2}$ are explicitly known

$$D_{\infty} = \frac{3 \ln 3}{2 \ln 2} - 2 \approx 0.377, \quad D_{1/2} = \frac{\ln 3}{2 \ln 2} \approx 0.792. \quad (12)$$

When $R \to \infty$, $\ln A_R = R^2 \ln(3\sqrt{3}/4) + O(R)$. Such quadratic in $N$ behaviour is a particular case of the emptiness formation probability of a string of $n$ aligned spins with $n \sim N^{2/3}$. This asymptotics means that
negative moments of the GS wave function in antiferromagnetic case require a scaling different from $\gamma_-$ and hence will not be considered here. The fractal dimensions for a few values of parameter $\Delta$ are presented in Fig. \ref{fig:fractal_dim}. The numerical calculations were performed by extrapolation of the Rényi entropy separately for odd and even $N = 3 - 13$. With available precision, fractal dimensions for odd and even $N$ are the same but sub-leading terms in the Rényi entropy \cite{30} are different.

- **The XYZ model** differs from the XXZ model by anisotropy $\gamma \neq 0$ in the $(x,y)$ plane. In zero fields its GS wave function has been found \cite{31}. A soluble example with factorized GS \cite{32} is $\alpha = 0$, $\lambda = \lambda_f$ \cite{19} where

$$
\lambda_f = \sqrt{(1 - \Delta)^2 - \gamma^2}, \quad \cos^2 2\theta = \frac{1 - \gamma - \Delta}{1 + \gamma - \Delta}.
$$

At this field GS wave function corresponds to the binomial measure and fractal dimensions are given by \cite{33}.

The combinatorial point for the XYZ model in zero fields where an additional information about GS is known (or conjectured) is $\Delta = (\gamma^2 - 1)/2$ \cite{24}. In Fig. \ref{fig:fractal_dim_xyz} we present fractal dimension in the zero fields XYZ model with $\gamma = 0.6$ for a few values of $\Delta$ including the combinatorial point. Qualitatively the curves are similar to the XXZ model and to $D_q$ with positive $q$ for the XY models.

- **Summary.** Wave functions are the most fundamental objects of any quantum-mechanical model. For many-body problems their structure is complicated and numerous questions remain open. We consider here practically all standard one-dimensional spin-$z$ models and demonstrate that their GS wave functions in the natural spin-$z$ basis are multifractals with, in general, non-trivial fractal dimensions. For special values of parameters and/or certain dimensions we get exact analytical formulas which prove rigorously the existence of fractal dimensions. In other cases we rely on numerical calculations. The multifractality in spin chains is a very robust phenomenon. It exists for integrable and non-integrable models, for ferro and anti-ferro magnetic states, as well as for critical and non-critical systems.

A common point of all these models is that their $M \times M$ Hamiltonian matrix in spin-$z$ basis is such that in each row and column there exist only $K \sim \ln M$ non-zero matrix elements of the same order. As $M \gg K$ this specific form resembles a tree structure with branching number $K$. As $K \to \infty$ when $M \to \infty$ and it is known \cite{30, 31} that on a tree with large branching number (with other parameters fixed) the Anderson localization is unlikely, states are delocalized. On the other hand, the full ergodicity on a tree is, in general, also improbable \cite{31}. The remaining possibility corresponds to delocalized but not ergodic states, i.e. to multifractality, which may explain its ubiquity. The multifractality is related finally not with explicit randomness but with internal complexity of models considered. Such arguments are not restricted to one dimension and/or spin chains but can be applied to various many-body problems with local interactions and we conjecture that multifractality (i.e. a non-trivial scaling of different quantities with the number of particles) is a generic property of a large class of many-body models.

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