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Arbitrarily Slow Decay of Correlations in Quasiperiodic Systems

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For diffusive motion in random media it is widely believed that the velocity autocorrelation function $c(t)$ exhibits power law decay as time $t \to \infty$. We demonstrate that the decay of $c(t)$ in quasiperiodic media can be arbitrarily slow within the class of integrable functions. For example, in $d = 1$ with a potential $V(x) = \cos x + \cos kx$, there is a dense set of irrational k's such that the decay of $c(k, t)$ is slower than $1/t^{(1+\varepsilon)}$ for any $\varepsilon > 0$. The irrationals producing such a slow decay of $c(k, t)$ are *very* well approximated by rationals.

KEY WORDS: Long-time tails; quasiperiodic media; velocity autocorrelation function; time-dependent transport coefficients; modulated structures.

1. It has been noted[1–6] that the velocity autocorrelation function (VAF) for particle motion in a variety of random systems exhibits a power-law long-time tail. For example, it is argued in ref. 4 that the VAF $c(t)$ for diffusion in stationary random media in $\mathbb{R}^d$ decays in time like $1/t^{(1+d/2)}$ as $t \to \infty$. In this paper we remark that for diffusion in certain quasiperiodic media, the VAF has no such universal law, be it algebraic, logarithmic, or whatever. In particular, for diffusion $\mathbf{X}_t$ in the drift field $\nabla V(\mathbf{x})$, where $V(\mathbf{x})$ is a suitable quasiperiodic potential in $\mathbb{R}^d$, the "VAF" $c(t) = \langle\!\langle \nabla V(\mathbf{X}_0) \cdot \nabla V(\mathbf{X}_t) \rangle\!\rangle$ (where $\langle\!\langle \cdot \rangle\!\rangle$ denotes averaging over diffusion paths and the phase in the potential) exhibits decay which is arbitrarily slow within the class of integrable functions. Furthermore, our arguments indicate that the rate of decay depends on the Diophantine properties of

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the irrational parameters which characterize the quasiperiodicity—the better the approximation by rationals, the slower the decay. We also obtain similar results for other transport coefficients.

For example, in $d=1$ with $V(x)=\cos x+\cos kx$, there is a dense set Γ of irrational k's for which the following statements hold. First, for $k\in\Gamma$, the decay of $c(k, t)$ is slower than $1/t^{(1+\varepsilon)}$ for any $\varepsilon>0$. Related to $c(k, t)$ is the time-dependent diffusion coefficient $\mathscr{D}(k, t)=\langle\langle \mathbf{X}_t^2\rangle\rangle/t$, which converges as $t\to\infty$ to the effective diffusion coefficient D^*. For $k\in\Gamma$, $|\mathscr{D}(k, t)-D^*|$ decays to zero *extremely* slowly, for example, more slowly than $1/\log\cdots\log t$, for any fixed number of iterations of the logarithm. This is arbitrarily slow decay with no condition of integrability. The Laplace (Fourier) transform of the VAF corresponds to the frequency (ω)-dependent effective diffusivity $D(\omega)$ (conductivity $\sigma(\omega)$) of the medium. For $k\in\Gamma$, $|D(k,\omega)-D^*|$ decays to zero as $\omega\to 0$ more slowly, for example, than $1/\log\cdots\log(1/\omega)$, for any fixed number of iterations of the logarithm. This situation markedly contrasts that in random media,[4] where it is believed that $|D(\omega)-D^*|\sim\omega^{d/2}$ as $\omega\to 0$. In addition to the above quantities, we have also obtained similar results concerning the behavior near the origin of the spectral measure of ∇V for the (suitably defined) self-adjoint generator of the process.

The above statements about rates of decay are actually easy consequences of much stronger results which we state in the body of the paper and have the following form. For example, in the one-dimensional case, there exists a dense set of k's such that $c(k, t)\to 0$ more slowly than *any* positive function integrable on $[0, \infty)$ which is "expressible," i.e., that can be written down, either explicitly or implicitly.

Our results are based on the discontinuous dependence of D^* on the wavelengths of V, which was observed in ref. 7. For example, with $V(x)=\cos x+\cos kx$ in $\mathbb{R}^1$, $D^*(k)$ has the same value $\bar{D}$ for all irrational k, but differs from $\bar{D}$ and depends on k for k rational, where it is thus discontinuous. Moreover, $D^*(k)$ is continuous at irrational k. This pathology is reflected in the behavior of $\mathscr{D}(k, t)$ $[\to_{t\to\infty} D^*(k)]$ for irrational k that are well approximated by rationals k_n. In this case $\mathscr{D}(k, t)$ has "plateaus" around the values $D^*(k_n)$.[7,8] The closer k_n is to k (i.e., the closer the rational approximant), the longer the corresponding plateau. The existence of irrationals k for which $\mathscr{D}(k, t)$ decays arbitrarily slowly then follows easily. The behavior of $D(k,\omega)$, $\omega\to 0$, arises in a similar manner.

2. Let $\mathbf{X}_t$ be the position of a particle at time t diffusing in a medium with a bounded (sufficiently smooth) potential V according to

$$d\mathbf{X}_t=-\sigma_0\nabla V(\mathbf{X}_t)+(2D_0)^{1/2}\,d\mathbf{W}_t \qquad (1)$$

where $\mathbf{W}_t$ is standard Brownian motion, $\langle W_t^i W_t^j \rangle = \delta_{ij} t$, $i, j = 1,..., d$, and σ_0 and D_0 are the "bare" mobility and diffusion constants. The density $\rho(\mathbf{x}, t)$ associated with (1) satisfies the diffusion equation

$$\partial\rho/\partial t = D_0 \Delta\rho + \nabla \cdot (\sigma_0 \nabla V \rho) \tag{2}$$

which has the equilibrium density $\rho \sim \exp(-\beta V)$, $\beta = \sigma_0/D_0$, as per the Einstein relation. With $\mathbf{X}_0 = 0$, $\rho(\mathbf{x}, 0) = \delta(\mathbf{x})$.

It is known[9-11] that for V periodic, quadiperiodic, or stationary random ergodic,

$$\mathscr{D}_{ij}(V, t) = \langle\!\langle X_t^i X_t^j \rangle\!\rangle / t \xrightarrow[t \to \infty]{} D_{ij}^*(V) \tag{3}$$

where $\mathsf{D}^*(V)$ is a positive-definite effective diffusion tensor. [The actual trajectories are asymptotically Brownian with diffusion tensor $\mathsf{D}^*(V)$.]

Consider quasiperiodic $V(\mathbf{x}) = \hat{V}(x_1 \mathbf{k}_1 + \cdots + x_d \mathbf{k}_d) = \hat{V}(\mathsf{k}\mathbf{x})$ in $\mathbb{R}^d$, where $\hat{V}$ is a smooth function on the unit n-torus $T^n = \mathbb{R}^n/\mathbb{Z}^n$, which is equivalent to the unit n-cube with opposite faces identified; $\mathbf{k}_1,..., \mathbf{k}_d$ are linearly independent vectors in $\mathbb{R}^n$; and $\mathsf{k} = [\mathbf{k}_1,..., \mathbf{k}_d]$. The potential $V(\mathbf{x})$ can naturally be regarded as a member of a family $V_k(\mathbf{x}, \boldsymbol{\theta})$ depending on phase $\boldsymbol{\theta} \in T^n$ defined by $V_k(\mathbf{x}, \boldsymbol{\theta}) \equiv V(\mathsf{k}\mathbf{x} + \boldsymbol{\theta})$. The matrix k defines a group action $\tau_{\mathbf{x}}$ of $\mathbb{R}^d$ on T^n by $\tau_{\mathbf{x}} \boldsymbol{\theta} = \theta + \mathsf{k}\mathbf{x}$. This action leaves Lebesgue measure $\mathbf{d}\theta$ invariant. It is also ergodic relative to $\mathbf{d}\theta$ when the equations $\mathbf{k}_i \cdot \mathbf{j} = 0,..., \mathbf{k}_d \cdot \mathbf{j} = 0$ have no simultaneous integral solutions $\mathbf{j} \in \mathbb{Z}^n$. We say that k is "irrational" in this case and is "rational" otherwise. When $n = 2$, $d = 1$, and $\mathsf{k} = \mathbf{k} = [k_1, k_2]^T$, such as for $V(x) = \cos k_1 x + \cos k_2 x$, then k is irrational when k_2/k_1 is irrational, and is rational when k_2/k_1 is rational. When $n > d + 1$, k can have various "degrees" of rationality, depending on the dimension of the ergodic components of $\tau_{\mathbf{x}}$.

Let $\mathbf{X}_t$ be the diffusion process associated with $V_{\mathsf{k}}(\cdot, \boldsymbol{\theta})$. We shall be interested in the trace of the left side of (3).

$$\mathscr{D}(V_{\mathsf{k}}, t) = \langle\!\langle \mathbf{X}_t^2 \rangle\!\rangle / t \tag{4}$$

where $\langle\!\langle \cdot \rangle\!\rangle$ denotes averaging of the phase $\boldsymbol{\theta}$ over T^n with weight $\sim \exp[-\beta \hat{V}(\boldsymbol{\theta})]$ (which defines the equilibrium measure on T^n), as well as over Brownian motion paths $\mathbf{W}$. $\mathscr{D}(V_{\mathsf{k}}, t)$ has the representation

$$\mathscr{D}(V_{\mathsf{k}}, t) = D^*(\mathsf{k}) + \frac{1}{t} \int_0^t ds \int_s^\infty du\, c(u) \tag{5}$$

where $c(t) = \langle\langle \nabla V(\mathbf{X}_0) \cdot \nabla V(\mathbf{X}_t) \rangle\rangle$, $D^*(\mathsf{k}) = \mathrm{tr}[\mathsf{D}^*(\mathsf{k})]$, $\sigma_0 = 1$, and $D_0 = \frac{1}{2}$ in (1). We shall also be interested in[12]

$$D(\omega) = \int_0^\infty e^{-\omega t}\, c(t)\, dt \tag{6}$$

3. In the statement of our results, we utilize the notion of an expressible function, i.e., one which can be defined, either explicitly or implicity, using standard mathematical symbols. An example of such an implicitly defined function is one that satisfies, say, a polynomial or integral equation which has a unique solution. Since any expressible function is determined by a finite string of symbols from a finite alphabet, there are only countably many such functions. (To make this notion completely precise, one should consider a formal language, but we do not wish to go into this here.)

It is easy to see that $\mathscr{D}(\mathsf{k}, t)$ is continuous in k and $t \geqslant 0$. Moreover, $\lim_{t \to \infty} \mathscr{D}(\mathsf{k}, t) = D^*(\mathsf{k})$ exists, with $D^*(\mathsf{k})$ having the discontinuity properties described above. Now, it can be shown that any function with these properties exhibits arbitrarily slow decay.

More precisely, for any two functions $g(t)$ and $h(t)$, we write $g(t) >_{\text{i.o.}} h(t)$ as $t \to \infty$ if there is a sequence $t_n \to \infty$ such that $g(t_n) > h(t_n)$ for all n. The expression $g >_{\text{i.o.}} h$ says that h does not dominate g, not even asymptotically ($t \to \infty$). Then:

(*) If $f(\mathsf{k}, t)$ is any function continuous in $\mathsf{k} \in \mathbb{R}^N$ and $t \in [0, \infty)$, with $\lim_{t \to \infty} f(\mathsf{k}, t) = f(\mathsf{k})$ discontinuous for a dense set of k's, there is a dense set $\Gamma \subset \mathbb{R}^N$ such that for each $\mathsf{k} \in \Gamma$, $|f(\mathsf{k}, t) - f(\mathbf{k})| >_{\text{i.o.}} g(t)$ for every expressible g with $\lim_{t \to \infty} g(t) = 0$.

We may similarly define $g(\omega) >_{\text{i.o.}} h(\omega)$ as $\omega \to 0$ and formulate an analogous result for a function $f(\mathsf{k}, \omega)$ with $\omega \to 0$.

The discontinuous nature of $D^*(\mathsf{k})$ arises as follows. In one dimension, there is an exact formula (see, e.g., ref. 7) for D^*. In the example $V_k(x) = \hat{V}(x, kx)$, $\hat{V}(x, y) = \cos x + \cos y$, this formula involves integrations of functions of $\hat{V}$ on T^2 over a trajectory of the flow $(\dot{\theta}_1, \dot{\theta}_2) = (1, k)$, which is ergodic only when k is irrational. In this case, the integration is over all of T^2. However, when k is rational, the trajectory degenerates to a closed orbit, over which the integrals are different from their values over all of T^2, which is the source of the discontinuity.

There is no such general argument in higher dimensions $d \geqslant 2$, where an explicit formula for $\mathsf{D}^*(\mathsf{k})$ is absent. Nevertheless, we believe for the following reasons that, as in one dimension, there is typically a dense set of k's in $\mathbb{R}^N$ at which $\mathsf{D}^*(\mathsf{k})$ is discontinuous. First, as argued in ref. 7, the integrals involved in representation formulas for D^* suffer the same "discontinuity" in the domain of integration, caused by the breakdown of ergodicity for rational k, as in one dimension. It would thus be *surprising* if the discontinuous behavior of $D^*(\mathrm{k})$ is *not* generic. Second, in addition to the specific examples of the discontinuity provided in ref. 7, we constructed in ref. 8 a whole class of two-component media for which the effective conductivity $\sigma^*(\mathrm{k})$ is discontinuous. Henceforth, we shall consider only quasiperiodic potentials in $\mathbb{R}^d$, $d \geqslant 1$, generated by $\hat{V}$ which are "typical," i.e., for which $D^*(\mathrm{k})$ is discontinuous on a dense set in $\mathbb{R}^N$.

Let $\hat{V}$ on T^n be typical. Then from the previous discussion we may conclude that there is a dense set Γ of k's having the following properties:

(i) For any $\mathrm{k} \in \Gamma$, $\phi(\mathrm{k}, t) = |\mathscr{D}(\mathrm{k}, t) - D^*(\mathrm{k})| >_{\text{i.o.}} g(t)$ for every positive, expressible g with $\lim_{t \to \infty} g(t) = 0$.

(ii) For any $\mathrm{k} \in \Gamma$, $c(\mathrm{k}, t) >_{\text{i.o.}} h(t)$ for every positive, expressible h integrable on $[0, \infty)$.

(iii) For any $\mathrm{k} \in \Gamma$, $|D(\mathrm{k}, \omega) - D^*(\mathrm{k})| >_{\text{i.o.}} g(\omega)$ for every positive, expressible g with $\lim_{\omega \to 0} g(\omega) = 0$.

In order to state the last result about the spectral measure, let $\hat{L} = \frac{1}{2}\Delta_{\mathrm{k}} - \nabla_{\mathrm{k}} V \cdot \nabla_{\mathrm{k}}$, where ∇_k is gradient arising from the action τ_{x} of $\mathbb{R}^d$ on T^n, and Δ_{k} is the Laplacian corresponding to ∇_{k}. $\hat{L}$ is self-adjoint on $L^2(T^n, d\rho)$, where ρ is the equilibrium measure on T^n, and has negative spectrum contained in $(-\infty, 0]$ with projection-valued measures P_λ on $(-\infty, 0]$. We consider the spectral measure of P_λ in the state $\nabla_{\mathrm{k}} \hat{V}$, $\mu(d\lambda) = \langle \nabla_{\mathrm{k}} \hat{V} \cdot P(d\lambda) \nabla_{\mathrm{k}} \hat{V} \rangle$, where $\langle \cdot \rangle$ here means integration over T^n with respect to ρ. Using the semigroup $\exp(\hat{L}t) = \int \exp(\lambda t)\, dP_\lambda$, one can write

$$c(t) = \int_{-\infty}^{0} e^{\lambda t}\, d\mu(\lambda) \tag{7}$$

Now, for typical $\hat{V}$:

(iv) For any $\mathrm{k} \in \Gamma$, $\mu_{\mathrm{k}}(d\lambda) >_{\text{i.o.}} \nu(d\lambda)$ as $\lambda \to 0$ for every expressible measure ν on $(-\infty, 0]$ such that $\int_{-\infty}^{0} \nu(d\lambda)/|\lambda| < \infty$.

[By $\mu >_{\text{i.o.}} \nu$ as $\lambda \to 0$ we mean there is a sequence of intervals (t_n, s_n), $t_n \to 0$, such that $\mu(t_n, s_n) > \nu(t_n, s_n)$ for all n.]

The logical relationship among our results is as follows: (*) $\Rightarrow$ (i) $\Rightarrow$ (ii) $\Rightarrow$ (iv) and (*) $\Rightarrow$ (iii). Properties (i) and (iii) are direct consequences of (*). Property (i) $\Rightarrow$ (ii) because the failure of (ii) would provide, via (5), an expressible positive function dominating $\phi(\mathrm{k}, t)$. Similarly, using (7), (ii) $\Rightarrow$ (iv). [The fact that the same set Γ is appropriate in (iii) and in (i), (ii), and (iv) follows from a slightly improved version of (*).]

We remark that no contradiction is involved in (i)–(iv), even though, for example, $\phi(\mathrm{k}, t)$ in (i) satisfies $\lim_{t \to \infty} \phi(\mathrm{k}, t) = 0$ and $\phi(\mathrm{k}, t) >_{\text{i.o.}} \phi(\mathrm{k}, t)$

is clearly false. The point is that the k in Γ are not expressible and there is therefore no reason why functions defined in terms of these k should be.

To emphasize how slowly these functions decay, observe that, say for (i), $\phi(\mathrm{k}, t) >_{\text{i.o.}} (\log \cdots \log t)^{-1}$, $t \to \infty$, for any fixed number of iterations of the logarithm. Indeed, no law, be it algebraic, logarithmic, or whatever, can capture the behavior of $\phi(\mathrm{k}, t)$, not even in the weak sense of upper bounds.

While Γ is dense, it is of Lebesgue measure zero, so that it is analytically "small." However, under a further assumption about $D^*(\mathrm{k})$, Γ can be shown to be dense $\mathcal{G}_\delta$ set, i.e., it is a dense countable intersection of open sets, which is topologically "large." This assumption, which may be found in ref. 13, is typically true in one dimension, and is presumably true in higher dimensions.

Detailed proofs of the results in this paper are given in ref. 13.

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