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Classical Transport in Quasiperiodic Media

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Abstract. Classical transport coefficients such as the effective conductivity or diffusivity of a quasiperiodic medium were observed [1] to depend discontinuously on the frequencies of the quasiperiodicity. For example, for a one-dimensional medium with a potential $V(x) = \cos x + \cos kx$, the effective diffusion coefficient $D^*(k)$ has the same value $\overline{D}$ for all irrational k, but differs from $\overline{D}$ and depends on k for k *rational*, where it is thus discontinuous. Here we review some recent progress [2–4] in understanding this discontinuous behavior. In particular, a class of examples which explicitly exhibit the discontinuity in dimensions $d \geq 2$ is constructed. In addition, we examine some rather surprising consequences of the discontinuity for the rate of approach to limiting behavior of diffusion or conduction in quasiperiodic media as time or volume becomes infinite. It is found that these rates can be "arbitrarily slow," which contrasts with the power laws observed for random media. A very general theorem yielding such slow rates is described, and its consequences for quantum transport are also discussed.

1. Introduction. Quasiperiodic systems exhibit fascinating properties and arise in many settings. An example of such a system is a one-dimensional medium with a potential $V(x) = \cos x + \cos kx$. When k is irrational, $V(x)$ is quasiperiodic, and when k is rational, $V(x)$ is periodic. Mathematically, quasiperiodic media represent a special case of stationary random ergodic media, and can be thought of as "interpolating" between periodic and random. One way in which quasiperi-

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odicity can arise is in a modulated structure, i.e., a periodic structure such as a crystal lattice which is perturbed or modulated periodically with a period different from that of the underlying structure. For example [5], $Ti_{50}Ni_{47}Fe_3$ alloy subjected to charge density waves forms a modulated structure, where the periods of the alloy and the wave can be commensurate (rationally related) or incommensurate (irrationally related). Another way in which quasiperiodicity can arise is apparently through the lattice structure itself, as evidenced by the exciting discovery of so-called "quasicrystals" [6], where the atoms are believed to be arranged in a quasiperiodic manner.

In systems such as modulated structures where the period of the applied wave can be tuned to be commensurate or incommensurate with that of the underlying structure, one is interested in how the physical properties of the system change as this is done. It was observed in [1] that classical transport coefficients of a quasiperiodic medium in $\mathbb{R}^d$ with a potential $V(\underline{x})$ and/or conductivity $\sigma(\underline{x})$ depend discontinuously on the frequencies of the quasiperiodicity. For example, with $V(x) = \cos x + \cos kx$ in $d = 1$, the effective diffusion coefficient $D^*(k)$ has the same value $\overline{D}$ for all *irrational* k but differs from $\overline{D}$ and depends on k for k *rational*, where it is thus discontinuous. (Furthermore, $D^*(k)$ is continuous at irrational k.)

Here we give an overview of some recent progress [2–4] in analyzing this discontinuous behavior displayed by quasiperiodic media. The results are of two different types. The first type concerns explicit examples of the discontinuity in dimensions $d \geq 2$, where the general argument given in [1] for $d = 1$ does not apply. In these systems, for example in $d = 2$, we take a plane slice of a three-dimensional checkerboard of cubes with conductivities σ_1 and σ_2. When the plane, characterized by a matrix $\mathbf{k}$, is at an "irrational" angle, the resulting quasiperiodic medium has an effective conductivity tensor $\boldsymbol{\sigma}^*(\mathbf{k})$ which is invariant under interchange of σ_1 and σ_2. The Keller interchange equality [7, 8] then yields the surprising result that $\det(\boldsymbol{\sigma}^*)$ has the same value $\sigma_1\sigma_2$ for all *irrational* planes. The discontinuity is obtained by exhibiting a particular rational angle for which $\det(\boldsymbol{\sigma}^*)$ has a value different from $\sigma_1\sigma_2$. The checkerboard is but a special case of a general class of examples that yield the discontinuity in this way.

The second class of results concerns some striking consequences of the discontinuity for the rate of approach to limiting behavior of diffusion or conduction in quasiperiodic media as time or volume becomes infinite. For example, we consider diffusion $\underline{X}_t$ in a quasiperiodic potential $V(\underline{x})$ in $\mathbb{R}^d$, where $\lim_{t\to\infty} \mathscr{D}(t) = \lim_{t\to\infty} E[\underline{X}_t^2]/t = D^* = \mathrm{tr}\,(\mathbf{D}^*(V))$, $\mathbf{D}^*(V)$ is the effective diffusion tensor, and E denotes averaging over diffusion paths and the phase in the potential (see Section 2). We find that when the irrational parameters characterizing $V(\underline{x})$ are very well approximated by rationals, $\mathscr{D}(t)$ approaches its limit through a series of "plateaus" which correspond to the rational approximants, where the better the approximation, the longer the plateau. In fact, say in $d = 1$ with $V(x) = \cos x + \cos kx$, there is a dense set Γ such that for each $k \in \Gamma$, $|\mathscr{D}(k, t) - D^*(k)|$, roughly speaking, approaches zero as $t \to \infty$ "arbitrarily slowly," i.e., more slowly than any positive function $g(t) \to 0$ as $t \to \infty$ which can be *explicitly* written down (expressible). For example, when $k \in \Gamma$, $|\mathscr{D}(k, t) - D^*(k)| \to 0$ more slowly than $1/\log \cdots \log t$, for any fixed number of iterations of the logarithm. (Note that the k's in Γ are not expressible.) We can also prove corresponding statements for related functions such as the "velocity" autocorrelation function as $t \to \infty$ and the frequency (ω) dependent diffusivity as $\omega \to 0$, as well as for $|\boldsymbol{\sigma}^*(\mathbf{k}, L) - \boldsymbol{\sigma}^*(\mathbf{k})| \to 0$ as $L \to \infty$ for the length (L) dependent conductivity $\boldsymbol{\sigma}^*(\mathbf{k}, L)$ of a finite sample of a quasiperiodic medium.

The arbitrarily slow approach that we see for quasiperiodic media is in marked contrast to the behavior in random systems [**9–12**], where the rates of approach are widely believed to have power law structure. Our results demonstrate that in quasiperiodic systems, the functions characterizing the approach to limiting behavior obey no such universal law, be it algebraic, logarithmic, or whatever.

The above results about rates of approach are based on a very general theorem about any function $f(\mathbf{k}, t)$ which is continuous in $\mathbf{k}$ and t, but for which $F(\mathbf{k}) = \lim_{t\to\infty} f(\mathbf{k}, t)$ is discontinuous on a dense set of $\mathbf{k}$'s. In this case, there is always a dense set of $\mathbf{k}$'s for which the rate of approach of $f(\mathbf{k}, t)$ to $F(\mathbf{k})$ is arbitrarily slow.

Due to the generality of the above theorem, any system which exhibits discontinuous limiting behavior can display the arbitrarily slow approach. For example, in quantum transport in quasiperiodic potentials [**13, 14**], it is found that the nature of the wave functions satisfying the time dependent Schrödinger equation with a potential $q(x) = \cos x + \alpha \cos(kx + \theta)$ depends very sensitively on the rationality of k. Presumably, similar results to the above hold for appropriately defined time dependent functions characterizing the approach to limiting behavior, which will be briefly discussed in the lattice case at the end.

2. Formulation. We first formulate the notion of a quasiperiodic local conductivity or potential field in $\mathbb{R}^d$. Subsequently we consider the effective conductivity and diffusion problems in such quasiperiodic media.

Let $\hat{\sigma}(\underline{\theta})$ be a function on the unit n-torus $T^n = \mathbb{R}^n/\mathbb{Z}^n$, $\underline{\theta} \in T^n$, which we identify with its periodic extension to all of $\mathbb{R}^n$. The local conductivity field $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta})$ on $\mathbb{R}^d$ is obtained from $\hat{\sigma}$ via

$$\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta}) = \hat{\sigma}(\underline{\theta} + \mathbf{k}\underline{x}) = \hat{\sigma}(\tau_{\underline{x}}^{\mathbf{k}}\underline{\theta}) \, , \tag{2.1}$$

with translations on $\mathbb{R}^n$ given by

$$\tau_{\underline{x}}^{\mathbf{k}}\underline{\theta} = \underline{\theta} + \mathbf{k}\,\underline{x} = \underline{\theta} + \sum_{i=1}^{d} \underline{k}_i x_i \, , \tag{2.2}$$

where $\mathbf{k}$ is an n by d matrix $\mathbf{k} = [\underline{k}_1^{\mathrm{T}}, \ldots, \underline{k}_d^{\mathrm{T}}]$, $\underline{k}_i \cdot \underline{k}_j = 0$, $i \neq j$, $\underline{k}_i \in \mathbb{R}^n$. A local potential field $V_{\mathbf{k}}(\underline{x}, \underline{\theta})$ on $\mathbb{R}^d$ is obtained similarly from some $\widehat{V}(\underline{\theta})$ on T^n.

The "flow" on T^n induced by (2.2) leaves invariant Lebesgue measure $d\underline{\theta}$ on T^n. It is also ergodic relative to $d\underline{\theta}$ when the equations $\underline{k}_1 \cdot \underline{i} = 0, \ldots, \underline{k}_d \cdot \underline{i} = 0$ have no simultaneous integral solutions $\underline{i} \in \mathbb{Z}^n$, $\underline{i} \neq 0$ **[15]**. We say that $\mathbf{k}$ is "irrational" in this case, i.e., when $\tau_{\underline{x}}^{\mathbf{k}}$ is ergodic, and is "rational" otherwise. When $n = 2$, $d = 1$ and $\mathbf{k} = \underline{k} = [k_1, k_2]^{\mathrm{T}}$, $\mathbf{k}$ is irrational when k_2/k_1 is irrational. When $n > d + 1$, $\mathbf{k}$ can have various degrees of rationality depending on the dimension of the ergodic components of $\tau_{\underline{x}}^{\mathbf{k}}$.

Given $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta})$, we consider the electric field $\underline{E}_j(\underline{x}, \underline{\theta}) = \widehat{\underline{E}}_j(\underline{\theta} + \mathbf{k}\underline{x})$ and current field $\underline{J}_j(\underline{x}, \underline{\theta}) = \widehat{\underline{J}}_j(\underline{\theta} + \mathbf{k}\underline{x})$ satisfying

$$\underline{J}_j(\underline{x}, \underline{\theta}) = \sigma_{\mathbf{k}}(\underline{x}, \underline{\theta}) \underline{E}_j(\underline{x}, \underline{\theta}), \tag{2.3}$$

$$\nabla \cdot \underline{J}_j = 0, \tag{2.4}$$

$$\nabla \times \underline{E}_j = 0, \tag{2.5}$$

$$⨍_{\mathbb{R}^d} \underline{E}_j(\underline{x}, \underline{\theta}) d\underline{x} = \underline{e}_j \, , \tag{2.6}$$

where $\underline{e}_j$ is a unit vector in the jth direction in $\mathbb{R}^d$, and the integral in (2.6) is an infinite volume average of $\underline{E}_j(\underline{x}, \underline{\theta})$ over $\mathbb{R}^d$.

We shall be most interested in two-component media, arising from

$$\hat{\sigma}(\underline{\theta}) = \sigma_1 \hat{\chi}_1(\underline{\theta}) + \sigma_2 \hat{\chi}_2(\underline{\theta}) , \tag{2.7}$$

where σ_1, $\sigma_2 > 0$, and the indicator functions $\hat{\chi}_i(\underline{\theta})$, $i = 1, 2$, satisfy $\hat{\chi}_1 + \hat{\chi}_2 = 1$. Due to the absence of smoothness in this case, equations (2.4) and (2.5) should be understood to hold weakly in an appropriate subspace of $L^2(T^n, d\underline{\theta})$ [16], where $\frac{\partial}{\partial x_i}$ is identified with the generator of translations in the direction of $\underline{k}_i$.

The effective conductivity tensor $\boldsymbol{\sigma}^* \equiv \boldsymbol{\sigma}^*(\mathbf{k}, \underline{\theta})$ is defined via

$$\boldsymbol{\sigma}^* \underline{e}_j = \fint_{\mathbb{R}^d} \sigma_{\mathbf{k}}(\underline{x}, \underline{\theta}) \underline{E}_j(\underline{x}, \underline{\theta})\, d\underline{x} , \tag{2.8}$$

which is symmetric. If $\mathbf{k}$ is irrational, $\boldsymbol{\sigma}^*(\mathbf{k}, \underline{\theta})$ is almost surely (with respect to $d\underline{\theta}$) a constant independent of $\underline{\theta}$, while if $\mathbf{k}$ is rational, $\boldsymbol{\sigma}^*$ will depend on $\underline{\theta}$ only through the ergodic component to which $\underline{\theta}$ belongs. In any dimension [16],

$$\boldsymbol{\sigma}^*(\mathbf{k}, \underline{\theta}) = \lim_{L\to\infty} \boldsymbol{\sigma}^*(L, \mathbf{k}, \underline{\theta}) , \tag{2.9}$$

where $\boldsymbol{\sigma}^*(L, \mathbf{k}, \underline{\theta})$ is the conductivity of a sample of side $2L$ of $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta})$, which in one dimension has the form

$$[\sigma^*(L, \underline{k}, \underline{\theta})]^{-1} = \frac{1}{2L} \int_{-L}^{L} [\sigma_{\underline{k}}(x, \underline{\theta})]^{-1} dx , \tag{2.10}$$

and the convergence in (2.9) is in $L^2(T^n, d\underline{\theta})$. The integration on the right side of (2.10) can be viewed as integration over a trajectory of the flow $\dot{\underline{\theta}} = \underline{k}$, which is ergodic only when $\underline{k}$ is irrational. In this case, the integration is over all of T^n, so that

$$[\sigma^*]^{-1} = \int_{T^n} [\hat{\sigma}(\underline{\theta})]^{-1} d\underline{\theta} \tag{2.11}$$

is independent of $\underline{k}$. However, when $\underline{k}$ is rational, the trajectory degenerates to a closed orbit, over which the integration is different from its value over all of T^n, which is the source of the discontinuity.

We shall also be interested in diffusion in a potential $V_{\mathbf{k}}(\underline{x}, \underline{\theta}) = \widehat{V}(\underline{\theta} + \mathbf{k}\underline{x})$, $\underline{x} \in \mathbb{R}^d$, $\underline{\theta} \in T^n$, which is uniformly bounded and smooth, i.e., having uniformly bounded derivatives to third order. Given $V_{\mathbf{k}}$, we consider the $\mathbb{R}^d$-valued process $\underline{X}_t$ governed by

$$d\underline{X}_t = -\nabla V_{\mathbf{k}}(\underline{X}_t) dt + d\underline{W}_t , \tag{2.12}$$

where $\underline{X}_0 = 0$ and $\underline{W}_t$ is standard Brownian motion with mean 0 and covariance matrix tI, where I is the identity. The transition density $u(\underline{x}, t)$ satisfies the (forward) equation

$$\frac{\partial u}{\partial t} = L^* u , \qquad \lim_{t \downarrow 0} u(\underline{x}, t) = \delta(\underline{x}) , \tag{2.13}$$

where

$$L^* = \frac{1}{2}\Delta + \nabla \cdot (\nabla V_{\mathbf{k}} \cdot) . \tag{2.14}$$

For $\underline{X}_t$ governed by (2.12), $\varepsilon \underline{X}_{t/\varepsilon^2}$ converges as $\varepsilon \to 0$ [see, e.g., **17**] to $\underline{W}_t(\mathbf{D}^*(\mathbf{k}))$, with $\mathbf{D}^*(\mathbf{k}) = \lim_{t\to\infty} \mathbf{D}(\mathbf{k}, t)$, $D_{ij}(\mathbf{k}, t) = E[X_t^i X_t^j]/t$, where E denotes expectation over Brownian motion paths in (2.12) as well as an average over T^n with respect to the "equilibrium" measure

$$\mu(d\underline{\theta}) = e^{-2\widehat{V}(\underline{\theta})} d\underline{\theta} \Big/ \int_{T^n} e^{-2\widehat{V}(\underline{\theta})} d\underline{\theta} . \tag{2.15}$$

We shall be interested in $\mathscr{D}(\mathbf{k}, t) = \mathrm{tr}(\mathbf{D}(\mathbf{k}, t))$ and $D^*(\mathbf{k}) = \mathrm{tr}(\mathbf{D}^*(\mathbf{k}))$. As in the case of conduction, there is an exact formula for $D^*(\underline{k})$ in $d = 1$ [see, e.g., **1**],

$$[D^*(\underline{k})]^{-1} = \fint e^{2V_{\underline{k}}} dx \fint e^{-2V_{\underline{k}}} dx . \tag{2.16}$$

3. Higher-dimensional examples of discontinuous behavior of $\sigma^*(\mathbf{k})$. We now construct explicit examples of systems for which $\sigma^*(\mathbf{k})$ is discontinuous in $\mathbf{k}$. First we look at the one-dimensional case $\sigma_k(x) = \hat{\sigma}(x, kx)$ where $\hat{\sigma}$ is a checkerboard on T^2, and then we consider its higher-dimensional analogs.

3.1. $d = 1$. Let $\hat{\sigma}(\underline{\theta})$ on the unit 2-torus T^2 be defined as follows. Divide T^2 into four equal squares with the common vertex $(\frac{1}{2}, \frac{1}{2})$. On the squares let $\hat{\sigma}(\underline{\theta})$ take the positive values σ_1 or σ_2 in a checkerboard arrangement, with, say, σ_2 on the square nearest the origin. Extend this by periodicity to the whole plane, $\mathbb{R}^2$, and define

$$\sigma_k(x) = \sigma_k(x, \underline{\theta} = \underline{0}) = \hat{\sigma}(x, kx) , \tag{3.1}$$

which we visualize as the restriction of $\hat{\sigma}$ to a trajectory of slope k passing through the origin.

Now for $\sigma_k(x)$ in (3.1),

$$[\sigma^*(k)]^{-1} = p_1(k)/\sigma_1 + p_2(k)/\sigma_2 , \tag{3.2}$$

where $p_j(k)$ is the proportion of length that the line of slope k in $\mathbb{R}^2$ spends in regions (squares) where $\hat{\sigma} = \sigma_j$, $j = 1, 2$, for the above described checkerboard. For further simplicity we assume that $\sigma_1 = 1$ and $\sigma_2 = \infty$.

Then we have

THEOREM 3.1. *For $\sigma_k(x) = \hat{\sigma}(x, kx)$ with $\hat{\sigma}$ the above checkerboard of squares of $\sigma_1 = 1$ and $\sigma_2 = \infty$, and $k > 0$,*

(3.3)
$$\frac{1}{\sigma^*(k)} = \begin{cases} \frac{1}{2}, & k \text{ irrational} \\ \frac{1}{2} - \frac{1}{2pq}, & k = \frac{p}{q},\ p, q = \text{odd, relatively prime integers} \\ \frac{1}{2}, & k = \frac{p}{q}, \text{ otherwise.} \end{cases}$$

The proof, by D. Barsky, is contained in the Appendix of [2].

3.2. $d = 2$. The analog of the checkerboard for T^3 is obtained by dividing it into eight equal cubes with common vertex $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ with $\hat{\sigma}$ taking the values σ_1 and σ_2 in a checkerboard fashion. Given $\mathbf{k}$ and this $\hat{\sigma}$, (2.1) defines $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta})$, which is quasiperiodic when $\mathbf{k}$ is irrational and periodic when the coordinates of both $\underline{k}_1 = (k_{11}, k_{21})$ and $\underline{k}_2 = (k_{12}, k_{22})$ are rational.

As indicated in the Introduction, we obtain a discontinuity in $\det(\boldsymbol{\sigma}^*)$ by first examining it for $\mathbf{k}$ irrational, and then by exhibiting a particular rational for which its value is separated from those in the irrational case.

Our principal tool will be the Keller interchange equality [7, 8]: let $\boldsymbol{\sigma}^*(\sigma_1, \sigma_2)$ be the effective conductivity tensor of any ergodic two-component material and let $\boldsymbol{\sigma}^*(\sigma_2, \sigma_1)$ be the effective tensor of the material with σ_1 and σ_2 interchanged. Then

$$\sigma_1^*(\sigma_1, \sigma_2)\sigma_2^*(\sigma_2, \sigma_1) = \sigma_1\sigma_2, \tag{3.4}$$

where $\sigma_1^* \le \sigma_2^*$ are the eigenvalues of the symmetric matrix $\boldsymbol{\sigma}^*$. The following observation allows (3.4) to provide information about $\det(\boldsymbol{\sigma}^*)$.

LEMMA 3.1. *For $\mathbf{k}$ irrational, the quasiperiodic medium $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta})$ arising from the checkerboard on T^3 satisfies*

$$\boldsymbol{\sigma}^*(\mathbf{k}; \sigma_1, \sigma_2) = \boldsymbol{\sigma}^*(\mathbf{k}; \sigma_2, \sigma_1), \tag{3.5}$$

i.e., $\boldsymbol{\sigma}^*(\mathbf{k})$ is invariant under the interchange of the components.

PROOF. Suppose $\mathbf{k}$ is irrational; then $\boldsymbol{\sigma}^*(\mathbf{k})$ is independent of $\underline{\theta}$ almost surely. However, interchange of the components σ_1 and σ_2 is induced by $(\theta_1, \theta_2, \theta_3) \mapsto (\theta_1 + \frac{1}{2}, \theta_2, \theta_3)$ on T^3. Thus $\boldsymbol{\sigma}^*(k)$ is interchange invariant. □

As an immediate consequence of (3.4) and Lemma 3.1, we have

THEOREM 3.2. *Let* $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta}) = \hat{\sigma}(\underline{\theta} + \mathbf{k}\underline{x})$, $\underline{x} \in \mathbb{R}^2$, *where* $\hat{\sigma}$ *is a checkerboard of* σ_1 *and* σ_2 *on* T^3. *Then for all irrational* $\mathbf{k}$,

$$\det\left(\boldsymbol{\sigma}^*(\mathbf{k})\right) = \sigma_1\sigma_2 . \tag{3.6}$$

We now obtain the discontinuity. Let the cube nearest the origin in $T^3(\simeq [0, 1]^3)$ have conductivity σ_2. Consider the plane passing through $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$, and then translate it downward so that it passes through $(0, 0, 3/4)$. Let $\mathbf{k}_0$ span this plane and let $\underline{\theta}_0 = (0, 0, 3/4)$. The resulting pattern $\sigma_{\mathbf{k}_0}(\underline{x}, \underline{\theta}_0)$ is a periodic array of six-pointed stars with a central hexagon of σ_1, which is "isotropic", $\sigma^*_{ij}(\mathbf{k}_0; \underline{\theta}_0) = \sigma^*(\mathbf{k}_0; \underline{\theta}_0)\delta_{ij}$, due to the six-fold symmetry about the center of the hexagon. However, this array is *not* interchange invariant, since $p_1 = \frac{3}{4}$ while $p_2 = \frac{1}{4}$, which indicates that we should *not* expect that $\det(\boldsymbol{\sigma}^*(\mathbf{k}_0; \underline{\theta}_0)) = \sigma_1\sigma_2$.

LEMMA 3.2. *There exist* σ_1 *and* σ_2 *such that for the resulting* $\hat{\sigma}$ *and* $\mathbf{k}_0$, $\underline{\theta}_0$ *as above,*

$$\det\left(\boldsymbol{\sigma}^*(\mathbf{k}_0; \underline{\theta}_0)\right) \neq \sigma_1\sigma_2 . \tag{3.7}$$

The proof is obtained by using the isotropy of $\sigma^*_{ij}(\mathbf{k}_0, \underline{\theta}_0) = \sigma^*\delta_{ij}$ and the arithmetic mean upper bound on σ^*.

Theorem 3.2 and Lemma 3.2 together yield a discontinuity in $\det\left(\boldsymbol{\sigma}^*(\mathbf{k})\right)$ at $\mathbf{k} = \mathbf{k}_0$. Since $\det(\boldsymbol{\sigma}^*)$ is a continuous function of $\boldsymbol{\sigma}^*$, we have

COROLLARY 3.1. *Let* σ_1 *and* σ_2 *be as in Lemma* 3.2. *Then* $\boldsymbol{\sigma}^*(\mathbf{k})$ *is discontinuous at* $\mathbf{k} = \mathbf{k}_0$.

We have constructed here only one example of a rational $\mathbf{k}$ for which the discontinuity can be proven. When the denominators in the rational numbers in $\mathbf{k}$ are much larger, so that p_1 and p_2 are both very close to $\frac{1}{2}$, the proof involving the simple bound will not work, as much tighter bounds on $\boldsymbol{\sigma}^*$ would be required. Nevertheless, we expect that $\boldsymbol{\sigma}^*(\mathbf{k})$ is discontinuous at "most" rational $\mathbf{k}$.

3.3. $d \geq 3$. For $d \geq 3$, the inequality

$$\sigma^*_i(\sigma_1, \sigma_2)\sigma^*_j(\sigma_2, \sigma_1) \geq \sigma_1\sigma_2 \tag{3.8}$$

replaces (3.4), for all pairs of eigenvalues σ_i^* and σ_j^*, which was first proved by Shulgasser [18]. Since Lemma 3.1 holds for T^n as well as T^3, slight manipulation of (3.8) yields

THEOREM 3.3. *Let* $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta}) = \hat{\sigma}(\underline{\theta} + \mathbf{k}\underline{x})$, $\underline{x} \in \mathbb{R}^d$, $d \geq 3$, *where* $\hat{\sigma}$ *is a checkerboard of* σ_1 *and* σ_2 *on* T^n, $n \geq d+1$. *Then for all irrational* $\mathbf{k}$,

$$\det(\boldsymbol{\sigma}^*(\mathbf{k})) \geq (\sigma_1\sigma_2)^{d/2} . \tag{3.9}$$

The discontinuity is established by finding rational $\mathbf{k}$ for which there are σ_1 and σ_2 such that $\det(\boldsymbol{\sigma}^*(\mathbf{k})) < (\sigma_1, \sigma_2)^{d/2}$.

We remark that whenever interchange of σ_1 and σ_2 in the ambient environment $\hat{\sigma}$ on $\mathbb{R}^n$ is induced by a change in realization $\underline{\theta} \to \underline{\theta}'$, which, in fact, can be assumed to be a translation, the conclusions of Theorem 3.2 for $d = 2$ or Theorem 3.3 for $d \geq 3$ hold. This observation yields a large class of media which exhibit the discontinuity in the same way as the checkerboard.

3.4. *Phase averaging.* Let us consider explicitly the "phase" $\underline{\theta}$ of the local conductivity field, for example in one dimension with $\sigma_k(x, \underline{\theta}) = A + \cos(x + \theta_1) + \cos(kx + \theta_2)$, $A > 2$. Then $\sigma^*(k, \underline{\theta})$ will depend on $\underline{\theta}$ for k rational but not for k irrational. For the $d = 2$ checkerboard example one can see this as well by observing that for $\mathbf{k}$ irrational the relative volume fractions p_1 and $p_2 = 1 - p_1$ of σ_1 and σ_2 are independent of phase, with $p_1 = p_2 = \frac{1}{2}$, while for $\mathbf{k}$ rational they depend on phase. In other words, the discontinuity in $\boldsymbol{\sigma}^*$ arises from a discontinuity in the microgeometry, as characterized by the volume fractions. It is surprising that even after averaging over phase, the discontinuity persists, which we can prove in $d = 1$. Given $\sigma_{\underline{k}}(x, \underline{\theta}) = \hat{\sigma}(\underline{\theta} + \underline{k}x)$, $\underline{\theta} \in T^n$, define

$$\sigma^*_{\mathrm{av}}(\underline{k}) = \int_{T^n} \sigma^*(\underline{k}, \underline{\theta}) d\underline{\theta} , \tag{3.10}$$

where $\sigma^*(\underline{k}, \underline{\theta})$ is the effective conductivity of $\sigma_k(x, \underline{\theta})$. Also let $[\overline{\sigma}]^{-1}$ be given by the right side of (2.11). Then, using Jensen's inequality, we can prove

THEOREM 3.4. *For* $d = 1$,

$$\sigma^*_{\mathrm{av}}(\underline{k}) \geq \overline{\sigma} . \tag{3.11}$$

Furthermore, equality holds in (3.11) *if and only if* $\sigma^*(\underline{k}, \underline{\theta})$ *is independent of* $\underline{\theta}$ *(almost surely with respect to* $d\underline{\theta}$ *on* T^n*).*

While we believe but have not yet *proven* that the discontinuity is generally present in higher dimensions for $\sigma^*_{\text{av}}(\mathbf{k})$, which is the analog of (3.10) for $d \geq 1$, we *can* prove

THEOREM 3.5. *For* $d \geq 1$, $\sigma^*_{\text{av}}(\mathbf{k})$ *is upper semicontinuous in* $\mathbf{k}$.

4. Arbitrarily slow approach to limiting behavior. We now discuss the consequences of the discontinuity for the rate of approach to limiting behavior of diffusion and conduction in quasiperiodic media. First, we present a general result about functions with discontinuous limit from which all the results about diffusion and conduction follow.

4.1. *General results on approach to limits.* The statement of the basic theorem is aided by the following

DEFINITION. For two functions $g(t)$ and $h(t)$ with $\lim_{t\to\infty} g(t) = 0$ and $\lim_{t\to\infty} h(t) = 0$, we say that $g(t)$ is greater than $h(t)$ infinitely often,

$$g(t) \underset{\text{i.o.}}{>} h(t) \,, \tag{4.1}$$

if there is a sequence $t_n \to \infty$ such that

$$g(t_n) > h(t_n) \,, \quad \forall n \,. \tag{4.2}$$

We now state the principal result.

THEOREM 4.1. *Let* $f(\mathbf{k}, t) : \mathbb{R}^N \times [0, \infty) \to \mathbb{R}$ *satisfy the following conditions*:

(i) $f(\mathbf{k}, t)$ *is jointly continuous in* $\mathbf{k} \in \mathbb{R}^N$ *and* $t \in (0, \infty)$,
(ii) $\lim_{t\to\infty} f(\mathbf{k}, t) = F(\mathbf{k})$ *exists for all* $\mathbf{k} \in \mathbb{R}^N$,
(iii) $F(\mathbf{k})$ *is discontinuous on a dense set* $A \subset \mathbb{R}^N$.

Then for any sequence of functions $\{g_j(t), t \in [0, \infty)\}$ *with* $\lim_{t\to\infty} g_j(t) = 0$ *for each* j, *there exists a dense set* $\Gamma \subset \mathbb{R}^N$ *such that for each* $\mathbf{k} \in \Gamma$,

$$|f(\mathbf{k}, t) - F(\mathbf{k})| \underset{\text{i.o.}}{>} g_j(t) \,, \quad \forall j \,. \tag{4.3}$$

The idea of the proof is to construct each $\mathbf{k}$ in Γ as the limit of a sequence $\{\mathbf{k}_n\}$ such that F is discontinuous at each $\mathbf{k}_n$. Because of the discontinuity at $\mathbf{k}_n$, $F(\mathbf{k}_n)$ can be bounded away from $F(\mathbf{k})$ while $\mathbf{k}_n$ is arbitrarily close to $\mathbf{k}$. Then for a corresponding arbitrarily long time $f(\mathbf{k}, t)$ is close to $F(\mathbf{k}_n)$, which serves as a "plateau" for $f(\mathbf{k}, t)$. These arbitrarily long plateaus give rise to the slow decay of $|f(\mathbf{k}, t) - F(\mathbf{k})|$ as stated in the theorem.

A rather striking consequence of Theorem 4.1 involves the notion of an expressible function, i.e., one which can be defined, either explicitly or implicitly, using standard mathematical symbols. An example of such an implicitly defined function is one that satisfies, say, a differential 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. Clearly, then, we have

COROLLARY 4.1. *Let $f(\mathbf{k}, t)$ satisfy the conditions of Theorem* 4.1. *Then there exists a dense set $\Gamma \subset \mathbb{R}^N$ such that for each $\mathbf{k} \in \Gamma$,*

$$|f(\mathbf{k}, t) - F(\mathbf{k})| \underset{\text{i.o.}}{>} g(t) \;, \tag{4.4}$$

for every expressible function g with $\lim_{t\to\infty} g(t) = 0$.

We remark that there is no contradiction here because for $\mathbf{k} \in \Gamma$, $|f(\mathbf{k}, t) - F(\mathbf{k})|$ is not expressible.

To appreciate how slowly $|f(\mathbf{k}, t) - F(\mathbf{k})|$ decays for $\mathbf{k} \in \Gamma$, observe that $|f(\mathbf{k}, t) - F(\mathbf{k})| \underset{\text{i.o.}}{>} (\log\cdots\log t)^{-1}$, $t \to \infty$, for any fixed number of iterations of the logarithm. Indeed, no law, be it algebraic, logarithmic, or whatever can capture the behavior of $|f(\mathbf{k}, t) - F(\mathbf{k})|$, not even in the weak sense of upper bounds.

While Γ in the above results is dense, it is presumably of Lebesgue measure zero, so that it is analytically "small". However, by replacing condition (iii) above with a slightly stronger one, namely that $F(\mathbf{k}) = \varphi(\mathbf{k})$ for some continuous φ when $\mathbf{k} \notin A$ and $F(\mathbf{k}) \neq \varphi(\mathbf{k})$ when $\mathbf{k} \in A$, Γ can be shown to be a dense $\mathscr{G}_\delta$. That is, it is a dense, countable intersection of open sets, which is (topologically) generic.

4.2. *Diffusion in quasiperiodic potentials.* We now apply Corollary 4.1 to $\mathscr{D}(\mathbf{k}, t)$ and related functions. While conditions (i) and (ii) are clearly satisfied by, say, $\mathscr{D}(\mathbf{k}, t)$, we must discuss condition (iii). In one dimension, given any $\widehat{V}$, one can in principle check the explicit formula for $D^*(k)$ to see if it is discontinuous on a dense set in $\mathbb{R}$. Typically there is a dense set of rationals on which $D^*(k)$ is discontinuous. (In fact, typically $D^*(k)$ satisfies the stronger condition mentioned at the end of the previous section.) In higher dimensions, although an explicit formula for $\mathbf{D}^*(\mathbf{k})$ is lacking, we believe for the following reasons that typically $\mathbf{D}^*(\mathbf{k})$ is discontinuous on a dense set in $\mathbb{R}^N$. First, as argued in [1], the integrals involved in representation formulas for $\mathbf{D}^*$ are averages over trajectories on tori which depend discontinuously on $\mathbf{k}$, as in one dimension. Secondly, the findings of Section 3 for $\boldsymbol{\sigma}^*(\mathbf{k})$ (which can be defined via a diffusion process) suggest that the discontinuity is generic. Accordingly, we shall state our results for systems with this property, and make the following

Definition. A potential $\widehat{V}$ on T^n is "typical" if $\mathbf{D}^*(\mathbf{k})$ is discontinuous in $\mathbf{k}$ on a dense set in $\mathbb{R}^N$.

Now, applying Corollary 4.1 to $\mathscr{D}(t)$, we have

Theorem 4.2. *Let $\widehat{V}$ on T^n be typical. Then for diffusion $\underline{X}_t$ in $\mathbb{R}^d$ satisfying* (2.12) *with $V_{\mathbf{k}}(\underline{x}, \underline{\theta}) = \widehat{V}(\underline{\theta} + \mathbf{k}\underline{x})$, $\underline{x} \in \mathbb{R}^d$, $\underline{\theta} \in T^n$, there is a dense set $\Gamma \subset \mathbb{R}^N$ such that for every $\mathbf{k} \in \Gamma$,*

$$|\mathscr{D}(\mathbf{k}, t) - D^*(\mathbf{k})| \underset{\text{i.o.}}{>} g(t) \,, \tag{4.5}$$

for every expressible function $g(t)$ with $\lim_{t\to\infty} g(t) = 0$.

We remark that the $\mathbf{k}$'s in Γ here are irrationals that are *very* well approximated by rationals. Furthermore, in one dimension, and presumably in higher dimensions, Theorem 4.2 holds for a dense $\mathscr{G}_\delta$ set as well.

We now wish to state results corresponding to Theorem 4.2 for other functions of interest, namely the "velocity autocorrelation" function and the frequency dependent diffusivity. The "velocity autocorrelation" function (VAF) is defined by

$$c(t) = E[\nabla V(\underline{X}_0) \cdot \nabla V(\underline{X}_t)] \geq 0 \,, \tag{4.6}$$

which is related to $\mathscr{D}(\mathbf{k}, t)$ via

$$\mathscr{D}(\mathbf{k}, t) = D^*(\mathbf{k}) + \frac{1}{t}\int_0^t ds \int_s^\infty c(u)du \,. \tag{4.7}$$

Now, from Theorem 4.2 and (4.7) we can prove

Theorem 4.3. *Let $\widehat{V}$ on T^n be typical with $\underline{X}_t$ as in Theorem 4.2. Then there is a dense set $\Gamma \subset \mathbb{R}^N$ such that for every $\mathbf{k} \in \Gamma$,*

$$c(\mathbf{k}, t) \underset{\text{i.o.}}{>} h(t) \,, \tag{4.8}$$

for every expressible h which is integrable on $[0, \infty)$.

In order to state our last result of this subsection, we introduce the frequency dependent diffusivity

$$\widetilde{D}(\mathbf{k}, \omega) = \omega^2 \int_0^\infty e^{-\omega t} E[\underline{X}_t^2]dt \,, \tag{4.9}$$

which can also be written in terms of the VAF

$$\widetilde{D}(\mathbf{k}, \omega) = 1 - \int_0^\infty e^{-\omega t} c(\mathbf{k}, t)\, dt\,. \tag{4.10}$$

By applying an $\omega \to 0$ version of Corollary 4.1 to $\widetilde{D}(\mathbf{k}, \omega)$, where $\lim_{\omega\to 0} \widetilde{D}(\mathbf{k}, \omega) = D^*(\mathbf{k})$, we have

THEOREM 4.4. *Let $\widehat{V}$ on T^n be typical with $\underline{X}_t$ as in Theorem* 4.2. *Then there is a dense set $\Gamma \subset \mathbb{R}^N$ such that for every $\mathbf{k} \in \Gamma$,*

$$|\widetilde{D}(\mathbf{k}, \omega) - D^*(\mathbf{k})| \underset{\text{i.o.}}{>} g(\omega)\ , \quad \omega \to 0\ , \tag{4.11}$$

for every expressible function $g(\omega)$ with $\lim_{\omega\to 0} g(\omega) = 0$.

4.3. *Conduction in quasiperiodic media.* Recall from Section 2 that $\boldsymbol{\sigma}^*(L, \mathbf{k}, \underline{\theta})$ is the effective conductivity of a sample of side $2L$ of $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta})$, which in $d = 1$ has the form (2.10). We are interested in averaging $\boldsymbol{\sigma}^*(L, \mathbf{k}, \underline{\theta})$ over T^n to obtain

$$\boldsymbol{\sigma}^*(\mathbf{k}, L) = \int_{T^n} \sigma^*(\mathbf{k}, L, \underline{\theta}) d\underline{\theta}\ , \tag{4.12}$$

which is continuous in $\mathbf{k}$, as well as L. Then

$$\lim_{L\to\infty} \boldsymbol{\sigma}^*(\mathbf{k}, L) = \boldsymbol{\sigma}^*_{\text{av}}(\mathbf{k})\ , \tag{4.13}$$

where $\boldsymbol{\sigma}^*_{\text{av}}(\mathbf{k})$ is the same as in Section 3.4.

As in Section 3, we say that $\hat{\sigma}$ on T^n is "typical" if $\boldsymbol{\sigma}^*_{\text{av}}(\mathbf{k})$ is discontinuous in $\mathbf{k}$ on a dense subset of $\mathbb{R}^N$. We have again using Corollary 4.1,

THEOREM 4.5. *Let $\hat{\sigma}$ on T^n be typical. Then for $\boldsymbol{\sigma}^*(\mathbf{k}, L)$ in* (4.12) *arising from a local conductivity field $\sigma_{\mathbf{k}}(\underline{x}, \underline{\theta}) = \hat{\sigma}(\underline{\theta} + \mathbf{k}\underline{x})$, there exists a dense set $\Gamma \subset \mathbb{R}^N$ such that for each $\mathbf{k} \in \Gamma$*

$$|\boldsymbol{\sigma}^*(\mathbf{k}, L) - \boldsymbol{\sigma}^*_{\text{av}}(\mathbf{k})| \underset{\text{i.o.}}{>} g(L)\ , \quad L \to \infty\ , \tag{4.14}$$

for every expressible function $g(L)$ with $\lim_{L\to\infty} g(L) = 0$.

4.4. *Quantum transport in quasiperiodic potentials.* We consider the time dependent Schrödinger equation on the lattice $\mathbb{Z}$ in one dimension defined by the Hamiltonian

$$H = \Delta + \varepsilon \cos 2\pi k x_j\ , \quad x_j \in \mathbb{Z}\ , \tag{4.15}$$

where $\triangle$ is the discrete Laplacian in $d = 1$. When k is rational, H has purely absolutely continuous spectrum, and

$$b(k, t) = \sum_{j=-\infty}^{\infty} |e^{itH} f(x_j)|^2 x_j^2 , \tag{4.16}$$

which is a quantum analog of the mean squared displacement for some initial f of compact support, has "ballistic" asymptotic behavior. That is, when k is rational,

$$\lim_{t\to\infty} \mathscr{B}(k, t) = \lim_{t\to\infty} \frac{b(k, t)}{t^2} = B^*(k) > 0 . \tag{4.17}$$

However, when ε is large enough and k is irrational with good diophantine properties, then H has only localized states [**19, 20**]. In this case it can be shown [**21**] that

$$\lim_{t\to\infty} \mathscr{B}(k, t) = 0 , \tag{4.18}$$

so that $\mathscr{B}(k, t)$ apparently displays discontinuous limiting behavior similar to $\mathscr{D}(k, t)$ for classical diffusion, with $\mathscr{B}(k, t)$ continuous in k and t. Presumably $B^*(k)$ is discontinuous on a dense set. Then there exists a dense set Γ such that for each $k \in \Gamma$,

$$|\mathscr{B}(k, t) - B^*(k)| \underset{\text{i.o.}}{>} g(t) , \tag{4.19}$$

for every expressible function g with $\lim_{t\to\infty} g(t) = 0$. Presumably the k's in such a Γ are irrationals that are *very* well approximated by rationals.

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