

# On a “Structure Intermediate Between Quasiperiodic and Random”

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This paper proves rigorously that the structure factor of the “structure intermediate between quasiperiodic and random” introduced by Aubry, Godrèche, and Luck is purely singular continuous apart from a delta function at zero for “most” choices of the parameters. The result is based on a proof that a flow under a step function over an irrational circle rotation is weakly mixing for “most” parameters, and on the Wonderland Theorem.

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**KEY WORDS:** Diffraction; aperiodic structures; flow under a function; periodic approximation; weak mixing; singular continuous spectrum.

## 1. INTRODUCTION

Aubry *et al.*<sup>(1, 2)</sup> have considered a model of atoms on the line defined by an irrational rotation  $\alpha$  on the circle  $\mathbb{T} = \mathbb{R}/\mathbb{Z}$  in which the positions  $x_n$  of the atoms are given by

$$x_n - x_{n-1} = 1 + \xi 1_{(0, \beta)}(n\alpha) \quad (1)$$

where  $0 < \beta < 1$  and  $x_0, \xi \in \mathbb{R}$  are parameters. Changing  $x_0$  translates the structure. They have shown by a combination of scaling arguments and numerical work that for  $\beta = 1/2$ ,  $\alpha = \tau^{-1}[\tau = (\sqrt{5} + 1)/2]$ , and irrational  $\xi$  the “structure factor”

$$S := \lim_{L \rightarrow \infty} (2L)^{-1} \left| \sum_{x_k \in [-L, L]} e^{-2\pi i q x_k} \right|^2 \quad (2)$$

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is a purely singular continuous measure (apart from a delta function at 0). More generally they suggest that  $S$  is purely discrete if and only if  $\beta = k\alpha \pmod{1}$  for some  $k \in \mathbb{Z}$  (the “Kesten condition”<sup>(3)</sup>) and that it is continuous if the Kesten condition is not satisfied. The interest of the structure factor is that it describes how the model looks in diffraction experiments.<sup>(4, 5)</sup> Since  $S$  is absolutely continuous for random systems and purely discrete for quasiperiodic systems, Aubry *et al.* called their structure “intermediate between quasiperiodic and random”.

The main interest, in my opinion, of the work by Aubry *et al.* is their use of scaling to detect singular continuous spectrum.

This paper proves that  $S$  is purely singular continuous apart from the delta function at 0 for every irrational  $\xi$ , every  $\beta$ , and generic  $\alpha$  (Corollary 5.1). Here “generic  $\alpha$ ” means: for  $\alpha$  in a dense  $G_\delta$ , i.e., in a dense countable intersection of open sets. We also prove that  $S$  is continuous (apart from the delta function at 0) for *all* irrational  $\alpha$ , Lebesgue-a.e.  $\beta$ —depending on  $\alpha$ —and all  $\xi$  such that  $1/\xi$  is not rationally dependent on  $\alpha$ . In the special case that  $\alpha$  has bounded partial quotients the “Lebesgue-a.e.  $\beta$ ” can be replaced by “all  $\beta$  such that  $\beta \neq k\alpha$  for any  $k \in \mathbb{Z}$ ” (Corollary 4.1). In particular, this proves that  $S$  is continuous for the parameters of  $\beta = 1/2$ ,  $\alpha = \tau^{-2}$  considered by Aubry *et al.*

The principal ingredient for these results is a fairly complete determination of the parameters for which the flow under a step function is or is not weakly mixing (see Section 4). Then the Wonderland Theorem<sup>(6)</sup> gives that  $S$  is purely singular continuous apart from the delta function at 0 for generic  $\alpha$  (Proposition 5.2).

The structure of the paper is as follows. Section 2 recalls the definition of a flow under a function, sets up notation, and states some facts that will be needed later. Section 3 explains how  $S$  is related to the flow under a step function. Section 4 discusses for which parameters this flow is weakly mixing. This implies the results about the continuity of  $S$ . Section 5 uses the Wonderland theorem to prove that the flow has purely singular continuous spectrum for generic  $\alpha$ . It implies that  $S$  is purely singular continuous apart from a delta function at 0 for all  $\beta$ , all irrational  $\xi$ , and generic  $\alpha$ . The last section contains some comments on the results.

## 2. THE FLOW UNDER A FUNCTION

If  $\alpha \in \mathbb{T} = \mathbb{R} \setminus \mathbb{Z}$  and  $f: \mathbb{T} \rightarrow \mathbb{R}$  satisfies  $0 < a \leq f(x) \leq b$  for some  $a, b$  and all  $x \in \mathbb{T}$ , then the flow under the function  $f$  over the rotation  $\alpha$  is the flow  $T_t$  acting on  $\Gamma := \{(x, y) \mid x \in \mathbb{T}, 0 \leq y < f(x)\}$  by letting  $y$  increase with unit speed, and jumping from  $(x, f(x))$  to  $(x + \alpha, 0)$  whenever  $y$  hits the graph of  $f$ .<sup>(7)</sup> The Lebesgue measure  $\nu$  on  $\Gamma$  is invariant under  $T_t$ . The flow

is ergodic if and only if  $\alpha$  is irrational.<sup>(7)</sup> It is not hard to see that the flow is uniquely ergodic if it is ergodic, if  $f$  is Riemann integrable.

Let  $\mathcal{H} = L^2(\Gamma, \nu)$  and denote by  $U_t$  the strongly continuous group of unitary operators on  $\mathcal{H}$  associated to  $T_t$  by  $U_t f := f \circ T_t$ . An eigenfunction (for the flow, or of  $U$ ) is a  $\phi \in \mathcal{H}$  for which there is a  $\lambda \in \mathbb{R}$  (the eigenvalue) such that

$$U_t \phi = e^{2\pi i \lambda t} \phi \tag{3}$$

Eigenfunctions can be chosen such that (3) holds for all  $(x, y) \in \Gamma$  and all  $t$  (ref. 7, Section VI.2). If  $\phi$  is an eigenfunction with eigenvalue  $\lambda$ , then  $e^{-2\pi i \lambda y} \phi(x, y)$  is independent of  $y$ . So

$$\psi(x) := e^{-2\pi i \lambda y} \phi(x, y) \tag{4}$$

is a measurable function on  $\mathbb{T}$ , which is in  $L^2(\mathbb{T})$  since  $\phi \in \mathcal{H}$ . It satisfies

$$\psi(x + \alpha) = e^{2\pi i \lambda f(x)} \psi(x) \tag{5}$$

Conversely every  $\psi \in L^2(\mathbb{T})$  satisfying (5) gives an eigenfunction through (4) (ref. 7, Section VI.3). The flow is called weakly mixing if the constants are the only eigenfunctions of the flow.

Every  $\phi \in \mathcal{H}$  defines a spectral measure  $\mu_\phi$  on  $\mathbb{R}$  by

$$\int e^{2\pi i \lambda t} d\mu_\phi(\lambda) = (\phi, U_t \phi) \tag{6}$$

This is a real, bounded measure. Like any measure, it can be decomposed into a discrete part, an absolutely continuous part, and a singular continuous part. If  $\phi$  is an eigenfunction with eigenvalue  $\lambda$ , then  $\mu_\phi$  is a Dirac delta function at  $\lambda$ . The smallest closed subspace of  $\mathcal{H}$  containing all eigenfunctions is denoted by  $\mathcal{H}_d$ . A spectral measure  $\mu_\phi$  is purely discrete if and only if  $\phi \in \mathcal{H}_d$ . Note that  $\mathcal{H}_d$  is never empty, since the constants are eigenfunctions for  $\lambda = 0$ . For this reason it is convenient to introduce the symbol  $\mathcal{H}^\perp$  to denote the orthogonal complement in  $\mathcal{H}$  of the constant functions. Similarly,  $\mathcal{H}_{ac}$  and  $\mathcal{H}_{sc}$  are the largest closed subspaces for which  $\mu_\phi$  is absolutely continuous and purely singularly continuous, respectively. The three spaces are invariant under  $U$  and  $\mathcal{H} = \mathcal{H}_d + \mathcal{H}_{ac} + \mathcal{H}_{sc}$ . If  $\mathcal{H} = \mathcal{H}_d$ , then the flow is said to have purely discrete spectrum; if  $\mathcal{H}_d$  consists only of the constant functions then the flow is said to have purely continuous spectrum (strictly speaking, on  $\mathcal{H}^\perp$ ). This means that  $\mu_\phi$  is continuous for all  $\phi$  with  $\int \phi d\nu = 0$ , or, equivalently, that for all  $\phi \in \mathcal{H}$  the only possible discrete part of  $\mu_\phi$  is a delta function at 0. If the flow has

purely continuous spectrum then it is said to have purely singular continuous spectrum if  $\mathcal{H}_{ac} = \emptyset$ . This means that  $\mu_\phi$  is purely singular continuous for all  $\phi \in \mathcal{H}$  apart from a possible delta function at 0, which is absent if and only if  $\int \phi \, d\nu = 0$ , i.e., if  $\phi \in \mathcal{H}^\perp$ .

### 3. THE FLOW AND THE STRUCTURE FACTOR

The structure factor (2) is the Fourier transform (in the sense of tempered distributions) of the autocorrelation

$$\gamma = \lim_{L \rightarrow \infty} (2L)^{-2} \sum_{x_j, x_k \in [-L, L]} \delta_{x_j - x_k} \tag{7}$$

of the measure  $\mu = \sum_{n \in \mathbb{Z}} \delta_{x_n}$ .<sup>(5)</sup> Note that  $\gamma$  exists by the unique ergodicity of irrational circle rotations:  $\gamma = \sum n_a \delta_a$ , where the summation is over all possible vectors  $a$  of the form  $x_j - x_k$  and  $n_a$  is the density with which  $a$  occurs in the structure. It is clear that  $\gamma$  does not change if the structure is translated [nor when  $n\alpha$  is replaced by  $n\alpha + \theta$  in (1)]. The structure factor  $S = \hat{\gamma}$  has a delta function at 0 of weight  $n_0$ , the particle density.<sup>(5)</sup>

This section explains how  $S$  can be obtained as a limit of spectral measures of the flow under the function  $f(x) = 1 + \xi 1_{[0, \beta)}(x)$ . That will prove the following proposition.

**Proposition 3.1.** If the flow under  $f$  is weakly mixing, then  $S$  is continuous apart from the delta function at 0. If the flow has purely singular continuous spectrum on  $\mathcal{H}^\perp$ , then  $S$  is purely singular continuous apart from the delta function at 0.

*Proof.* Let  $\omega \geq 0$  be a  $C^\infty$ -function with support in  $|x| < \eta \ll 1$ . Put a copy of  $\omega$  at every  $x_n$ ; i.e., consider the function

$$\rho := \omega * \mu \tag{8}$$

where  $*$  denotes convolution. Its autocorrelation is given by<sup>(5)</sup>

$$\begin{aligned} \gamma_\rho(x) &= \lim_{L \rightarrow \infty} (2L)^{-1} \int_{-L}^L \rho(y+x) \overline{\rho(y)} \, dy \\ &= (\omega * \bar{\omega}) * \gamma \end{aligned}$$

where  $\bar{\omega}(x) = \overline{\omega(-x)}$  and the bar denotes complex conjugation. Now the structure factor of  $\rho$  is  $\hat{\gamma}_\rho = |\hat{\omega}|^2 \hat{\gamma}$ .

Observe that  $|\hat{\omega}|^2 > 0$  in some neighborhood  $(-a, a)$  of the origin, since  $\hat{\omega}(0) = \int \omega \, dx > 0$ . For  $\varepsilon > 0$  the function  $\omega_\varepsilon(x) := \varepsilon^{-1} \omega(x/\varepsilon)$  has Fourier transform  $\hat{\omega}_\varepsilon(\zeta) = \varepsilon \hat{\omega}(\varepsilon \zeta)$ , so  $|\hat{\omega}_\varepsilon(\zeta)|^2 > 0$  for  $\zeta \in (-a/\varepsilon, a/\varepsilon)$ . Hence

$\hat{\gamma}$  is purely (singular) continuous on  $\mathbb{R} \setminus \{0\}$  if and only if  $\hat{\gamma}_{\rho_\varepsilon}$  is purely (singular) continuous on  $(-a/\varepsilon, 0) \cup (0, a/\varepsilon)$  for every  $\varepsilon > 0$ .

Define  $g_\varepsilon \in \mathcal{H}$  by

$$g_\varepsilon(x, y) := \begin{cases} \omega_\varepsilon(y) & \text{if } 0 \leq y < \eta \\ \omega_\varepsilon(y - f(x)) & \text{if } f(x) - \eta < y \leq g(x) \\ 0 & \text{otherwise} \end{cases} \quad (9)$$

Choose  $u_0 = 0$ . If  $\rho_\varepsilon = \omega * \mu$ , then  $\rho_\varepsilon(t) = (U_t g_\varepsilon)(0, 0)$ ; replacing  $(0, 0)$  by  $T_{\omega}(0, 0)$  translates the structure. Now

$$\gamma_{\rho_\varepsilon}(x) = \lim_{L \rightarrow \infty} (2L)^{-1} \int_{-L}^L \rho_\varepsilon(t+x) \overline{\rho_\varepsilon(t)} dt \quad (10)$$

$$= \lim_{L \rightarrow \infty} (2L)^{-1} \int_{-L}^L U_t(\overline{g_\varepsilon} U_x g_\varepsilon)(0, 0) dt \quad (11)$$

$$= (g_\varepsilon, U_x g_\varepsilon) \quad (12)$$

Equation (12) holds because (i) the flow is uniquely ergodic and (ii) the function  $g_\varepsilon$  is continuous (ref. 8, Theorem 1.8.2).

If the flow is weakly mixing (has purely singular continuous spectrum on  $\mathcal{H}^\perp$ ), then the Fourier transform of (12) is a measure that is purely (singular) continuous apart from a delta function at 0. This also shows that  $S = \hat{\gamma}$  is purely discrete if the flow has purely discrete spectrum. ■

The significance of Proposition 3.1 is that it links  $S$  to spectral measures of a dynamical system—the flow under  $f$ —that can be explicitly analyzed. Given any configuration of points (in any dimension) with a hard-core condition, one can consider the set of all its translates and close it in the topology of hard-sphere particle systems (see, e.g., ref. 9, Appendix B). This gives a compact metric space with an action of  $\mathbb{R}^d$  by translations. Dworkin <sup>(12)</sup> showed in this general setup that the Fourier transform of the autocorrelation of (8) is a spectral measure of the unitary group action of  $\mathbb{R}^d$  on the  $L^2$ -space of an ergodic measure on this metric space.

#### 4. SPECTRUM OF THE FLOW

This section studies for which parameters  $\alpha, \beta, \xi$  the flow under the function  $1 + \xi 1_{[0, \beta)}(x)$  is weakly mixing or not. The flow is weakly mixing if (5) has no solutions  $\psi \in L^2(\mathbb{T})$  for any  $\lambda \neq 0$ ; it is not weakly mixing if there is  $\lambda \neq 0$  for which (5) has a solution in  $L^2(\mathbb{T})$ . To make use of results from ergodic theory we need some definitions.

A measurable function  $g: \mathbb{T} \rightarrow \mathbb{T}$  is called a multiple of a coboundary (in, e.g., ref. 11) or a projective coboundary (in, e.g., ref. 12) if there is an  $a \in \mathbb{R}$  for which there is a measurable  $\psi: \mathbb{T} \rightarrow \mathbb{T}$  such that

$$\psi(x + \alpha) = e^{2\pi i a} g(x) \psi(x) \tag{13}$$

(Lebesgue-a.e.). The function  $g$  is called a coboundary if there is a measurable solution to (13) with  $a = 0$ . Proving existence or nonexistence of solutions to (13) for given  $g$  and  $\alpha$  is a classic problem in ergodic theory (see, e.g., refs. 13–15).

The question for which parameters  $\alpha, \beta, s$  the function  $g_{\beta, s}(x) := \exp\{2\pi i s 1_{[0, \beta)}(x)\}$  is a multiple of a coboundary has been studied, among others, by Merrill.<sup>(11)</sup> Since  $f(x) = \xi 1_{[0, \beta)}(x) + 1$ , Eq. (5) can be written as

$$\psi(x + \alpha) = e^{2\pi i \lambda} g_{\beta, \lambda \xi}(x) \psi(x) \tag{14}$$

and we see that  $\lambda$  is an eigenvalue of the flow under  $f$  if and only if  $g_{\beta, \lambda \xi}$  is a particular multiple of a coboundary, namely with  $a = \lambda$ . In this way, results from ref. 11 can be used to prove that the flow under  $f$  is or is not weakly mixing for certain parameters. [Note that  $|\psi(x)|$  is constant a.e. since  $\alpha$  is irrational, so  $\psi \in L^2(\mathbb{T})$  if  $\psi$  is measurable.]

The solvability of (13) depends on the continued-fraction representation  $[a_1, a_2, \dots]$  of  $\alpha$ . The  $a_n$  are called partial quotients of  $\alpha$ . We say that  $\alpha$  has bounded partial quotients if there is an  $N$  such that  $a_n < N$  for all  $n$ . Otherwise it has unbounded partial quotients. Lebesgue-a.e.  $\alpha$  has unbounded partial quotients (ref. 16, Theorem 196). A continued fraction is called periodic if there are integers  $k, L > 0$  such that  $a_l = a_{l+k}$  for all  $l > L$ . A number  $\alpha$  has a periodic continued-fraction representation if and only if it is a quadratic number, i.e., if  $p\alpha^2 + q\alpha + r = 0$  for some  $p, q, r \in \mathbb{Z}$  (ref. 16, Theorem 176).

**Proposition 4.1.** For every irrational  $\alpha$ , if  $\beta = \{k\alpha\}$  for some integer  $k$ , then for all  $\xi \in \mathbb{R}$  the flow under  $f$  has eigenvalues  $\lambda = (m\alpha + n)/(\xi\{k\alpha\} + 1)$ , with  $n, m \in \mathbb{Z}$ .

*Proof.* If  $\beta = \{k\alpha\}$  then for all  $s \in \mathbb{R}$  the function  $g_{\beta, s}$  is a multiple of a coboundary with  $a = -s\{k\alpha\} + m\alpha + n, m, n \in \mathbb{Z}$  [see pp. 326–327 of ref. 11; the solutions to (13) are also given there]. If  $\alpha, \beta = \{k\alpha\}$  and  $\xi$  are fixed, then  $s = \lambda\xi$  and the condition that  $a = \lambda$  imply  $\lambda = (m\alpha + n)/(\xi\{k\alpha\} + 1)$ . ■

The numbers  $\alpha$  and  $1/\xi$  are called rationally independent if  $m\alpha + n/\xi = p$  has no solutions  $m, n, p \in \mathbb{Z}$  except  $m = n = p = 0$ . Otherwise they are called rationally dependent. Note that rational independence

implies that  $\xi$  is irrational if  $\alpha$  is irrational. The next proposition shows that the flow under  $f$  is not weakly mixing if  $\alpha$  and  $1/\xi$  are rationally dependent.

**Proposition 4.2.** For every irrational  $\alpha$  and every  $\beta$ , the flow under  $f$  has an eigenvalue  $\lambda = m/\xi$  for some  $m \in \mathbb{Z}$  if and only if  $\alpha$  and  $1/\xi$  are rationally dependent.

*Proof.* If  $\lambda = m/\xi$  is an eigenvalue of the flow, then there is by (5) a  $\psi \in L^2(\mathbb{T})$  such that

$$\psi(x + \alpha) = e^{2\pi i \lambda} \psi(x) \tag{15}$$

since  $f = \xi 1_{[0, \beta)} + 1$ . This means that  $\lambda$  is an eigenvalue of rotation over  $\alpha$ . Hence  $\lambda = r\alpha + s$ ,  $r, s \in \mathbb{Z}$  (see, e.g., ref. 7) and  $\alpha$  and  $1/\xi$  are rationally dependent.

Conversely, if  $\alpha$  and  $1/\xi$  are rationally dependent, then  $m/\xi = r\alpha + s$  for some  $m, r, s \in \mathbb{Z}$ . Since  $r\alpha + s$  is an eigenvalue of rotation over  $\alpha$ , there is a  $\psi \in L^2(\mathbb{T})$  such that

$$\psi(x + \alpha) = e^{2\pi i (r\alpha + s)} \psi(x) \tag{16}$$

and this  $\psi$  satisfies (5) if  $\lambda = m/\xi$ . ■

**Proposition 4.3.** If  $\alpha$  has bounded partial quotients and is rationally independent of  $1/\xi$ , then the flow under  $f$  is weakly mixing if and only if  $\beta \neq \{k\alpha\}$  for all  $k \in \mathbb{Z}$ .

*Proof.* If the flow under  $f$  is weakly mixing, then  $\beta \neq \{k\alpha\}$  by Proposition 4.1.

Conversely, if  $\beta \neq k\alpha$ , then Theorem 2.4 in ref. 11 gives that  $g_{\beta, s}$  is not a multiple of a coboundary if  $s \neq 0$ . Since  $\xi > 0$ ,  $s = \lambda\xi = 0 \pmod{1}$  gives  $\lambda = m/\xi$  for some  $m \in \mathbb{Z}$ . But by Proposition 4.2,  $\lambda = m/\xi$  is an eigenvalue of the flow under  $f$  if and only if  $\alpha$  and  $\xi$  are rationally dependent. ■

Note that this proposition shows that  $\hat{\gamma}$  is continuous apart from a delta function at 0 in the case  $\beta = 1/2$ ,  $\alpha = \tau^{-2}$  if and only if  $1/\xi$  is rationally independent of  $\alpha$ . These are the parameters considered by Aubry *et al.*<sup>(1, 2)</sup> Since almost every  $\alpha$  has unbounded partial quotients Proposition 4.3 applies to a set of  $\alpha$ 's of Lebesgue measure 0. Note, however, that Proposition 4.3 suffices to prove the results in the next section.

To treat the case of  $\alpha$ 's with unbounded partial quotients, we shall use the following result of Katok and Stepin.<sup>(14)</sup> The condition on  $\alpha$  is equivalent to  $\alpha$  having unbounded partial quotients.

**Proposition 4.4.**<sup>(14)</sup> Suppose there is a sequence  $p_n/q_n$  of irreducible fractions such that  $\lim_{n \rightarrow \infty} q_n^2 |\alpha - p_n/q_n| = 0$ . Suppose that  $\beta$  satisfies

$$\limsup_{n \rightarrow \infty} \min_{k=0}^{q_n-1} q_n |\beta - k/q_n| > 0 \tag{17}$$

Let  $h(x) := \eta_1 1_{[0, \beta)}(x) + \eta_2 1_{[\beta, 1)}(x)$ , where  $|\eta_1| = |\eta_2| = 1$  and  $\eta_1 \neq \eta_2$ . Then the equation

$$\psi(x + \alpha) = h(x) \psi(x) \tag{18}$$

has no nonzero solutions  $\psi \in L^2(\mathbb{T})$ .

**Proposition 4.5.** The set  $B := \{\beta \in \mathbb{T} \mid \beta \text{ satisfies (17)}\}$  has Lebesgue measure 1.

*Proof.* Since  $\alpha$  has unbounded partial quotients, we can assume that  $q_n/q_{n+1} < 1/2$  for all  $n$  by taking a subsequence of the  $p_n/q_n$ . Let  $\delta < 1/4$ . Then  $B \subset B' := \{\beta \mid \limsup_{j \rightarrow \infty} \min_{k=0}^{q_j-1} |q_j \beta - k| \leq \delta\}$ . We will show that the Lebesgue measure  $|B'|$  of  $B'$  is zero.

Let  $B_j := \{\beta \mid \min_{k=0}^{q_j-1} |q_j \beta - k| \leq \delta\}$ . Then  $B' = \bigcup_{j=1}^{\infty} \bigcap_{k=0}^{\infty} B_{j+k}$ . Note that  $B_j$  consists of  $q_j$  closed intervals of length  $2\delta/q_j$ . If  $I$  is any interval, then  $|B_j \cap I|$  is not more than the number of intervals of  $B_j$  intersecting  $I$  times  $2\delta/q_j$ , i.e.,  $|B_j \cap I| \leq \lceil q_j |I| \rceil 2\delta/q_j$ , where  $\lceil x \rceil$  is the integer satisfying  $\lceil x \rceil - 1 \leq x < \lceil x \rceil$ . Hence

$$\begin{aligned} &|B_j \cap B_{j+1} \cap \dots \cap B_{j+k}| \\ &\leq q_j \lceil q_{j+1} 2\delta/q_j \rceil \lceil q_{j+2} 2\delta/q_{j+1} \rceil \dots \lceil q_{j+k} 2\delta/q_{j+k-1} \rceil 2\delta/q_{j+k} \\ &\leq q_j (q_{j+1} 2\delta/q_j + 1) (q_{j+2} 2\delta/q_{j+1} + 1) \dots (q_{j+k} 2\delta/q_{j+k-1} + 1) 2\delta/q_{j+k} \\ &\leq (2\delta + \frac{1}{2})^k 2\delta \rightarrow 0 \quad \text{as } k \rightarrow \infty \end{aligned}$$

This proves that  $|B'| = 0$ . ■

**Proposition 4.6.** If  $\alpha$  has unbounded partial quotients, then for Lebesgue-a.e.  $\beta$  the flow under  $f$  is weakly mixing for all  $\xi$  such that  $1/\xi$  is rationally independent of  $\alpha$ .

*Proof.* Let  $\alpha$  have unbounded partial quotients and suppose that  $1/\xi$  is rationally independent of  $\alpha$ . Let  $\beta \in B$ ; the set  $B$  has full Lebesgue measure by Proposition 4.5.

Suppose the flow is not weakly mixing. Then there is a  $\lambda \neq 0$  and a  $\psi \in L^2(\mathbb{T})$  such that (5) holds. Proposition 4.4 shows this can only happen if  $\eta_1 = \eta_2$  where  $\eta_1 = e^{2\pi i \lambda (1 + \xi)}$  and  $\eta_2 = e^{2\pi i \lambda}$ . It follows that  $\lambda = m/\xi$  for



some  $m \in \mathbb{Z}$ . But then  $\alpha$  and  $1/\xi$  are rationally dependent by Proposition 4.2. ■

**Corollary 4.1.** If  $\alpha$  is rationally independent of  $1/\xi$ , then the structure factor  $S$  is a continuous measure apart from a delta function at 0:

- (i) If  $\alpha$  has bounded partial quotients, if and only if  $\beta \neq k\alpha \pmod{1}$  for any integer  $k$ .
- (ii) If  $\alpha$  has unbounded partial quotients, for Lebesgue-a.e.  $\beta$ .

Proposition 4.6 also follows from results by Veech<sup>(15)</sup> and Steward,<sup>(17)</sup> (see ref. 11 and pp. 792–793 in ref. 18). In fact, these results give the slightly stronger conclusion that the flow is also weakly mixing for all irrational  $\alpha$ , all  $\xi$  such that  $1/\xi$  is rationally independent of  $\alpha$ , and all rational  $\beta$  (Theorem 1.12.5.d in ref. 18). Note, however, that we have not excluded the possibility that the flow can fail to be weakly mixing for some  $\alpha$  with unbounded partial quotients, a  $\xi$  such that  $1/\xi$  is rationally independent of  $\alpha$ , and a  $\beta$  that is not a multiple of  $\alpha$ .

## 5. PURELY SINGULAR CONTINUOUS SPECTRUM

Simon's Wonderland Theorem<sup>(6)</sup> can now be used to prove that for generic  $\alpha$  the flow has purely singular continuous spectrum on  $\mathcal{H}^\perp$ . Knill<sup>(19)</sup> has recently used the Wonderland theorem to give a new proof of the fact that, in the weak topology, measure preserving transformations generically have purely singular continuous spectrum in the orthocomplement of the constant functions. The Wonderland Theorem can be formulated as follows. Let  $\mathcal{X}$  be a complete metric space of self-adjoint operators on a separable Hilbert space for which convergence in the metric implies strong resolvent convergence. Suppose the sets of operators that have purely continuous spectrum and purely discrete spectrum are dense in  $\mathcal{X}$ . Then there is a generic set in  $\mathcal{X}$  of operators that have purely singular continuous spectrum. (Recall that a set is called generic if it is a dense  $G_\delta$ .)

**Proposition 5.1.** Suppose that for some  $\beta, \xi$  the flow is weakly mixing for a dense set of  $\alpha$ . Then there is a generic  $A_{\beta, \xi} \subset \mathbb{T}$  such that the flow with parameters  $\alpha, \beta, \xi$  has purely singular continuous spectrum on  $\mathcal{H}^\perp$  for all  $\alpha \in A_{\beta, \xi}$ .

*Proof.* Note that  $\mathcal{H}$  depends on  $\beta$  and  $\xi$  but not on  $\alpha$ . Take  $\mathcal{H}^\perp$  as Hilbert space. Write  $U_t^\alpha$  to stress the dependence on  $\alpha$ . By Stone's theorem

there is a self-adjoint operator  $C^\alpha$  on  $\mathcal{H}$  such that  $U_t^\alpha = \exp(2\pi i t C^\alpha)$ . The spectral measures  $d\mu_\phi^\alpha$  of  $C^\alpha$ , defined by

$$\int e^{2\pi i \lambda t} d\mu_\phi^\alpha = (\phi, e^{2\pi i t C^\alpha} \phi)$$

(see e.g., p. 263 in ref. 20), coincide with those defined for  $U_t^\alpha$  in (6). Let  $\mathcal{X} = \{C^\alpha \mid \alpha \in \mathbb{T}\}$  with the metric of  $\mathbb{T}$ . If  $\alpha_n \rightarrow \alpha$  in  $\mathbb{T}$ , then  $U_t^{\alpha_n} \rightarrow U_t^\alpha$  strongly in  $\mathcal{H}$  for each  $t$ . This implies that  $C^{\alpha_n} \rightarrow C^\alpha$  in strong resolvent sense (see, e.g., Theorem VIII.21 in ref. 20).

By the hypothesis of weak mixing, there is dense set of  $U_t^\alpha$  with purely continuous spectrum on  $\mathcal{H}^\perp$ . For rational  $\alpha$  the flow is quasiperiodic ( $\mathbb{T}$  partitions into finitely many intervals on which the period is constant) and therefore has purely discrete spectrum. Hence the Wonderland Theorem implies the conclusion of the theorem. ■

**Proposition 5.2.** For every  $\beta \in \mathbb{T}$  and every irrational  $\xi$  there is a generic set  $A_{\beta, \xi} \subset \mathbb{T}$  such that for all  $\alpha \in A_{\beta, \xi}$  the flow with parameters  $\alpha, \beta, \xi$  has purely singular continuous spectrum on  $\mathcal{H}^\perp$ .

*Proof.* The numbers  $\alpha_p = \sqrt{p} \pmod{1}$ , with  $p$  a prime number, are rationally independent. There is at most one prime  $p_1$  such that  $m\alpha_{p_1} = k\beta \pmod{1}$  for some non-zero integers  $m, k$ , and at most one prime  $p_2$  such that  $\alpha_{p_2}$  is rationally dependent on  $1/\xi$ . Hence there is a prime  $p_3$  such that  $\alpha = \alpha_{p_3}$  is rationally independent of  $\beta$  and  $1/\xi$ . Then  $m\alpha_{p_3} = k\beta \pmod{1}$  has no solutions in  $\mathbb{Z}$  other than  $m = k = 0$ . Since any quadratic number has a periodic continued fraction and hence bounded partial quotients, the flow under  $f$  with parameters  $n\alpha, \beta, \xi$  is weakly mixing by Proposition 4.3. The numbers  $n\alpha$  are dense in  $\mathbb{T}$ . Hence Proposition 5.1 gives the desired result. ■

**Corollary 5.1.** For every  $\beta \in \mathbb{T}$  and every irrational  $\xi$  the structure factor  $S$  is a purely singular continuous measure apart from a delta function at 0 for a generic set of  $\alpha$ 's.

## 6. DISCUSSION

To conclude, we would like to mention some results from the literature. Von Neumann<sup>(7)</sup> proved that the flow under  $f$  is weakly mixing for all irrational  $\alpha$  if  $f$  is piecewise  $C^1$  with points of discontinuity  $x_1, \dots, x_n$  at which (i) the left and right limits of  $f'$  exist and (ii) it has jumps  $\delta_i = \lim_{x \uparrow x_i} f(x_i) - \lim_{x \downarrow x_i} f(x_i)$  such that  $\sum_{i=1}^n \delta_i \neq 0$ . This shows that it is not really remarkable for a model of atoms on the line of the form  $u_n - u_{n-1} = f(n\alpha)$  to have a structure factor that is continuous apart from the delta

function at zero. Von Neumann<sup>(7)</sup> gives an example of a continuous function for which the flow is weakly mixing for certain  $\alpha$ . Indeed, he conjectures that the flow should be weakly mixing for “most” continuous functions. In this direction Kočergin<sup>(21)</sup> has proved that for every irrational  $\alpha$  and every  $L^1$ -function  $f > 0$  on  $\mathbb{T}$  there exists a continuous function  $\Delta f$  with  $\sup_{x \in \mathbb{T}} |\Delta f(x)|$  arbitrarily small such that the flow under  $f + \Delta f$  is strongly mixing, hence weakly mixing. This shows that discontinuities in  $f$  are not necessary for weak mixing.

Kočergin<sup>(22)</sup> has also shown that the flow is not strongly mixing if  $f$  has bounded variation. It follows that  $\mathcal{H}_{sc} \neq \emptyset$  (cf. ref. 23, p. 50) if  $f(x) = 1 + \xi 1_{[0, \beta)}(x)$  whenever  $\alpha$ ,  $\beta$ , and  $\xi$  are such that the flow under  $f$  is weakly mixing. So if  $\mu$  is replaced by  $\rho$  of (8), which amounts to modeling the structure by electron clouds instead of pointlike atoms, then the structure factor (i.e., the Fourier transform of  $\gamma_\rho$ ) typically has a singular continuous part whenever the flow is weakly mixing. Here “typically” means that every ball in  $\mathcal{H}$  around  $g_\omega$  [ $g_\omega = g_1$  in (9)] contains a  $g'_\omega$  for which the structure factor has a singular continuous part.

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