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Spectra of Nonlocally Bound Quantum Systems

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Abstract. We discuss a class of nonlinear and nonlocal models for the dynamics of a composite quantum system. The models in question depend on the following constituents: on two subsystem Hamiltonians (denoted by H and $\hat{H}$), an analytic function (f), and a real parameter (s). As demonstrated elsewhere before, the stationary states can be described in these models fairly explicitly. In this article, we build upon that result, and discuss the topological as well as statistical characteristics of the spectra. Here, we concentrate on the special case $f = \log$. It turns out that an energy spectrum of the nonlocally bound system substantially differs from that of its components. Indeed, we show rigorously that, if H is the harmonic oscillator and $\hat{H}$ is completely degenerate with one energy level, then the energy spectrum of the composite system has the topology of the Cantor set (for $s > 2$). In addition, we show that, if H is replaced by the logarithm of the harmonic oscillator, then the spectrum consists of finitely many intervals separated by gaps (for s sufficiently large). In the last case, the key analytic object is the series $\sum n^{-s}$. In particular, as an interesting offshoot, this structure furnishes a nontautological immersion of fundamental number-theoretic functions into the quantum formalism.

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1. INTRODUCTION

In this article, we examine the spectra of quantum systems modelled by a special type of nonlinear, nonlocal, and nondissipative dynamics defining the evolution of a quantum state. We claim that these systems can be designed, by an appropriate choice of the model constituents, to have a rich spectral structure, for example, of a Cantor-set type, of a union of intervals interspersed with band-gaps, or of discrete type. Our analysis is based on the characterization of stationary states obtained in [1].

It seems helpful to begin with a few examples of spectra of microscopic and mesoscopic objects. Objects like molecules, quantum dots, or atomic nuclei have discrete energy spectra, but their complexity varies from fairly simple (atoms) to very complex (molecules). Next, crystals and metalattices, characterized by periodic potentials, have spectra that comprise quasi-continuous intervals interspersed with energy gaps. Moreover, when lattices are coupled to an external magnetic field, the resulting spectrum, in some regimes, may take the form of a topologically nontrivial Cantor set [2]. Another interesting example is that of the Josephson–junction circuits, whose importance is underscored by a suggested application to superconducting qubit quantum computing [3]. The spectra depend on the device architecture, e.g., the spectrum in the *flux qubit* regime is simply discrete, whereas in the *phase qubit* regime the spectrum consists of continuous-energy bands interspersed with segments containing discrete energy levels, see, e.g., [4]. In addition, the spectra of *small superconducting islands* are essentially discrete but display broadening due to the presence of low-lying quasi-particle states [5].

In very many instances of structure calculations, the spectra of a quantum system are determined via an eigenvalue problem for a single-particle Schrödinger operator. This linear differential operator is obtained via quantization of the classical model. The potential function alone decides the complexity of the spectrum, but its effect can be quite subtle, so that even a seemingly minor alteration can give a strong effect. This is well illustrated by the famous Hénon–Heiles dynamics, see, e.g., [6]. In this example, in spite of the relative simplicity of the potential, the spectrum is fairly complex, and its eigenvalues may be divided into two types; this reflects the presence of chaos in the underlying classical system. In general, the problem of determining the spectrum is highly

nontrivial. The effective solutions typically rely on approximate methods, like semi-classical ones, and some of these approaches have been developed only recently. Examples include the Gutzwiller formulas, [7, 8, 9], and the method of approximate eigenfunctions, which is based on Maslov's canonical operator, [10, 11, 12]. An interesting point of view at the semiclassical machinery is discussed in [13].

However, not all quantum dynamics comes from quantization. A notable exception is encountered in the framework of cavity QED, particularly the Jaynes–Cummings model of interaction of light with an atom in a cavity ([14, 15]). The Jaynes–Cummings model relies on composite system theory. The system in question consists of two subsystems, namely, a two-level atom with the energy gap $\hbar\omega_0$, and a harmonic oscillator with energy values $n\hbar\omega$, $n = 1, 2, \ldots$ (the ground state energy $\hbar\omega/2$ is suppressed as unessential). The model introduces an interaction term, and predicts composite eigenstates at the energy levels

$$E_{\pm}(n) = \left(n - \frac{1}{2}\right)\hbar\omega \pm \frac{\hbar}{2}\Omega(n), \quad \text{where } \Omega(n) = \left[(\omega - \omega_0)^2 + 4\lambda^2 n\right]^{1/2}.$$

The energy gaps characteristics of the composite are essentially different than those of either one of its components, and these depend on the coupling constant λ via the Rabi frequencies $\Omega(n)$. The Jaynes–Cummings model is linear; however, it is somewhat conceptually related to the nonlocal dynamics considered in this article.

Nonlocal dynamics, see equation (6), results from a nonlinear perturbation (small or large) of a linear problem, where the perturbation term depends on an analytic function f. In addition, the dynamics *is not* derived via the quantization of a classical problem. Instead, one postulates a nonlinear Hamiltonian dynamics directly in the phase space of the quantum system. Most importantly, the resulting evolution of the subsystems is localized and linear. In other words, the evolution of the reduced density matrices, i.e., the mixed states, only depends on the local Hamiltonians. In particular, there is no transfer of energy from one subsystem to another. This type of separability is necessary for a quantum theory to be realistic. (The reader may wish to refer to [16, 17] for a discussion of general "reality" constraints on nonlocal quantum dynamics.) At the same time, the *global* nonlinearity implies the existence of *nonlocal* stationary states, and thus leads to the notion of nonlocal bonding, first explored in [18]. The nonlocal dynamics seems unique in that it allows for a direct characterization of its stationary states, and subsequently its spectrum. It ought to be emphasized, however, that the description starts at a higher level of generality, as we assume that the "linear part" of the problem is given *a priori* with its spectral decomposition. Given this, the operators that represent stationary states are constructed out of the two subsystem Hamiltonians and the function f. This fact facilitates a rigorous and explicit description of the corresponding nonlocal spectra. As it turns out, the spectra can have an intricate topological structure. Our focus here is on the special case $f = \log$. We show that, for a certain specific choice of the Hamiltonians in (6), the spectrum is a topological Cantor set (more precisely the image of the standard Cantor set under a logarithmic mapping). For another choice of the Hamiltonians, the spectrum is obtained via the set of all subseries (rarefied sums) of the series $\sum n^{-s}$. Remarkably, it turns out that, in this case, the ground state is tied to the sum of the full series, i.e. $\zeta(s)$, [19]. In particular, its energy can be expressed via an integral formula known already to Riemann, which ties the zeta function to the prime-counting function; see formula (30) below. The resulting relation between fundamental number theoretic functions and the ground state is nontautological, namely, the function is not being inserted as a constituent, but rather emerges naturally from the structure of quantum theory and from the specific properties of equation (6). Overall, these examples shed new light at the nature of the nonlocal bonding scenario. In particular, they show that the spectral characteristic of a nonlocally bound system typically is drastically different from that of its components.

In general, one expects a large variety of spectrum types in terms of quantitative variety, i.e., having prescribed levels of stationary state energies with a given topological type. The quantitative characteristic will depend on the choice of constituents in (6). This property of the nonlocal dynamics makes it universally applicable to the task of modelling a complex quantum system, providing an attractive alternative in those situations when the inherent system complexity makes the *ab initio* approach impractical. At the same time, the proposed nonlocal model, and the resulting notion of nonlocal bonding, may in fact be fundamental; see [20] for a discussion of this problem.

Since fractal type spectra are the most exotic, and have received a lot of attention in the physics literature, let us briefly outline some of the key points as background for results presented in

Section 4.1. As we have already mentioned, fractal type energy spectra feature most prominently in the theory of Bloch electrons in magnetic fields. It is worthwhile repeating that this theory is fully based on linear quantum dynamics. The multi-scale structure of the spectrum of such systems has been described theoretically already in the 1970s by Hofstadter, [2]. Hofstadter based his analysis on a tight-binding approximation of the dynamics with periodic potential, which results in Harper's equation. The spectrum related to Harper's equation depends on one real parameter, α, which represents the number of flux quanta through one lattice cell. In particular, Hofstadter proved that, if α is an irrational number, then the corresponding spectrum can only be a Cantor-type set. However, he also pointed out a difficulty in proving that the spectrum coincides in fact with the implicated Cantor set; namely, it is hard to demonstrate the conjecture that all points in the spectrum correspond to a bounded eigenfunction. Interestingly enough, Harper's equation has also been at the foundation of one of the mathematical approaches to the integer quantum Hall effect, see [21, 22]. In general, the topic of the dynamics of a single electron in the periodic lattice potential and transversal magnetic field has received a lot of attention. An ample review of the mathematical literature, alongside interesting new results, can be found in [11, 12]. A discussion of the theoretical and numerical aspects of the specific problem of spectrum Cantorization in periodic metastructures can be found in [23], wherein the problem is approached via the theory of Green's function.

The article is organized as follows. In Sections 2 and 3, we recapitulate the relevant facts about nonlocal dynamics and its stationary states. While the main result comes from [1], we state it here in a modified form well-adapted to the discussion that follows. The spectrum structure is discussed in Sections 4 and 5. We highlight two particular examples of nonlocal dynamics which are viewed as fairly representative, although not exhaustive of interesting spectra types. The main observation is that the energy spectra of systems considered here consist of the subseries (also known as rarefied sums) of an infinite series. General level studies of this particular object can be found in the mathematical literature going back to the 1940s. The foundational concepts have been developed by a group of mathematicians, most of all J. D. Hill, H. von Hornich, H. Pollard, and S. Ulam (see [24–26]). The approach they have taken combines elements of topology, measure theory, and probability, especially Kolmogorov's version of the zero-one law. It seems that the problem at hand was considered at the time without any particular applications in mind. Nevertheless, those classical results became unexpectedly relevant to the mathematical/theoretical physics problem considered here, many years later. Most notably, Hill's theorem assists in the numerical work with the spectra; see equation (39) and discussion in Subsection 5.2.

Finally, it seems appropriate to mention that many different types of nonlinear operator equations have been discussed in the physics and mathematics literature, see, e.g., [27–30], and other sources. There are similarities and differences between these types, and they have been considered for many different purposes. Just as better known nonlinear partial differential equations, each type of an operator equation requires its own methods. A more detailed comparison of many different nonlinear operator equations can be found in [1]. The procedure of identifying the combined state vector with an operator, denoted by K, which endows the nonlocal dynamics with a physical interpretation (see the introduction below), was previously used in [31], and (independently) in [20]. It has been used in this role implicitly, as a transform mediating between two subsystems of a quantum system, already in [32–34]. Also, many authors have taken advantage of the possibility to formally factorize the density operator into a product $\rho = K^*K$ for various purposes; see, e.g., [35].

2. NONLOCAL DYNAMICS

2.1. Evolution of Composite States

In this section, we describe the fundamentals of nonlocal dynamics. This brief exposition summarizes relevant results published in our previous articles. We organize the material in a way suitable for the discussion of energy spectra. Let us begin with a pair of quantum systems. When the two systems are considered separately, the states of the first system (of the second one, respectively) correspond to unit vectors in two Hilbert spaces, namely, in $\mathbf{H}$ (in $\widehat{\mathbf{H}}$, respectively). The dynamics of the first (second, respectively) system is prescribed by Hamiltonian H ($\hat{H}$, respectively). Throughout the paper, we assume that both the Hamiltonians have pure-point spectra consisting of the eigenvalues. Let $\mathbb{N} = \{1, 2, \dots\}$ stand for the set of natural numbers. To fix the notation, we

set

$$H = \sum_{n\in\mathbb{N}} h_n |e_n\rangle\langle e_n|, \tag{1}$$

where $h_0 \leqslant h_1 \leqslant \cdots$, and $(e_n)_{n\in\mathbb{N}}$ is an orthonormal basis of $\mathbf{H}$. Analogously, let

$$\hat{H} = \sum_{n\in\mathbb{N}} \hat{h}_n |f_n\rangle\langle f_n|, \tag{2}$$

where $\hat{h}_0 \leqslant \hat{h}_1 \leqslant \cdots$, and $(f_n)_{n\in\mathbb{N}}$ is an orthonormal basis of $\widehat{\mathbf{H}}$. The operators H and $\hat{H}$ are densely defined and self-adjoint but need not be bounded, i.e., either one or both of the sequences (h_n) and $(\hat{h}_n)$ may diverge to infinity. The two eigenbases will be considered fixed but they do not need to be defined uniquely, e.g., taking $\hat{H} = h\,I$ allows one to consider an arbitrary orthonormal basis (f_n) in correspondence to the uniform energy level $h = \hat{h}_0 = \hat{h}_1 = \hat{h}_2 = \cdots$. In general, the phases of the eigenfunctions are not defined uniquely; this ambiguity has no effect on the analysis below.

Next, we consider the composite system consisting of the pair of subsystems $\mathbf{H}$ and $\widehat{\mathbf{H}}$. The composite states are represented by unit vectors in $\widehat{\mathbf{H}} \otimes \mathbf{H}$. Furthermore, the Hermitian product on $\mathbf{H}$ allows us to identify composite states with operators, so that the state

$$|\Psi\rangle = \sum_{m,n} k^*_{mn} |f_m\rangle \otimes |e_n\rangle \in \widehat{\mathbf{H}} \bigotimes \mathbf{H}$$

will be identified with

$$K = \sum k_{mn} |f_m\rangle\langle e_n|.$$

Note that the normalizing condition $\|\Psi\|^2 = 1$ translates into

$$\operatorname{Tr} K^*K = 1.$$

In particular, the operators K that admit physical interpretation have the Hilbert–Schmidt property, and are *a fortiori* bounded. One easily verifies that $\operatorname{Tr}_{\widehat{\mathbf{H}}} |\Psi\rangle\langle\Psi| = K^*K$. In other words, the corresponding mixed state of the $\mathbf{H}$ subsystem is $\rho = K^*K$. Similarly $\hat{\rho} = KK^*$ is the mixed state of the hatted subsystem.

Representing states via operators K rather than vectors $|\Psi\rangle$ has an advantage, namely, since the space of operators has an algebra structure, it is possible to consider nonlinear expressions in K, such as $f(K^*K)$, where f is an analytic function. This is the type of nonlinearity we are to consider. Note that, if K^*K is a self-adjoint bounded operator, then one can interpret $f(K^*K)$ via the spectral decomposition theorem.

Next, let us prescribe the dynamics of the composite system. We assume that f is an analytic function, well-defined on the entire positive semi-axis $(0, \infty)$, where it takes real values. In addition, let F be the antiderivative of f, $F' = f$. We consider a model for nonlocal dynamics that is prescribed by the following composite-system Hamiltonian:

$$\Xi(K) = \operatorname{Tr}\left[K^*KH + K^*\hat{H}K + \frac{1}{s}\,F\,(K^*K)\right] \quad (s = \text{ real parameter}). \tag{3}$$

Under certain technical assumptions [20], the gradient of Ξ can readily be calculated, and it is seen to induce the Hamiltonian flow

$$-i\hbar\dot{K} = KH + \hat{H}K + \frac{1}{s}Kf(K^*K). \tag{4}$$

Since K is identified with the composite state, the equation is taken to describe the evolution of the composite system. We conclude this section with the following general observations.

Remark 1. It is easily seen that (4) implies

$$i\hbar\dot{\rho} = [H, \rho], \qquad i\hbar\dot{\hat{\rho}} = [\hat{\rho}, \hat{H}]. \tag{5}$$

Therefore, the mixed states evolve according to the von Neumann equations based on the local Hamiltonians. This means, in particular, that the subsystems cannot nonlocally feed into the evolution of each other.

Remark 2. In the better known theory of nonlinear Schrödinger equations, the nonlinearity is introduced by means of expressions such as $f(|\psi(x)|^2)$. This presupposes that the state vectors admit an interpretation as functions defined over a certain geometric domain $x \to \psi(x)$. In contrast, in our approach, geometry is essentially removed from the picture. However, it can be implicitly present in the picture. Indeed, this is the case in which the Hamiltonians (1), (2) stem from differential operators on manifolds.

2.2. Solutions of the Stationary Problem

Substituting $e^{i\nu t/\hbar}K$ for K into (4), we obtain

$$KH + \hat{H}K + \frac{1}{s}Kf(K^*K) = \nu K \quad (K \text{ time-independent}). \tag{6}$$

The solutions of this equation represent the stationary states of the composite system. It has been demonstrated in [1] that all Hilbert-Schmidt solutions (in fact, even a broader class of solutions) can be represented in the form

$$K = K_{J,\sigma}(s) := \sum_{n\in J} r_n^\sigma(s)\, |f_{\sigma(n)}\rangle\langle e_n|, \tag{7}$$

where $J \subseteq \mathbb{N}$, $\sigma\colon J \overset{1-1}{\longrightarrow} \mathbb{N}$ is an arbitrary immersion of J into $\mathbb{N}$, and, in addition, the coefficients satisfy the condition

$$r_n^\sigma(s)^2 = f^{-1}\left[s\left(\nu - h_n - \hat{h}_{\sigma(n)}\right)\right] \text{ for all } n \in J. \tag{8}$$

(If f differs from $1-1$, then any point of the preimage gives rise to an admissible solution. The main example in this article is $f = \log$, in which case $f^{-1} = \exp$.) Note that the phases of the eigenfunctions remain unconstrained. In the subsequent analysis, we do not distinguish between stationary states that differ only by phases of $|f_{\sigma(n)}\rangle\langle e_n|$.

Note that, if the composite system is in the state $K_{J,\sigma}$, then the two subsystem mixed states are

$$\rho_{J,\sigma}(s) = \sum_{n\in J} \rho^n_{J,\sigma}(s)|e_n\rangle\langle e_n|, \quad \rho^n_{J,\sigma}(s) := r_n^\sigma(s)^2, \tag{9}$$

and

$$\hat{\rho}_{J,\sigma}(s) = \sum_{n\in J} \rho^n_{J,\sigma}(s)|f_{\sigma(n)}\rangle\langle f_{\sigma(n)}| \quad (\text{same eigenvalues as } \rho_{J,\sigma}(s)). \tag{10}$$

The physical solutions satisfy

$$\operatorname{Tr}\, \rho_{J,\sigma}(s) = \operatorname{Tr}\,[K_{J,\sigma}(s)^* K_{J,\sigma}(s)] = \sum_{n\in J} \rho^n_{J,\sigma}(s) = 1. \tag{11}$$

In the next section, we use this constraint to determine ν, and subsequently the energy spectrum.

3. THE SET OF STATIONARY STATES, AND THE ENERGY SPECTRUM

3.1. The Set of Stationary States

From now on, assume that $F(x) = x\log x - x$, and therefore, $f(x) = \log x$ and $f^{-1}(x) = e^x$. Hence (8) and (9) imply

$$\rho^n_{J,\sigma}(s) = e^{s(\nu - h_n - \hat{h}_{\sigma(n)})}. \tag{12}$$

This agrees with the Boltzmann distribution of states if we interpret s as $1/kT$. Physical solutions are obtained by selecting ν to satisfy (11), i.e.,

$$\sum_{n\in J} e^{s(\nu - h_n - \hat{h}_{\sigma(n)})} = 1.$$

This determines $\nu = \nu_{J,\sigma}(s)$ for every choice of J and σ. A direct calculation shows that

$$\nu_{J,\sigma}(s) = -\frac{1}{s}\log\sum_{n\in J} e^{-(h_n + \hat{h}_{\sigma(n)})s} = -\frac{1}{s}\log D_{J,\sigma}(s), \tag{13}$$

where

$$D_{J,\sigma}(s) := \sum_{n\in J} e^{-s(h_n + \hat{h}_{\sigma(n)})} = \sum_{n\in\sigma(J)} e^{-s(h_{\sigma^{-1}(n)} + \hat{h}_n)}. \tag{14}$$

Note that, if J is finite, then $D_{J,\sigma}(s)$ is an analytic function well-defined for all s. Consider an infinite J, say, $J = \{j_1, j_2, \dots\}$. Since all terms of the series are positive, convergence automatically implies uniform convergence. In particular, the ordering of terms does not matter. In general, the convergence of each $D_{J,\sigma}(s)$ is resolved separately. However, if $D_{J,\sigma}(s) < \infty$ for some real s, then it is defined in the maximal semi-axis, say, $\{s > s_0\}$, and $D_{J,\sigma}(s) \to \infty$ for $s \to s_0+$.

Substituting (13) into (12), we obtain

$$\rho^n_{J,\sigma}(s) = e^{-(h_n + \hat{h}_{\sigma(n)})s}/D_{J,\sigma}(s), \quad n \in J. \tag{15}$$

The operators

$$\rho_{J,\sigma}(s) = \sum_{n\in J} \rho^n_{J,\sigma}(s)|e_n\rangle\langle e_n|$$

and

$$\hat{\rho}_{J,\sigma}(s) = \sum_{n\in J} \rho^n_{J,\sigma}(s)|f_{\sigma(n)}\rangle\langle f_{\sigma(n)}|$$

are well defined mixed states as long as $D_{J,\sigma}(s) < \infty$. For J infinite, the density operator is well defined in $\{s > s_0\}$, but it degenerates to 0 at the pole at $s = s_0$.

Next, consider the set of stationary states,

$$\mathrm{States}(s) := \{(J,\sigma) : K_{J,\sigma}(s) \text{ satisfies } (7), (8), (11)\} \tag{16}$$

The stationary states correspond to those pairs (J,σ) for which $D_{J,\sigma}(s)$ is well defined. As s decreases, some of the $D_{J,\sigma}(s)$ may blow up to infinity, and the corresponding states $K_{J,\sigma}(s)$ can be lost. Therefore,

$$s_1 < s_2 \Longrightarrow \mathrm{States}(s_1) \subseteq \mathrm{States}(s_2).$$

Note that, if $s < 0$, then $K_{J,\sigma}(s) \in \mathrm{States}(s)$ if and only if J is finite. Properties of $\mathrm{States}(s)$ depend on the choice of H and $\hat{H}$. This is illustrated by a few examples in Section 4.

Remark. If we admit complex values of s, then $D_{J,\sigma}(s)$ can be regarded as a generalized Dirichlet series. It is a Dirichlet series in the proper sense [36], if the sequence $(h_{\sigma^{-1}(j_n)} + \hat{h}_{j_n})_{n=1}^{\infty}$ contains no repetitions, and the last property cannot be guarantied for a general σ, H, and $\hat{H}$. The complex variable interpretation suggests the possibility of working with analytic extensions of operators such as $K_{J,\sigma}(s)$, but we do not undertake it here.

3.2. The Energy Levels

Let us evaluate the energy of a stationary state (J,σ) via (3):

$$\Xi_{J,\sigma}(s)=\Xi[K_{J,\sigma}(s)]=\sum_{n\in J}\rho^n_{J,\sigma}(h_n+\hat{h}_{\sigma(n)})+\frac{1}{s}F(\rho^n_{J,\sigma}).$$

Recall that $F(x)=x\log x-x$. Therefore,

$$\Xi_{J,\sigma}(s)=-\frac{1}{s}\left(1+\log D_{J,\sigma}(s)\right)=-\frac{1}{s}+\nu_{J,\sigma}(s). \tag{17}$$

It is also interesting to note that the corresponding state entropy is

$$S_{J,\sigma}(s)=-\mathrm{Tr}\ \left[\rho_{J,\sigma}(s)\log\rho_{J,\sigma}(s)\right]=\left(1-s\frac{d}{ds}\right)\log D_{J,\sigma}(s). \tag{18}$$

We also wish to consider a probability distribution on States(s), assuming that all stationary states of equal energy occur (in an ensemble) with the same frequency and that the distribution is insensitive to shifting all energies by a constant. Naturally, this mirrors the assumption of *equal* a priori *probability* used in Statistical Mechanics [37]. The probability distribution is thus represented by a formal expression

$$P(s)=\frac{1}{\tilde{Z}}\,e^{-s\Xi_{J,\sigma}(s)}\,[d(J,\sigma)], \tag{19}$$

where $[d(J,\sigma)]$ is a suitable measure on States(s), and $\tilde{Z}$ is a normalizing constant, i.e., P is the partition function. Substituting (17) into (19), we directly obtain

$$P(s)=\frac{1}{Z}\,D_{J,\sigma}(s)\,[d(J,\sigma)] \tag{20}$$

with $Z=\tilde{Z}/\exp(1)$. In Section 5, we give a rigorous interpretation (limited to some interesting special cases) to the measure $[d(J,\sigma)]$.

4. TOPOLOGY OF THE SPECTRUM

In this section, our main objective is to discuss qualitative properties of the set

$$\mathrm{Sp}(s):=\{\Xi_{J,\sigma}(s)=\Xi[K_{J,\sigma}(s)]:K_{J,\sigma}(s)\in\mathrm{States}(s)\}.$$

In fact, we accomplish slightly more, and describe the graph

$$\mathrm{States}(s)\ni K_{J,\sigma}(s)\mapsto\Xi_{J,\sigma}(s)\in\mathrm{Sp}(s).$$

It is convenient to define the *pre-spectrum* P_s as the set of all Dirichlet sums corresponding to physical states, i.e.,

$$P_s=\left\{D_{J,\sigma}(s):(J,\sigma)\text{ such that }K_{J,\sigma}(s)\in\mathrm{States}(s)\right\}. \tag{21}$$

In view of (17), P_s can be taken onto the actual spectrum via

$$\mathrm{Sp}(s)=-\frac{1}{s}\left(1+\log P_s\right). \tag{22}$$

It is interesting to ask whether or not the pre-spectrum (and, consequently, the spectrum as well) has gaps, and, if yes, to describe their structure. It turns out the answer strongly depends on the

type of the Hamiltonians H and $\hat{H}$. In particular, the pre-spectrum can be a Cantor type set, or a continuum with finitely many holes. In the following sections, we illustrate this claim by examples based on two choices of the Hamiltonian pairs (1), (2) (see also Remark at the end of Subsection 4.2).

Few questions about the spectrum can be resolved by using general considerations. However, it is typically easy to check whether or not the pre-spectrum P_s is bounded above. Note that, if P_s is bounded above and $s > 0$, then the spectrum $\mathrm{Sp}(s)$ is bounded below (22), and so the system has a ground state. Indeed,

$$2e^{-s(h_n+\hat{h}_{\sigma(n)})} \leqslant e^{-2sh_n} + e^{-2s\hat{h}_{\sigma(n)}},$$

and '=' holds only if $h_n = \hat{h}_n$. Therefore,

$$D_{J,\sigma}(s) = \sum_{n\in J} e^{-s(h_n+\hat{h}_{\sigma(n)})} \leqslant \frac{1}{2}\sum_{n\in J} e^{-2h_n s} + \frac{1}{2}\sum_{n\in J} e^{-2\hat{h}_{\sigma(n)} s} \leqslant \frac{1}{2}\sum_{n=1}^{\infty} e^{-2h_n s} + \frac{1}{2}\sum_{n=1}^{\infty} e^{-2\hat{h}_n s}.$$

For example, let $H = \hat{H}$. In this case, P_s has the following properties:

$$\text{if } D_{\mathbb{N},Id}(s) < \infty, \text{ then } P_s \subseteq (0, D_{\mathbb{N},Id}(s)]\,. \tag{23}$$

In the complementary case, P_s contains all partial sums of the divergent series $D_{\mathbb{N},Id}(s)$. Therefore,

$$\text{If } D_{\mathbb{N},Id}(s) = \infty, \text{ then } P_s \subseteq (0,\infty) \text{ is unbounded above.} \tag{24}$$

4.1. Fractal Type

Let $H = \sum n|e_n\rangle\langle e_n|$ and $\hat{H} = h\sum |f_n\rangle\langle f_n|$. Since the second Hamiltonian is a multiple of the identity, the eigenbasis (f_n) is not determined uniquely; namely, it can be an arbitrary orthonormal basis. Nevertheless, the results discussed above still apply, and the only effect of degeneracy for the stationary states (7) is that they can now be constructed starting from an arbitrary (f_n). Inserting the corresponding eigenvalues into (14), we obtain

$$D_J(s) = D_{J,\sigma}(s) = \sum_{n\in J} e^{-s(n+h)} = e^{-sh}\sum_{n\in J} e^{-sn}. \tag{25}$$

We drop the subscript σ, because the sums do not depend on σ. Note that $D_{\mathbb{N}}(s)$ is a geometric series, and

$$D_{\mathbb{N}}(s) = e^{-sh}\sum_{n=1}^{\infty} e^{-sn} = e^{-sh}\frac{1}{e^s - 1}.$$

In addition, $P_s = \{D_J(s) : J \subseteq \mathbb{N}\}$ consists of sums of all the subseries. For clarity, it is convenient to separate the scale factor and to represent the pre-spectrum in the form

$$P_s = e^{-sh}\tilde{P}_s.$$

Then $\tilde{P}_s$ does not depend on h, and it consists of the sums

$$\tilde{P}_s = \left\{\sum_{n=1}^{\infty} \varepsilon_n e^{-sn} : (\varepsilon_n) \text{ can be any sequence with } \varepsilon_n = 0, 1\right\}.$$

Note that $\tilde{P}_s$ is a self-similar set satisfying the relation

$$\tilde{P}_s = e^{-s}\tilde{P}_s \cup \left(e^{-s} + e^{-s}\tilde{P}_s\right).$$

In particular, $\tilde{P}_{\log 3}$ is the classical Cantor set,

$$\tilde{P}_{\log 3} = \frac{1}{3}\tilde{P}_{\log 3} \cup \left(\frac{1}{3} + \frac{1}{3}\tilde{P}_{\log 3}\right).$$

We can obtain sparser (denser) Cantor sets for larger (smaller) values of s. If $0 < s \leqslant \log 2$, then $\tilde{P}_s$ is a segment without gaps, and (22) shows that the spectra $\mathrm{Sp}(s)$ are of the same topological type as those of P_s or $\tilde{P}_s$.

4.2. Union-of-Intervals Type

Consider the pair of Hamiltonians

$$H = \sum \log n \, |e_n\rangle\langle e_n|, \qquad \hat{H} = h \sum |f_n\rangle\langle f_n|.$$

Substituting the eigenvalues into (14), we obtain

$$D_J(s) = \sum_{n\in J} e^{-s(\log n + h)} = e^{-sh} \sum_{n\in J} n^{-s} =: e^{-sh}\zeta_J(s).$$

Note that

$$\zeta_{\mathbb{N}}(s) = \sum_{n=1}^{\infty} n^{-s} = \zeta(s) \quad (s > 1),$$

where $\zeta(s)$ is the Riemann zeta function. This justifies our notation. As above, we are to characterize the set of all rarefied sums of the series. It seems that the type of argument needed to be engaged here was known already to von Hornich, [25]. Similar ideas can also be found in [38]. Here, we briefly discuss the problem in a manner suitable for our purposes.

Since the role of h is trivial, let us set $h = 0$, and consider the pre-spectrum

$$P_s := \{\zeta_J(s) : J \subseteq \mathbb{N}\} = \left\{ \sum_{n=1}^{\infty} \varepsilon_n n^{-s} : (\varepsilon_n) \text{ can be any sequence with } \varepsilon_n = 0, 1 \right\}.$$

We focus on the case $s > 1$, $P_s \subseteq (0, \zeta(s)]$, and show that, in this case, P_s is a continuum with finitely many holes. More precisely,

$$(0, \zeta(s)] \setminus P_s \text{ either is the empty set or consists of finitely many open intervals.} \tag{26}$$

In order to see this, let us fix $s > 1$ and observe that

$$\frac{1}{s-1}(k+1)^{1-s} = \int_{k+1}^{\infty} \frac{1}{x^s} dx < \sum_{n=k+1}^{\infty} \frac{1}{n^s} < \int_{k}^{\infty} \frac{1}{x^s} dx = \frac{1}{s-1} k^{1-s}.$$

This implies that for all k but finitely many, k^{-s} is dominated by the tail $\sum_{n=k+1}^{\infty} n^{-s}$. Indeed, if only $k + 1 > (s-1)2^s =: N(s)$, then

$$\frac{k+1}{s-1} > 2^s \geqslant \left(\frac{k+1}{k}\right)^s,$$

so that

$$k^{-s} < \frac{1}{s-1}(k+1)^{1-s} < \sum_{n=k+1}^{\infty} \frac{1}{n^s}.$$

Let us focus on the set of partial sums of the series $\zeta_+(s) := \sum_{n=N(s)+1}^{\infty} n^{-s}$. We claim that

$$\text{every point } z \in (0, \zeta_+(s)] \text{ may be expressed as a rarefied sum of } \sum_{n=N(s)+1}^{\infty} n^{-s}. \tag{27}$$

Before we shall proceed with the proof of this fact, we note the following: P_s consists of finitely many right shifts of $(0, \zeta_+(s)]$ by quantities $\sum_{n=1}^{N(s)} \varepsilon_n n^{-s}$ with arbitrary $\varepsilon_n = 0, 1$. Also note that, even though 0 is not in the spectrum, its shifts are. Therefore, (27) implies that $(0, \zeta(s)] \setminus P_s$ is

either empty or consists of finitely many open intervals, as claimed in (26). Let us now present a short proof of (27).

Proof of (27). If $z = \zeta_+(s)$, then there is nothing to show. Assume that $0 < z < \zeta_+(s)$. Let us construct a $0-1$ sequence $\varepsilon_n = \varepsilon_n(z)$ such that

$$\sum_{n=N(s)+1}^{\infty} \varepsilon_n(z) n^{-s} = z. \tag{28}$$

We initially set $\varepsilon_n = 0$ for all n, and alter this sequence recursively as follows:

(1) Step 1. Find $n_1 = \min\{m > N(s) : m^{-s} \leqslant z\}$, and set $\varepsilon_{n_1}(z) = 1$. If $n_1^{-s} = z$, stop; otherwise move to the next step.
(2) Step 2. Find $n_2 = \min\{m > n_1 : n_1^{-s} + m^{-s} \leqslant z\}$, and set $\varepsilon_{n_2}(z) = 1$. If $n_1^{-s} + n_2^{-s} = z$, stop; otherwise move to the next step.
(3) Sep 3. Find $n_3 = \min\{m > n_2 : n_1^{-s} + n_2^{-s} + m^{-s} \leqslant z\}$, and set $\varepsilon_{n_3}(z) = 1 \ldots$ etc.

The algorithm either stops after a finite number of steps or never stops. In the former case, z can be expressed as a rarefied sum, and there is nothing more to prove. Therefore, assume that $\varepsilon_n(z) = 1$, for infinitely many n. Since $z < \zeta_+(s)$, there is an $m > N(s)$ such that $\varepsilon_m(z) = 0$. We claim that, in fact, $\varepsilon_m(z) = 0$ for infinitely many m. Indeed, since $\varepsilon_m(z) = 0$, it follows that

$$0 < z - \sum_{n=N(s)+1}^{m-1} \varepsilon_n(z) n^{-s} < m^{-s}, \tag{29}$$

and since $m > N(s)$, we have

$$m^{-s} < \sum_{n=m+1}^{\infty} n^{-s}.$$

Therefore, there is an $m' > m$ such that $\varepsilon_{m'}(z) = 0$. Since this argument can be repeated with m' instead of m, we have $\varepsilon_m(z) = 0$ for infinitely many m, as was claimed above. It follows that (29) holds for infinitely many m. Passing to the limit as $m \to \infty$ implies (28). This completes the proof of (27).

Remark. It is of interest to note that, in the case of $\hat{h}_n = h_n = \log n$, the pre-spectrum consists of generalized zeta functions

$$D_{J,\sigma}(s) = \zeta_{J,\sigma}(s) = \sum_{n \in J} [n\sigma(n)]^{-s}$$

indexed by pairs (J, σ). Note that $\zeta_{\mathbb{N},Id}(s) = \zeta(2s)$ for $s > \frac{1}{2}$. It follows from (23) that $P_s \subseteq (0, \zeta(2s)]$ in this case. Moreover, the complement of the pre-spectrum to this interval can be only an empty set or a union of finitely many open intervals. Indeed, P_s contains, in particular, all the sums

$$\zeta_{J,Id}(s) := \sum_{n \in J} n^{-2s},$$

so that the claim follows from (26). Naturally, in this case, the graph

$$\mathrm{States}(s) \ni K_{J,\sigma}(s) \mapsto \Xi_{J,\sigma}(s) \in \mathrm{Sp}(s)$$

has a more complex structure than that in the case of $\hat{h}_n = h$.

4.3. Information Inherent in the Ground State $K_{\mathbb{N}}(s)$

We continue discussing the example from Subsection 4.2. Note that, as long as $s > 1$, $K_{\mathbb{N}}(s)$ represents the ground state of the system. Indeed, $D_{\mathbb{N}}(s) > D_J(s)$ for any proper subset $J \subseteq \mathbb{N}$. Therefore, (17) implies that $\Xi_{\mathbb{N}}(s) < \Xi_J(s)$. If $0 < s < 1$, the series diverges, $D_{\mathbb{N}}(s) = \infty$, and the system has no ground state. Instead, there is a sequence of states whose energies tend to $-\infty$. If s is negative, then the ground state reappears, but it is no longer $K_{\mathbb{N}}(s)$. Namely, for $s < 0$, the ground state corresponds to $J = \{1\}$, which minimizes $D_J(s)$ and gives the minimal energy

$$\Xi_{\{1\}} = -\frac{1}{s} - \frac{1}{s}\log D_{\{1\}}.$$

We now assume that $s > 1$ and evaluate the energy and the entropy of the ground state $K_{\mathbb{N}}$. Rewriting (17) with the help of well-known integral formulas for $\log\zeta(s)$, see [19], we have

$$\Xi_{\mathbb{N}}(s) = h - \frac{1}{s} - \frac{1}{s}\log\zeta(s) = h - \frac{1}{s} - \int_0^\infty \frac{\pi(x)}{x(x^s-1)}dx = h - \frac{1}{s} - \int_0^\infty J(x)x^{-s-1}dx \quad (s>1), \tag{30}$$

where $\pi(x)$ stands for the prime-counting function, and

$$J(x) = \sum_n \frac{1}{n}\pi(x^{1/n}).$$

Similarly, the entropy (18) can be represented as

$$S_{\mathbb{N}}(s) = \log\zeta(s) - s\frac{\zeta'(s)}{\zeta(s)} = s\int_0^\infty J(x)x^{-s-1}dx + s^2\int_0^\infty \psi(x)x^{-s-1}dx \quad (s>1), \tag{31}$$

where $\psi(x) = \sum_{p^k<x}\log p$ (here p ranges over the prime integers) is the Chebyshev function.

The guest appearance of the fundamental number theoretic functions in the description of a state of a quantum system is as buffling as it is beautiful. The reader can note that these functions have not been introduced here by brute force (say, by hand-inserting a refined analytic function directly into the model); instead, these are a consequence of the choice of the Hamiltonians and the nonlocal coupling based on the *log* function. The model seems to bridge quantum mechanics to number theory in a new way. It is natural to ask if the ground states of an s-parametrized family of quantum systems can be used to determine either one of the fundamental number theoretic functions, but this problem is not addressed here.

Remark. Note that the degeneracy of $\hat{H}$ is not essential for the "number theoretic" ground state. Indeed, the case $\hat{h}_n = h_n = \log n$ results in similar formulas for the ground state, cf. Remark in Subsection 4.2.

5. STATE STATISTICS

In this concluding section, we consider only a special type of systems, such as those discussed in Subsections 4.1 and 4.2. The following assumptions will underly the discussion of state statistics.

(1) $H = \sum h_n|e_n\rangle\langle e_n|$ with all h_n distinct, and $\hat{H} = \sum h|f_n\rangle\langle f_n|$, so that $\hat{H}$ has just one degenerate energy level. In this case, $D_{J,\sigma}(s) = D_J(s)$ does not depend on σ.
(2) Recall that the stationary states are described in (7). The states that differ only by σ or by a choice of the orthonormal basis $|f_n\rangle$ will be viewed as indistinguishable.
(3) Unless otherwise stated, s is assumed to be large enough to ensure the condition $D_{\mathbb{N}}(s) < \infty$.

Under these assumptions, the set of states can be identified with the set of all subsets of the index set, i.e., $\text{States}(s) = \{J : J \subset \mathbb{N}\}$. In the following subsections, we show how every $D_J(s)$ can be identified with a function of real variable $x \to D(x,s)$, $x \in [0,1]$. We shall also define the measure $[d(J,\sigma)] = [d(J)]$ as $[d(J)] := dx$, where dx is the standard Lebesgue measure on $[0,1]$. This will enable us to give a rigorous interpretation of formulas (19), (20) and to conduct a quantitative and numerical analysis of the energy spectra.

5.1. Identification of States(s) with $[0,1]$ *and the Probability Measure*

Subsets $J \subset \mathbb{N}$ can be identified with points $x \in [0,1]$ as follows: Every J determines a binary sequence $(\alpha_n)_{n=1}^{\infty}$: $\alpha_n = 1$ for $n \in J$ and $\alpha_n = 0$ otherwise. The binary sequence in turn determines $x = \sum \alpha_n 2^{-n}$, which is written in the binary notation as $0.\,\alpha_1\,\alpha_2 \ldots \alpha_n \ldots$. The identification $J \longleftrightarrow x$ is $1-1$ everywhere in $[0,1]$ except for the countable set of points of the form $x = k/2^N$ (reduced fraction), which can be represented either as $x = 0.\,\alpha_1\,\alpha_2 \ldots \alpha_{N-1}\,1$ or as $x = 0.\,\alpha_1\,\alpha_2 \ldots \alpha_{N-1}\,011111 \ldots$.

It is often convenient to use the Rademacher functions defined as

$$r_n(x) = -\operatorname{sgn}\sin(2^n \pi x), \quad x \in [0,1], \quad n \in \mathbb{N}.$$

Let $\alpha_n(x)$ denote the nth digit in the binary expansion of x. If x *is not* a binary fraction, then

$$\alpha_n(x) = \frac{1 + r_n(x)}{2}. \tag{32}$$

For a binary fraction $x = k/2^N$, we have $\frac{1+r_n(x)}{2} = \frac{1}{2}$ for all $n \geqslant N$.

Recall the definition of States(s) in (16). Identifying each J with a binary sequence, and subsequently with $x \in [0,1]$, gives an identification

$$\text{States}(s) = [0,1]. \tag{33}$$

The identification is '$1-1$', except for a countable set of dyadic fractions. Next, we define the measure $[d(J,\sigma)] = [d(J)]$ as

$$[d(J)] := dx, \tag{34}$$

where dx is the standard Lebesgue measure on $[0,1]$.

Finally, we identify $D_J(s)$ with a function of x. Recall that $D_J(s) = \sum_{n\in J} e^{-s(h_n+h)}$, so that

$$D_J(s) = D(x,s) = \sum_{n=1}^{\infty} \alpha_n(x) e^{-s(h_n+h)}. \tag{35}$$

Here, x is determined from the condition $\alpha_n(x) = 1$ for $n \in J$ and $\alpha_n(x) = 0$ otherwise. The function $x \to D(x,s)$ is well defined almost everywhere. Substituting Rademacher functions (32) gives a useful formula

$$D(x,s) = \sum_{n=1}^{\infty} \frac{1 + r_n(x)}{2} e^{-s(h_n+h)}. \tag{36}$$

The identifications (33), (35), and (34) enable us to replace the formal formulas (19) and (20) by a rigorous definition of the probability measure on the set of states. Namely, we write

$$P(s) = \frac{1}{Z}\, D(x,s)\, dx, \quad \text{where } Z = \int_0^1 D(x,s)\, dx < \infty. \tag{37}$$

The integral is well defined. Indeed, the integrability of the rarefied sum functions such as $x \to D(x,s)$ has already been proved by Hill [24]. It is necessary to assume, as we have, that the full series $D(1,s)$ converges in order to obtain $Z > 0$. Note also that, since the set of binary fractions is countable, and therefore of measure zero, one need not worry about the nonuniqueness of $D(x,s)$ at those points. Finally, recall that (17) gives $\Xi(x,s)$ as a function of $D(x,s)$. Therefore, the average state energy may be expressed as

$$\langle \Xi(s) \rangle = \frac{1}{Z} \int_0^1 \Xi(x,s) D(x,s)\, dx. \tag{38}$$

5.2. Numerical Simulations and Quantitative Analysis

We now have all the required ingredients to explicitly compute the spectra. First, the average value of $D(x,s)$ is

$$Z = \int_0^1 D(x,s)\,dx = \int_0^1 \sum_n \alpha_n(x) e^{-s(h_n+h)}\,dx = \frac{1}{2}\sum_n e^{-s(h_n+h)} = \frac{1}{2}D(1,s). \tag{39}$$

This result has been established by Hill [24]. It is natural, whereas its rigorous proof is nontrivial. (One needs to show that the integrand is in fact a measurable function, and that the sum and the integral can be transposed.) We use (39) to control the accuracy of numerical simulations. Namely, the accuracy is defined as

$$\text{accuracy} = \left|\frac{D^{\text{av}} - Z}{Z}\right|, \tag{40}$$

where D^{av} is the computed average value of $D = D(x,s)$. In practice, $Z = 0.5 \cdot D(1,s)$ is estimated numerically via a partial sum.

The figure depicts graphs of $D(x,s)$ for the two highlighted regimes: fractal (described in Subsection 4.1), here denoted D^f, and zeta-function (described in Subsection 4.2), here denoted D^z. Since the effect of h is trivial, we set $h = 0$. These graphs have been generated by a direct calculation of (36) based on the first twenty Rademacher functions. We have compared this method to an obvious Monte Carlo type method based on randomization of the sequence α_n in (35). Both algorithms have been implemented on a standard desktop computer with a 32 bit Intel Core 2 processor.
At the picture resolution, the images obtained from the two methods are indistinguishable. However, the numerics show that the approach based on the Rademacher-function gives a more accurate estimate of the average value of $D(x,s)$. The accuracy of this method typically tops the other by three to five orders of magnitude.

The Rademacher-function method is used also to estimate the average system energies by computational evaluation of the integral (38). The table below shows the numerical estimates of the mean system energy, as well as the corresponding accuracy (40), for the two convergent cases illustrated in the figure. The energy is expressed in units in which the eigenvalues of H are integers, $n = 1, 2, \ldots$. Note that we cannot assign meaningful values of mean energy, or accuracy, to the divergent case of $s = -0.01$, because $Z = \infty$ in the case.

spectrum type	parameter$s$	accuracy	mean energy$\langle \Xi_s \rangle$
Fractal	Log3	$6.3 \cdot 10^{-8}$	.0775
Zeta	3	$7.6 \cdot 10^{-8}$	$-.3059$

Remark 1. In the [24] cited above, Hill observed in particular that, for an absolutely convergent series, the rarefied sum functions, like $x \to D(x,s)$, are continuous at all $x \in [0,1]$ except for the dyadic fraction points. Note that the set of dyadic fractions is everywhere dense in $[0,1]$, so that in spite of the continuity almost everywhere, the graphs will typically look manifestly discontinuous. This is noticeable in the figures provided in this article.

Remark 2. It follows from well-known results that, if the full series converges, i.e., $D(1,s) < \infty$, then the set P_s of all rarefied sums, see (21), is topologically *perfect*. Recall that a perfect set is a set with no isolated points. (This observation concerning the rarefied sums of certain series has been made already by S. Ulam, who privately communicated it to Pollard [26]. More general results have been proven later by Hornich [25].) Automatically, $\mathrm{Sp}(s)$ is also perfect, see (22). In other words, every point in $\mathrm{Sp}(s)$ is a limit of a sequence of points in $\mathrm{Sp}(s)$. This means that, if $D(1,s) < \infty$, then the energy levels of a composite system are never isolated on both sides.

Remark 3. Pollard gave a proof of Hill's theorem (39) based on the Rademacher representation (36), see [26]. Furthermore, Pollard's results imply that the set

$$\mathrm{States}(s) = \{x \in [0,1] : D(x,s) < \infty\}$$

has measure either 1 or 0, depending on whether $D(1,s) < \infty$, or $D(1,s) = \infty$. One of the main tools in Pollard's work is the zero-one law. Here we have only considered the case of convergent series.

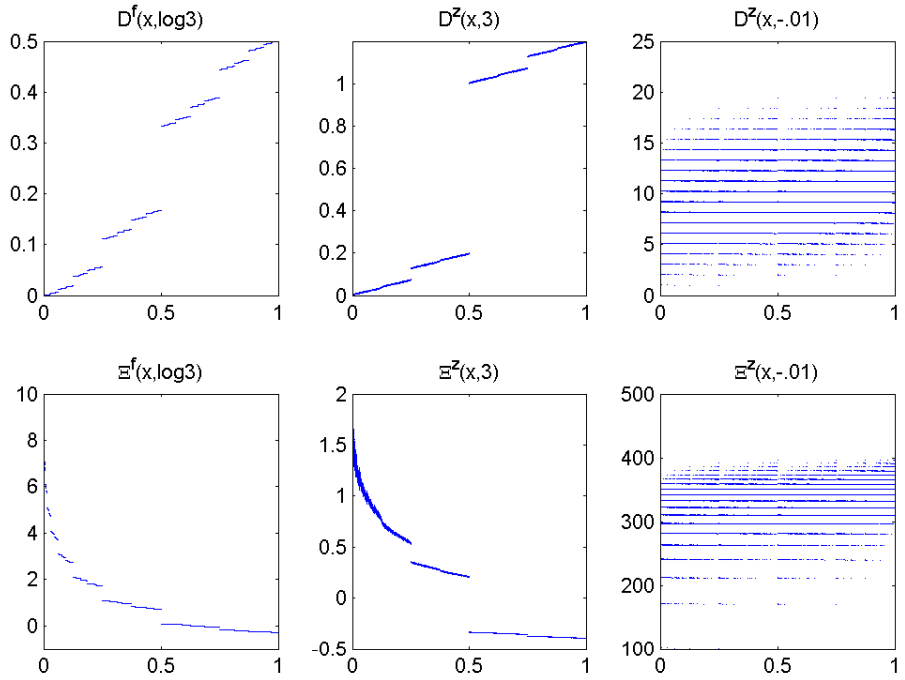

Figure. The graphs of $D^f(x, \log 3)$, $D^z(x,3)$, $D^z(x,-0.01)$ (top row), as well as the corresponding energy functions Ξ (bottom row). As explained in the text, the variable x indexes groups of quantum states of the composite system. The image of $D^f(x, \log 3)$ is a rescaled copy of the standard Cantor set. Note the self-similarity of the graph, and a multi-scale system of gaps. In comparison, the image of $D^z(.\,s)$ has only finitely many gaps (for $s > 1$), and the energy spectrum inherits this property. This is illustrated here for $s = 3$, in which case we see three gaps. One of those in the graph of $\Xi^z(x,3)$ is too tight to be visible at the current picture resolution. For $s < 1$ (here we take $s = -0.01$), the image of $D^z(x,s)$ and the corresponding spectrum display a sequence of gaps.

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