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On Computability of Decaying and Nondecaying States in Quantum Systems with Cantor Spectra

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We study Hamiltonians with singular spectra of Cantor type with a constant ratio of dissection. The decay properties of the states in such systems depend on the nature of the dissection rate that can be characterized in terms of the algebraic number theory. We show that in spite of simplicity of the considered model the computational modeling of nondecaying states is in general impossible.

KEY WORDS: decay; singular spectrum; S-number; computability; quantum system.

1. INTRODUCTION

Singular spectra were regarded for a long time as "unphysical" and neglected. This situation has changed dramatically in the last decades. Nowadays it is easy to find genuine "physical" systems for which singular spectra not only appear but they are even generic (Antoniou *et al.*, 1998, 1999; Antoniou and Shkarin, 2001; Antoniou and Suchanecki, 2000; Avron and Simon, 1981a,b; Bellisard, 1982; Damanik *et al.*, 2000; del Rio *et al.*, 1994; Jitomirskaya and Simon, 1994; Pearson, 1978). The simplest of them are Cantor-like (or fractal) sets which we study in this paper. Cantor-type sets are easier tractable than the other singular sets. There is a simple recursive procedure of the construction of Cantor sets and many theoretical results about their nature. Cantor spectra in spite of their simplicity exhibit, however, all the complexity of the behavior of quantum systems with singular spectra and the property of decay in particular.

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The decay of a quantum system depends on the nature of its spectrum. If the Hamiltonian has point spectrum then each state is nondecaying. On the other hand an easy consequence of the Radon–Nikodym theorem is that if the Hamiltonian has an absolutely continuous spectrum then each state is decaying (Weidmann, 1980). If the Hamiltonian consists of both point and absolutely continuous spectrum then the underlying Hilbert space can be decomposed as a direct sum of two Hilbert spaces. Each of these spaces reduces the Hamiltonian and one of them consists only of decaying states while the other only of nondecaying. However, the spectrum of an arbitrary Hamiltonian does not necessarily consist of these two parts only. Hamiltonian systems with singular continuous spectra may have both decaying and nondecaying states. As we have shown recently (Antoniou and Shkarin, 2001; Antoniou and Suchanecki, 2000) the Hilbert space of an arbitrary Hamiltonian H can also be decomposed on two parts, which reduce H, in such a way that one Hilbert space consists of decaying states and the other of nondecaying. The division line between decaying and nondecaying states goes through the singular part of the spectrum, which means that singular spectra may behave like point spectra but may also behave as absolutely continuous spectra.

In this paper we restrict our study to the simplest class of singular spectra. We study Cantor-type sets with constant ratio of dissection (Salem, 1983), which provide constructive examples of fractal spectra and show strict connections with algebraic number theory. It is therefore surprising to learn that the possibility to construct nondecaying states in such systems is only theoretical. We clarify this point below. First, however, let us recall the basic notions and facts.

The pure states of a quantum mechanical system are wave functions regarded as elements of a separable Hilbert space $\mathcal{H}$ in the von Neumann formulation (Von Neumann, 1955) of quantum mechanics. The time evolution of a wave function $\psi \in \mathcal{H}$ is governed by the unitary group

$$U_t = e^{-itH}, \qquad t \in \mathbb{R},$$

on $\mathcal{H}$, which is the solution of the Schroedinger equation

$$\partial_t \psi = -iH\psi, \qquad \hbar = 1.$$

The Hamiltonian H is a self-adjoint operator on $\mathcal{H}$.

A (pure) state $\psi \in \mathcal{H}$ is called a *decaying state* if its *survival amplitude* decays asymptotically, $t \to \infty$

$$\langle \psi, U_t \psi \rangle = \int_{\mathbb{R}} e^{-i\lambda t} d\langle \psi, E_\lambda \psi \rangle \to 0,$$

where $\{E_\lambda\}$ is the spectral family of H. The *survival probability*, i.e., the probability that at time t the state ψ has not yet decayed is

$$p(t) \stackrel{\text{df}}{=} |\langle \psi, U_t \psi \rangle|^2.$$

For any given state $\psi \in \mathcal{H}$ we denote by $F(\lambda)$ the spectral distribution function:

$$F(\lambda) = \langle \psi, E_\lambda \psi \rangle, \quad \text{for } \lambda \in \mathbb{R}.$$

It can be shown (Weidmann, 1980) that each state ψ can be uniquely decomposed as

$$\psi = \psi_{\rm p} + \psi_{\rm sc} + \psi_{\rm ac}$$

in such a way that the corresponding spectral distribution function $F_{\rm p}$, $F_{\rm sc}$, and $F_{\rm ac}$ is discrete, singular, and absolutely continuous respectively. Obviously $\psi_{\rm p}$ is nondecaying and $\psi_{\rm ac}$ is decaying. It turns out that the singular continuous state $\psi_{\rm sc}$ can be uniquely decomposed further as a sum of two states such that one is nondecaying and the other decaying (Antoniou and Shkarin, 2001; Antoniou and Suchanecki; 2000). In fact the whole Hilbert space can be decomposed as a direct sum of two closed subspaces

$$\mathcal{H} = \mathcal{H}^{\rm D} \oplus \mathcal{H}^{\rm ND},$$

called decaying and no-decaying space respectively. Moreover the spaces $\mathcal{H}^{\rm D}$ and $\mathcal{H}^{\rm ND}$ reduce the Hamiltonian operator H, which means that the spectral properties of H can be studied separately and independently on these subspaces.

The decaying states can also be characterized in terms of their spectral measures as follows:

Proposition 1. *Suppose that the spectral measure μ which corresponds to a state $\psi \in \mathcal{H}$ consists only of the singular continuous component and that the support of μ is bounded. Let*

$$M_1 = M_1(\psi) = \inf\{\lambda : \lambda \in \operatorname{supp} \mu\} \quad \text{and} \quad M_2 = M_2(\psi) = \sup\{\lambda : \lambda \in \operatorname{supp} \mu\}.$$

The necessary and sufficient condition for ψ to be a decaying state is that for each a, b, $0 < a < b < M_2 - M_1$, holds

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} \chi_{a,b}\,(n\,(\lambda - M_1))\,\mu(d\lambda) = \frac{b-a}{M_2 - M_1}||\psi||^2, \tag{1}$$

where $\chi_{a,b}(\lambda)$ denotes the characteristic function of the interval $[a, b]$ repeated mod ($M_2 - M_1$), i.e., the indicator of the set

$$\bigcup_{k\in\mathbb{Z}} [a + k(M_2 - M_1), b + k(M_2 - M_1)].$$

Proof: Let us introduce the linear transformation $\phi : [0, 2\pi] \to [M_1, M_2]$

$$\phi(x) = \frac{M_2 - M_1}{2\pi} x + M_1.$$

Since the support of μ is contained in $[M_1, M_2]$

$$\int_{-\infty}^{\infty} \chi_{a,b}(n(\lambda - M_1))\mu(d\lambda) = \int_{\phi(0)}^{\phi(2\pi)} \chi_{a,b}(n(\lambda - M_1))\, dF(\lambda)$$
$$= \int_{0}^{2\pi} \chi_{a,b}(n(\phi(\lambda) - M_1))\, dF(\phi(\lambda)), \qquad (2)$$

where F is the spectral distribution function of ψ. However

$$\chi_{a,b}(n(\phi(\lambda) - M_1)) = \chi_{a',b'}(n\lambda),$$

where $a' = \frac{2\pi a}{M_2 - M_1}$, $b' = \frac{2\pi b}{M_2 - M_1}$. Applying to the right-hand side of (2) Theorem XII, 10.5 of Zygmund (1968) we see that the integral converges to

$$\frac{b' - a'}{2\pi}(F(\phi(2\pi) - F(\phi(0))) = \frac{b - a}{M_2 - M_1}(F(M_2) - F(M_1))$$
$$= \frac{b - a}{M_2 - M_1}(F(\infty) - F(-\infty))$$
$$= \frac{b - a}{M_2 - M_1}||\psi||^2$$

if and only if

$$\lim_{n\to\infty} \int_0^{2\pi} e^{in\lambda} dF(\phi(\lambda)) = 0. \qquad (3)$$

However

$$\int_0^{2\pi} e^{in\lambda} dF(\phi(\lambda)) = \int_{M_1}^{M_2} e^{in\phi^{-1}(x)} dF(\lambda) = e^{-\frac{2\pi i n M_1}{M_2 - M_1}} \int_{M_1}^{M_2} e^{\frac{2\pi i n \lambda}{M_2 - M_1}} dF(\lambda).$$

Replacing n in (3) by $\frac{M_2 - M_1}{2\pi}\, n$ and applying (Zygmund 1968) XII, Theorem 10.11 we obtain that

$$\lim_{n\to\infty} \int_{M_1}^{M_2} e^{in\lambda} dF(\lambda) = 0$$

if and only if (1) holds.

If the support of μ in the above proposition is unbounded then the necessary and sufficient condition for ψ to be a decaying state is

$$\lim_{n\to\infty} \int_{M_1}^{M_2} \chi_{a,b}\,(n\,(\lambda - M_1))\, \mu(d\lambda) = \frac{b - a}{M_2 - M_1}||\psi||^2, \qquad (4)$$

for arbitrary $-\infty < M_1 < M_2 < \infty$ and $0 < a < b < M_2 - M_1$. Indeed, the condition is necessary since if ψ is a decaying state then

$$\lim_{t\to\infty}\int_{-\infty}^{\infty} e^{it\lambda} dF(\lambda) = 0.$$

Therefore, by Lemma 2 of Antoniou and Shkarin (2001) the measure corresponding to $\mathbf{1}_{[M_1,-M_2]}(\lambda)dF(\lambda)$ is decaying, so we can apply (1). Conversely, for a given $\varepsilon > 0$ we can find such M_1 and M_2 that $\mu(\mathbb{R}\backslash[M_1 - M_2]) < \varepsilon$. By the assumption there is an N such that $|\int_{M_1}^{M_2} e^{it\lambda}\mu(d\lambda)| < \varepsilon$, for $t \geq N$. Thus $|\int_{-\infty}^{\infty} e^{it\lambda}\mu(d\lambda)| < 2\varepsilon$ which shows that condition (4) is also sufficient.

Singular spectra may already appear in Hamiltonian systems of the form $-\frac{d^2}{dx^2} + V$, where the potential V is an almost periodic function or even when V is a uniform limit of periodic functions. Each period in the potential creates a gap in the spectrum. In result the spectrum of such an operator is in general a Cantor-type set. □

A vast literature has been devoted to study of the classes of potentials that lead to singular spectra (see, for example, Avron and Simon, 1981a,b; Bellisard, 1982, and references therein). We shall not review these important results here. Instead, given a Hamiltonian with a specified singular spectrum, we shall study its properties. Let us, therefore, show first how to correspond a Hamiltonian to a given spectrum. Suppose that the required spectrum σ is a Borel subset of $\mathbb{R}$ and a measure μ, which we would like to regard as a spectral measure, is a Borel measure on σ. In the spectral representation, the Hamiltonian with spectral measure μ is the multiplication operator

$$Hf(\lambda) = \lambda f(\lambda) \tag{5}$$

on the Hilbert space $L^2(\sigma, \mu)$. The spectral projectors E_λ of H are

$$E_\lambda f(\lambda') = \begin{cases} f(\lambda), & 0 \leq \lambda' < \lambda \\ 0, & \text{otherwise.} \end{cases}$$

The spectral measure $\mu(d\lambda) = dF(\lambda)$ corresponds to the distribution function F associated with the cyclic vector $\psi = 1$:

$$F(\lambda) = \langle\psi, E_\lambda\psi\rangle. \tag{6}$$

We introduce now an important class of Cantor-type sets which will serve as the supports of singular measures. To simplify the notation, we restrict our considerations to the interval $[a, b]$. Let r be a real number, $0 < r < \frac{1}{2}$. In the first step divide the interval $[a, b]$ into three parts of the lengths proportional to r, $1 - 2r$, and r respectively. Then remove the middle open interval. In the second step divide each of two remaining intervals into three parts of lengths also proportional to r, $1 - 2r$, and r respectively. Then remove then middle open intervals, and so on. In this way we obtain in the kth step a closed set σ_k consisting of 2^k disjoint intervals, each one of the length $(b-a)r^k$. Denote $\sigma = \cap_k \sigma_k$ and observe that σ is a closed set with points of the form

$$x = a + (b-a)(1-r)\sum_{k=1}^{\infty} \varepsilon_k r^{k-1}, \tag{7}$$

where $\varepsilon_k = 0$ or 1. Cantor's ternary set on the interval [0, 1] with points $x = 2\sum_{k=1}^{\infty} \frac{\varepsilon_k}{3^k}$, is obtained by putting $a = 0$, $b = 1$, and $r = \frac{1}{3}$.

Let us focus our attention on Cantor-type sets on the interval $[0, 2\pi]$ with a constant ratio of dissection. Therefore each point $x \in \sigma$ has the form

$$x = 2\pi(1-r)\sum_{k=1}^{\infty} \varepsilon_k r^{k-1}. \tag{8}$$

On the set σ define the distribution function F putting for the points x of the form (8)

$$F(x) = \sum_{k=1}^{\infty} \frac{\varepsilon_k}{2^k}.$$

We extend F on $[0, 2\pi]$ putting

$$F(x) = \sup_{\substack{y\in\sigma \\ y\le x}} F(y).$$

The function F is nondecreasing and continuous with $F'(x) = 0$ for almost all $x \in [0, 2\pi]$ therefore singular.

According to the above prescription we can define a Hamiltonian system on the Hilbert space $\mathcal{H}$ of all functions f such that $\int_{\mathbb{R}} |f(x)|^2 dF(x) < \infty$ putting as H the multiplication operator.

It is easy to see that the function (*state*) $\psi \equiv 1$ is a cyclic vector for H, i.e., the set of all finite linear combinations of $H^n\psi$, $n = 0, 1, 2, \ldots,$ is dense in $\mathcal{H}$. Therefore, the operator H, considered as a Hamiltonian on $\mathcal{H}$, has purely singular continuous spectrum.

We would like to know whether the constructed in the previous section cyclic state $\psi = \psi(r)$ is decaying. It turns out that the decay of ψ depends on the ratio of dissection. In Antoniou and Suchanecki (2002) we have given the full answer to this question describing the algebraic properties of the ratio of dissection r that decide about the decay properties of the corresponding state ψ. We present below the algebraic characterization of decaying states associated with the Cantor-type sets with a constant ratio of dissection. First, however, recall some basic facts from algebraic number theory (see, for example, Stewart nd Tall, 1979).

An algebraic integer is a root of an equation of the form

$$a_n x^n + a_{n-1}x^{n-1} + \cdots + a_0 = 0, \tag{9}$$

where a_k are integer numbers and $a_n = 1$. If α is a root of the polynomial (9) which is irreducible, i.e., there is no polynomial of degree $m < n$ with integer coefficients and the leading coefficient having α as a root, then the other roots of (9) are called the conjugates of α. An algebraic integer $\alpha > 1$ such that each its conjugate α', $\alpha' \neq \alpha$, satisfies $|\alpha'| < 1$ is called an *S-number*.

We have (Antoniou and Suchanecki, 2002)

Proposition 2. *Let $\psi(r)$ be the cyclic state of the Hamiltonian H with the spectrum of Cantor type with a constant ratio of dissection r. The state $\psi(r)$ is nondecaying if and only if $1/r$ is an S-number. Correspondingly, $\psi(r)$ is decaying if and only if $1/r$ is not an S-number.*

To prove this proposition it is enough to show (Antoniou *et al.*, 1999; Zygmund, 1968) that the Fourier transform of the spectral measure $\mu_\psi(r)$, which is of the form

$$\mu_{\psi(r)}(t) = \frac{1}{2\pi}\int_0^{2\pi} e^{itx} dF(x) = \frac{1}{2\pi} e^{\pi it} \prod_{k=1}^{\infty} \cos \pi t r^{k-1}(1-r) \tag{10}$$

converges to 0 or not when $1/r$ is not or is, accordingly, an S-number. The behavior of (10) as $t \to \infty$ is, in turn, equivalent to the behavior of the function

$$u \mapsto \prod_{k=1}^{\infty} \cos \pi u r^k \tag{11}$$

as $u \to \infty$ (Zygmund, 1968). In this way the proof of Proposition 2 reduces to the proof that (11) converges if and only if $1/r$ is not an S-number and can be found in Salem (1983) (see also Zygmund, 1968).

The S-numbers include all integers $n > 1$. It is also easy to verify that any number of the form $\frac{1}{2}(p + \sqrt{p^2 + 4q})$, where $p, q \epsilon \mathbb{N}, q \leq p$, is an S-number (its only conjugate is $\frac{1}{2}(p - \sqrt{p^2 + 4q}) < 1$). For example the golden number $\frac{\sqrt{5}+1}{2}$ is an S-number. On the other hand, none of the irreducible rationals $\frac{p}{q}$ with $p, q \in \mathbb{N}\backslash\{1\}$ is an S-number. In fact such $\frac{p}{q}$ is not even an algebraic integer (Stewart and Tall, 1979). Therefore if the ratio of dissection is any irreducible rational number $k/n < 1/2$, where k and n are integers different from 1, then the corresponding cyclic state is decaying.

A natural question is whether decaying and nondecaying states can be in some sense separated. It is surprising that the answer to this question is negative. This follows from the fact that since the irreducible rationals are dense in IR, they are also arbitrary close to S-numbers. In other words, for any dissection rate r determining a nondecaying state $\psi(r)$ and any $\varepsilon > 0$ one can find a dissection rate r' with $|r - r'| < \varepsilon$, such that the state $\psi(r')$ is nondecaying.

It follows from the above considerations that it is impossible to isolate nondecaying states associated with Cantor-type sets. On the other hand the decaying states can be separated from nondecaying. In fact we have (Antoniou and Suchanecki, 2002)

Proposition 3. *For each ratio of dissection r, which determines a decaying state $\psi(r)$, there is $\delta > 0$ such that the nearest ratio of dissection r', which determines a nondecaying state $\psi(r')$ is at the distant larger than δ.*

In the proof of the above proposition we use the fact that the set of S-numbers is closed (Salem, 1983). Now, let r be a ratio of dissection which determines a decaying state. Since $\frac{1}{r}$ does not belong to the set of S-numbers, there is a neighborhood, i.e., some numbers α, β such that $\alpha < \frac{1}{r} < \beta$, and such that the interval (α, β) has empty intersection with the class S. This implies that the rate of dissection r is separated from the nearest ratio of dissection of a nondecaying state by some positive number $\delta = \delta(r)$.

2. CONCLUDING REMARKS

Proposition 2 shows how inappropriate the computational modeling of decaying and nondecaying states can be. In the case of Hamiltonians with fractal spectra the construction of decaying states amounts to the construction of a Cantor-type set with a given ratio of dissection. According to Proposition 3 it is possible to construct such decaying states $\psi(r)$ for which the distance δ of r from the nearest inverse of an S-number is within the computing accuracy. However any construction of a nondecaying state $\psi(r)$ for which r has an infinite dyadic expansion is completely unreliable. The reason is that we cannot perform computations on numbers with infinite dyadic expansion. Therefore any truncation of the dissection rate give us, in general, a decaying state instead. Physically speaking any finite approximation of such nondecaying state is a decaying state. Only in the infinite limit we obtain non decay. Moreover the possibility of construction of decaying states is also rather theoretical because very little is known about the localization of S-numbers.

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