Anomalous Diffusion Properties of Wave Packets on Quasiperiodic Chains

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In a perturbative limit, we derive the diffusion properties of initially localized wave packets on the Fibonacci chain. We establish a new relation between generalized diffusion exponents and fractal dimensions of the energy spectrum. We give an argument extending in general to other one dimensional quasiperiodic systems. An illustration is given taking the case of the Harper model. [S0031-9007(96)00305-5]

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Quite recently two families of models have greatly renewed the problem of quantum localization of a particle moving in one dimension. Generically these models are neither periodic nor randomly disordered but quasiperiodic (QP). Typical examples are, on one hand, kicked rotator and kicked Harper models from the field of *quantum chaos* and, on the other hand, Harper-like models and tight-binding Hamiltonians associated to quasiperiodic sequences [1,2]. For these kinds of systems, depending on the strength of the QP modulation, a correspondence has been established between the dynamics of wave packets (WPs) and the energy spectrum properties. Qualitatively, if an initially localized WP exhibits a ballistic spreading, then the spectrum is *absolutely continuous* (AC). This corresponds to a metallic regime as in periodic systems. In the strongly localized regime, WP spreading stops after a finite time and the spectrum is *pure point* (PP) as in randomly disordered systems. Finally, there is a critical nonuniversal regime at the metal insulator transition, where the WPs have an anomalous diffusive spreading and the spectrum is *singular continuous* (SC) within general multifractal properties.

For more quantitative relations many heuristic arguments based on the Thouless [3] picture of localization have been given. The spirit of these is the following: Instead of the QP infinite chain, consider a sequence of periodic approximant Hamiltonians of increasing period L. The idea is then that the typical variation ΔE of the energy levels with a change of boundaries conditions defines an energy scale that is the inverse of the time t^* that a WP needs to spread over the entire chain [i.e., $x^2(t^*) = L^2 = t^{*2\sigma}$ where σ is the diffusion exponent]. In cases of AC and PP spectra this argument gives the correct answer: $\Delta E \sim L^{-1} \Rightarrow \sigma = 1, x^2(t) \sim t^2$, and $\Delta E \sim e^{-L} \Rightarrow \sigma = \ln L/L \simeq 0$, respectively [4–7].

In the case of a SC spectrum, there are many energy scales, typically $\Delta E \sim L^{-1/\alpha}$ with a number $L^{g(\alpha)}$ of exponents α. Because of this, any simple relation between spectral and diffusion exponents seems difficult. Nevertheless, numerical results obtained for Harper and kicked Harper models seem to support the relation $\sigma = D_F$ where D_F is the Hausdorff dimension of the *local* spectral measure (SM) [8] of the initial WP [4,5]. Recently, however, other mathematical and numerical results have contested its generality and instead have stressed the following more general properties: (i) A WP spreading exhibits *multiscaling* and *intermittency* such that the moments $x^q(t)$ ($q \geq 0$ and even) satisfy $x^q(t) \simeq t^{q\sigma_q}$. (ii) The q dependent diffusion exponents satisfy $\sigma_q \geq D_1$ [9,10] where D_1 is now the information dimension of the *local* SM [7,9–11]. Although these last results seem to exclude any simple relation between spectral and diffusion exponents, no definite conclusion has been possible so far.

In this context the purpose of this paper is double. First, for a QP model on the Fibonacci chain, we characterize analytically the diffusion properties of WPs. More precisely, in the spirit of [12], using the same perturbative renormalization group (RG) of Niu and Nori [13], we derive the following: For a WP initially localized on a site i_0, the exponents σ_q associated with the moments $x^q(i_0, t)$ can be written as $\sigma_q = \alpha$, where α, dependent on i_0, is one of the singularity exponents of the *global* SM. In this perturbative limit, this diffusion is thus *quasinormal* and *inhomogeneous.* These results complete a pioneering study of Abe and Hiramoto [14,15]. Upon averaging on the QP disorder (initial site), the diffusion becomes *homogeneous*, but it now exhibits *multiscaling.* As a consequence, the exponents σ_q associated with the average moments $x^q(t)$ now satisfy $\sigma_q = D_{1-q}$, where the D_q are the dimensions that characterize the multifractality of the *global* SM. Second, we give a semiquantitative argument for the validity of the last relation in the case of other QP models with the SC spectrum. We then support it with numerical results for the Harper model.

In the following, we only give the qualitative reasoning and final relations, and defer certain analytical steps and numerical details to a future publication [16].

As in [12], we consider a tight-binding Hamiltonian H_n, defined on approximants of period F_n of the Fibonacci chain by the following Schrödinger equation on a site i:

$$E_n^l \psi_i^l = t_{i,i+1}\psi_{i+1}^l + t_{i-1,i}\psi_{i-1}^l\,, \tag{1}$$

where ψ_i^l denotes the wave-function component of the energy level E_n^l, on site i. The hopping amplitude $t_{i,i+1}$ from site i to site $i+1$ takes the value t_w (weak bond) or t_s (strong bond) according to the Fibonacci sequence. In the case we consider, the density of (t_w) bonds is $\omega_n = F_{n-1}/F_n$ and tends to the golden mean $\omega = (\sqrt{5}-1)/2$ in the quasiperiodic limit ($n \to \infty$). The density of bonds (t_s) is $\omega_n^2 = F_{n-2}/F_n$ and tends to ω^2 ($F_{n+1} = F_n + F_{n-1}$ and $F_n \simeq \omega^{-n}$). The energy spectrum $W_n(t_s, t_w)$ consists of the F_n levels E_n^l ($l = 1, \ldots, F_n$ and $E_n^l \leq E_n^{l+1}$ by convention). The variation of a level $E_n^l(k)$, with Bloch boundary conditions ($\psi_{i+F_n}^l = e^{ik}\psi_i^l$), defines an energy band of width $\Delta_n^l = |E_n^l(\pi) - E_n^l(0)|$.

In the strong modulation regime ($t_w/t_s \ll 1$), using the perturbative RG established by Niu and Nori [13], it was shown [12] that the spectrum $W_n(t_s, t_w)$ is composed of three clusters of bands; the two edge clusters are the spectrum $W_{n-2}(t_s, t_w)$ contracted by a factor $z = t_w/2t_s (\ll 1)$ and translated by $\pm t_s$. The central cluster is $W_{n-3}(t_s, t_w)$ contracted by $\bar{z} = t_w^2/t_s^2 (\ll 1)$.

As is schematically depicted in Fig. 1(a), the central cluster $\bar{z}W_{n-3}(t_s, t_w)$ is the spectrum of the effective sub-Hamiltonian $H_{n-3}(\bar{z}t_s, \bar{z}t_w)$ between the F_{n-3} sites of the chain F_n, which form isolated *atoms* in the limit $t_w = 0$. Similarly, the two edge clusters $[\pm t_s + zW_{n-2}(t_s, t_w)]$ are the spectra of the effective sub-Hamiltonian $H_{n-2}(zt_s, zt_w)$ between the sites which constituted the F_{n-2} isolated *molecules* of energy $\pm t_s$ [see Fig. 1(b)]. From this we can derive the *local* (on-site) properties of the RG that are necessary to calculate the diffusion properties of WPs. The first of these is a recurrence relation between wave-function components. More precisely, for an energy level $E_n^{l+F_{n-2}} (l = 1, \ldots, F_{n-3})$ in central cluster we have $|\psi_i^{l+F_{n-2}}(E)| = |\sqrt{\omega_n^3}\psi_{i'}^l(E/\bar{z})|$, where i is the *atom* site of F_n associated to site i' of F_{n-3} as shown in Fig. 1(a). This relation is approximate. It ignores the probability of being on *molecule* sites, which is lower by a factor $z^2 \ll 1$ for an energy in this cluster. Very similarly, for the levels E_n^l and $E_n^{l+F_{n-1}} (l = 1, \ldots, F_{n-2})$ of the two edges clusters, we get, respectively, $(1/\sqrt{2})(\psi_{i+}^l + \psi_{i-}^l)(E) = \sqrt{\omega_n^2}\psi_{i'}^l(E + t_s/z)$ and $(1/\sqrt{2})(\psi_{i+}^{l+F_{n-1}} - \psi_{i-}^{l+F_{n-1}}) = \sqrt{\omega_n^2}\psi_{i'}^l(E - t_s/z)$. The sites (i^+, i^-) of F_n are those linked by a bond t_s. They are now associated to i' on F_{n-2}, as shown in Fig. 1. The second and last property that is necessary is the following: As can be seen in Fig. 1, in terms of the number of bonds, the distance $|i - i_0|$ between two *atom* sites i_0 and i on F_n is nearly $\omega_n^{-3} = F_n/F_{n-3}$ times the distance $|i' - i_0'|$ between the associated sites on the chain F_{n-3}. As a result, we have $\sum_i = \omega_n^{-3}\sum_{i'}$. Similarly, for the distance between *molecule* sites (see Fig. 1), we get $|i^+ - i_0^{\pm}| \simeq |i^- - i_0^{\pm}| \simeq \omega_n^{-2}|i' - i_0'|$ and $\sum_{i^\pm} = \omega_n^{-2}\sum_{i'}$.

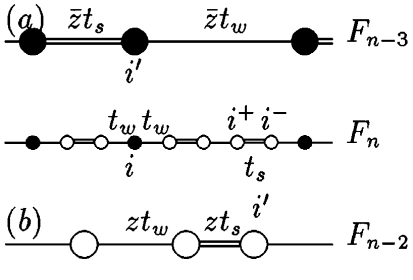

FIG. 1. (a) Relation between an atom (i) of F_n and its corresponding site (i') of F_{n-3}. (b) Relation between a *molecule* (i^+, i^-) of F_n and its corresponding site (i') of F_{n-2}.

Using these local properties of the RG, in the spirit of [12], we derive *local* recurrence relations between the diffusion properties on the chain F_n and those on chains F_{n-2} and F_{n-3}. Before calculating the diffusion moments of WPs, we first derive the probability distributions of the diffusion front. Apart for a normalization factor, this distribution is defined by $p_n(i_0, i, t) = |\mathcal{A}_n(i_0, i, t)|^2$ where $\mathcal{A}_n(i_0, i, t)$ represents the amplitude of probability to go from an initial site i_0 of a chain F_n to a final site i in a time t. In terms of the eigenfunctions and eigenenergies of the Hamiltonian H_n, the amplitude $\mathcal{A}_n(i_0, i, t)$ can be written $\mathcal{A}_n(i_0, i, t) = \sum_{l=1}^{F_n} e^{iE_n^l t}\overline{\psi_{i_0}^l}\psi_i^l$. Using this definition and the *local* properties of the RG, depending on the nature of the initial site, *atom* ($|_{\text{ato}}$) or *molecule* ($|_{\text{mol}}$), we obtain

$$\begin{aligned} p_n(i_0, i, t)|_{\text{ato}} &= \omega_n^3 p_{n-3}(i_0', i', \bar{z}t) + \mathcal{O}(z^2)\,, \\ p_n(i_0^{\pm}, i, t)|_{\text{mol}} &= \omega_n^2 p_{n-2}(i_0', i', zt) + \mathcal{O}(z^2)\,. \end{aligned} \tag{2}$$

For each line of Eq. (2), the distribution is normalized to $\sum_i p_n(i_0, i, t) = 1$. To find the second line of (2) we assume that i^+ and i^- play a symmetrical role, i.e., $\mathcal{A}_n(i_0^+, i^+, t) = \mathcal{A}_n(i_0^-, i^-, t)$ and $\mathcal{A}_n(i_0^+, i^-, t) = \mathcal{A}_n(i_0^-, i^+, t)$. We also neglect interference terms between probability amplitudes referring to left and right edge clusters [16]. Finally, the terms $\mathcal{O}(z^2)$ in each line signify that in our limit $t_w \ll t_s$, we can neglect the jump probability from *atom* to *molecule* sites (*molecule* to *atom*). The interpretation of the first line of Eq. (2) is then quite clear: The probability to go from an initial *atom* site i_0 of F_n to a final site i in a time t is w_n^3 times smaller than the probability to go from i_0' to i' (distance smaller by a factor ω_n^3) in a smaller time $\bar{z}t$.

We now examine the consequences of Eq. (2) and calculate the diffusion moment of order q (q even) defined by $x_n^q(i_0, t) = \sum_{i=1}^{F_n}(i - i_0)^q p_n(i_0, i, t)$. From Eq. (2) and the last property of the RG we get the following recurrence relations for each type of site:

$$\begin{aligned} x_n^q(i_0, t)|_{\text{ato}} &= \omega_n^{-6q} x_{n-3}^q(i_0', \bar{z}t)\,, \\ x_n^q(i_0^{\pm}, t)|_{\text{mol}} &= \omega_n^{-4q} x_{n-2}^q(i_0', zt)\,. \end{aligned} \tag{3}$$

Equations (3) and (2) provide a quantitative illustration of the qualitative remark in [14,15] that the time evolution of a WP can be viewed as successive recursions of the RG. In fact, for an initial site i_0, which is renormalized n_a times as an *atom* site and n_m times as a *molecule* site $(3n_a + 2n_m = n)$, the moments of a WP initially localized on i_0 verify $x_n^q(i_0, t) = \omega^{-2nq} x_0^q(\tilde{i}_0, \bar{z}^{n_a} z^{n_m} t)$, where $\tilde{i}_0$ is the *n*th iterated site corresponding to i_0. Now, by definition $x_0^q(\tilde{i}_0, t)$ represents the moments of a WP on the periodic chain of period $F_0 = 1$; the spreading is thus ballistic, $x_0^q(\tilde{i}_0, t) \sim t^q$. From this we deduce that $x_n^q(i_0, t) \sim (\mathcal{D}_n)^q t^q$, where the diffusion coefficient $\mathcal{D}_n$ decreases with the length F_n as $\mathcal{D}_n = F_n^{1-1/\alpha(x)}$, and $\alpha(x) = \ln\omega/(x \ln z/\bar{z}^{2/3} + \ln \bar{z}^{1/3}) \leq 1$ appears to be one of the singularity exponents of the *global* SM [12], with $x = n_m/n$ varying continuously in $[0, 1/2]$ in the limit $n \to \infty$. Having this, we see that the time t^* needed for each moment $x_n^q(i_0, t)$ to be spread over the entire chain F_n [i.e., $x_n^q(i_0', t) = F_n^q$] increases as $t^* \sim F_n^{1/\alpha}$. Assuming that the WP spreads now with a modified diffusive exponent instead of a size dependent diffusion coefficient [i.e., $x_n^q(i_0, t) \sim t^{q\sigma_q}$], then the last property gives $\sigma_q = \alpha$. This generalizes the results in [14,15]. More qualitatively, to conclude with this strict *local* point of view, since $\sigma_q = \alpha$ is independent of q but not on the initial site i_0, we can call the diffusion *quasinormal* but *inhomogeneous*. Note, however, that the *quasinormal* diffusion is just the approximate dominant behavior. More generally, we expect a multifractal diffusion due to the $\mathcal{O}(z^2)$ correction term in Eq. (2).

Instead of looking at the spreading of a WP initially localized on only one site, we now consider an average WP defined by its moments $x_n^q(t)$ that are statistical averages over all the $x_n^q(i_0, t)$: $x_n^q(t) = (1/F_n) \sum_{i_0=1}^{F_n} x_n^q(i_0, t)$. This procedure is equivalent to a quasiperiodic disorder averaging that makes the system *homogeneous*. Moreover, we believe that it also reincorporates in a self-consistent way the terms $\mathcal{O}(z^2)$ that were neglected in the strict local point of view. From Eq. (3) we deduce

$$x_n^q(t) = \omega_n^{3(1-q)} x_{n-3}^q(\bar{z}t) + 2\omega_n^{2(1-q)} x_{n-2}^q(zt), \qquad (4)$$

where the factors ω_n^3 $(2\omega_n^2)$ correspond to the fraction of *atom* (*molecule*) sites. In the limit of an infinite chain $(n \to \infty)$, or equivalently of infinite time, $x_n^q(t)$ will tend to an invariant $x^{q*}(t)$ which satisfies

$$x^{q*}(t) = \omega^{3(1-q)} x^{q*}(\bar{z}t) + 2\omega^{2(1-q)} x^{q*}(zt), \qquad (5)$$

This self-consistent equation (5) has two major consequences: (i) By definition $x^{q*}(t)$ is the moment of order q of an effective probability distribution $p^*(i, i_0, t)$. Since the diffusion is now *homogenous*, this distribution $p^*(i, i_0, t)$ depends only on the distance between the initial and final positions, i.e., $p^*(i, i_0, t) = p^*(r, t)$ where $r = |i - i_0|$. Furthermore, we can take the continuum limit and replace $\sum_i$ by $\int dr$. Using this, the diffusion moments $x^{q*}(t)$ are given by

$$x^{q*}(t) = \int dr\, r^q p^*(r, t). \qquad (6)$$

From Eqs. (6) and (5), we then deduce that $p^*(r, t)$ has to verify

$$p^*(r, t) = \omega^6 p^*(\omega^3 r, \bar{z}t) + 2\omega^4 p^*(\omega^2 r, zt), \qquad (7)$$

A first property of Eq. (7) is that the probability $p^*(0, t)$ to stay (or return) at the initial position, satisfies the relation derived in [12] by using only the form of the *global* SM. Thus we have $p^*(0, t) \sim t^{-D_2}$ where D_2 is one of the dimension D_q that characterizes the multifractal properties of the global SM. We now turn to a second property of Eq. (7). For a *quasinormal* and *homogeneous* diffusion, in one dimension and with a unique diffusion exponent σ, generically we would have obtained the following properties for the diffusion moments $x^{q*}(r, t)$ and the distribution $p^*(r, t)$:

$$\begin{aligned} x^{*q}(t) &= \lambda^{-q\sigma} x^{*q}(\lambda t) \Rightarrow \quad x^{*q}(t) = t^{q\sigma}, \\ p^*(r, t) &= \lambda^{\sigma} p^*(\lambda^{\sigma} r, \lambda t) \Rightarrow \quad p^*(r, t) = t^{-\sigma} f(r/t^{\sigma}), \end{aligned} \qquad (8)$$

where $f(\cdot)$ is a scaling function of the scaling variable r/t^{σ}. By comparison, Eqs. (5) and (7) show that for our model on the Fibonacci chain there are two characteristic length and time scales (*multiscaling*) [10]. More precisely, apart from the case $z = \bar{z}^{2/3}$ [17], we cannot put $p^*(r, t)$ in a simple form with only one characteristic exponent and scaling variable. Another possible interpretation of Eqs. (5) and (7) is the following: A fraction ω^3 of the WP has a tendency to spread with an exponent $\sigma = \ln\omega^3/\ln\bar{z}$, and the other fraction $2\omega^2$ spreads with an exponent $\sigma = \ln\omega^2/\ln z$.

(ii) The second property of Eq. (5) is the following: If we assume a power law behavior of the form $x^{q*}(t) \sim t^{q\sigma_q}$, then the diffusion exponents σ_q verify

$$\omega^{3(1-q)} \bar{z}^{q\sigma_q} + 2\omega^{2(1-q)} z^{q\sigma_q} = 1. \qquad (9)$$

This equation is similar to the self-consistent equation found in [12] for the dimensions D_q of the global SM. More precisely the exponents σ_q and D_q are related by

$$\sigma_q = D_{1-q}. \qquad (10)$$

From this relation we deduce that the diffusion exponents depend explicitly on *q*; in addition, since the D_q decrease with increasing q, we have $\sigma_q \geq D_1$, which means that the Guarneri inequalities [9,10] are verified for all *q*.

More generally, since Eq. (10) is independent of the parameters of our Hamiltonian, we conjecture that it is valid for other one dimensional quasiperiodic models with multifractal *global* SM. Our semiquantitative argument is the following: In the strictly *local* point of view, to each site i_0 we can associate a diffusion exponent $\sigma(i_0) = \alpha$ where α is a singularity exponent of the global SM. As a result, an averaging over i_0 is equal to an appropriate average over α, i.e., $x^{q*}(t) \sim \int t^{q\alpha} \rho(\alpha)\, d\alpha$. Now, as stated in [12], the bandwidth Δ associated to each energy level decreases with the period as $\Delta \sim F_n^{-1/\alpha}$, which is exactly the inverse of the time $t = t^*$. Furthermore, each band has a measure $F_n^{-1} = \Delta^{\alpha} = t^{-\alpha}$, and there

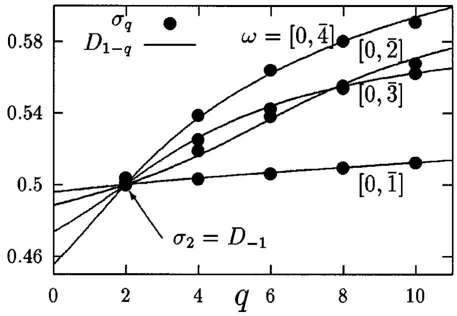

FIG. 2. Average diffusion exponents σ_q (filled circles) and spectral dimensions D_{1-q} (lines) of irrational $\omega = [0,\overline{n}]$ ($n = 1,\ldots,4$).

are $N(\alpha)d\alpha \sim \Delta^{-f(\alpha)}d\alpha$ bands with a given α. Using all these properties, we have $\rho(\alpha)d\alpha = \Delta^{\alpha}N(\alpha)d\alpha$ [18] such that in the limit of large time t (i.e., $\Delta \longrightarrow 0$), we get

$$x^{q*}(t) \sim \int d\alpha\, t^{f(\alpha)+(q-1)\alpha} = t^{qD_{1-q}}. \tag{11}$$

To check this conjecture, we consider the example of the Harper model in the critical regime. This is a Schrödinger equation with hopping amplitude $t_{i,i+1} = -1$ and on-site potential $v_i = 2\cos(2\pi\omega i + \phi)$ where ω is an irrational and ϕ an arbitarty phase. For this model, the diffusion exponents σ_q have been computed using WPs evolution (in terms of exact eigenfunctions) between time 10 and 2000 (in hopping term units), and for approximants $\frac{610}{987}$, $\frac{408}{985}$, $\frac{360}{1189}$, $\frac{305}{1292}$ of irrational $\omega = [0,\overline{n}]$ ($n = 1,\ldots,4$) (Fig. 2, filled circles). Initial WPs are delta functions on the central site. The initial site averaging is replaced by an average over 200 random values of ϕ. For each ω, the spectral dimensions D_{1-q} (lines) are computed using the energy bandwidths of four different approximants. Let us first examine the diffusion exponent σ_2: For all rational approximants r/s of ω, independently of ω, the spectrum Lebesgue measure decreases as $s^{-\delta}$ where $\delta = 1$ [19]. Now, by definition (see also [12]) we have $D_{-\delta} = 1/(1+\delta)$. We thus expect $\sigma_2 = D_{-1} = 1/2$, independent of ω, which is in good accord with the numerical results (Fig. 2) [4]. For other σ_q, we expect distinct behavior for different ω but still $\sigma_q = D_{1-q}$. Again, Fig. 2 confirms this.

In conclusion, in a perturbative limit we have described analytically the diffusion properties of WPs on the Fibonacci chain. After definition of an initial site or QC disorder averaging, we have found a new relation between the diffusion exponents and the dimensions that characterize the multifractal properties of the energy spectrum. We have conjectured this relation to hold for other one dimensional QP systems with singular continuous spectrum. We back this with a semiquantitative argument and provide support from numerical computations on the Harper model.

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