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Observation of log-periodic oscillations in the quantum dynamics of electrons on the one-dimensional Fibonacci quasicrystal

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We revisit the question of quantum dynamics of electrons on the off-diagonal Fibonacci tight-binding model. We find that typical dynamical quantities, such as the probability of an electron to remain in its original position as a function of time, display log-periodic oscillations on top of the leading-order power-law decay. These periodic oscillations with the logarithm of time are similar to the oscillations that are known to exist with the logarithm of temperature in the specific heat of Fibonacci electrons, yet they offer new possibilities for the experimental observation of this unique phenomenon.

Keywords: quasicrystals; Fibonacci quasicrystals; tight-binding model; electronic transport; quantum dynamics; log-periodic oscillations

1. Fibonacci electrons

The Fibonacci sequence of *Long* (L) and *Short* (S) intervals on the one-dimensional line – generated by the simple substitution rules $L \rightarrow LS$ and $S \rightarrow L$ – is a favorite textbook model for demonstrating the peculiar nature of electrons in quasicrystals [1–3]. The wavefunctions of Fibonacci electrons are neither extended nor exponentially localized, but rather decay algebraically; the spectrum of energies is neither absolutely continuous nor discrete, but rather singular-continuous, like a Cantor set; and the quantum dynamics is anomalous. In recent years, we have studied how these three electronic properties change as the dimension of the Fibonacci quasicrystal increases to two and three [4–8], by constructing square and cubic versions of the Fibonacci quasicrystal [9].

The one-dimensional *off-diagonal* Fibonacci tight-binding model is constructed by associating a unit hopping amplitude between sites connected by a *Long* interval, and a hopping amplitude $T > 1$ between sites connected by a *Short* interval, while assuming equal on-site energies that are taken to be zero. The resulting tight-binding Schrödinger equation, on an F_N-site model, is given by

$$T_{j+1}\psi(j+1) + T_j\psi(j-1) = E\psi(j), \quad j = 1, \ldots, F_N, \tag{1}$$

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where $\psi(j)$ is the value of an electronic eigenfunction on site j, E is the corresponding eigenvalue, F_N is the Nth Fibonacci number, and the hopping amplitudes T_j are equal to 1 or T according to the Fibonacci sequence $\{T_j\} = \{1, T, 1, 1, T, 1, T, 1,1,T,1, 1, T, 1, T, 1, 1, T, 1, T, \ldots\}$, as described above. The *diagonal* Fibonacci tight-binding model is constructed by taking all the hopping amplitudes to be equal to 1, and taking the on-site energies to have two values, V_L and V_S, arranged according to the Fibonacci sequence. These models have been studied extensively ever since the initial interest in the behavior of electrons in quasiperiodic potentials [10–13], and continue to offer mathematical challenges to this day [14].

Various two-dimensional extensions of the Fibonacci model were introduced soon thereafter [15–19], and strongly promoted recently [9] as models for quasicrystals without "forbidden" symmetries [20,21]. In our studies, we have shown that whereas Fibonacci electrons in one dimension always behave as described above for any $T > 1$, in two dimensions, and even more so in three, there is crossover – as the strength T of the quasiperiodicity is decreased – to a regime in which Fibonacci electrons behave more and more like electrons do in periodic crystals, particularly in the sense that their energy spectra develop continuous intervals [4–6]. These results were recently explained in a rigorous manner by Damanik and Gorodetzki [22]. More surprisingly, our studies of Fibonacci electrons have led us to new results also in the simple one-dimensional case. We have examined dynamical properties, such as the probability of an electron to remain in its original position as a function of time. The power-law decay of this quantity is commonly used for analyzing the dynamics. We have observed *log-periodic oscillations* on top of the power-law decay, implying the existence of an imaginary correction to the exponent. We wish to describe this new observation here, and indicate some directions for its analysis.

We note that while the model studied is that of an electronic tight-binding Hamiltonian, no reference is made to any particular electronic property, such as its statistics, the existence of a Fermi level, or the nature of electron–electron interactions. Therefore, the results of the model may apply to other quantum mechanical excitations hopping along the Fibonacci quasicrystal.

2. Quantum dynamics of electronic wavepackets

We consider the dynamics of electronic wavepackets, or states $|n\rangle$, that are initially localized at a single lattice site n of the one-dimensional Fibonacci quasicrystal, denoting their amplitude on site m at time t by $\phi_n(m,t)$. Thus, at time $t = 0$ the wavepacket is given by $\phi_n(m,0) = \langle m|n\rangle = \delta_{mn}$, where δ_{mn} is the Kronecker delta. At any later time $t > 0$ the wavepacket is given by $e^{iHt}|n\rangle$, which is simply the nth column of the matrix representation of the time evolution operator e^{iHt}, where H is the off-diagonal matrix representation of the Hamiltonian in Equation (1), and we take $\hbar = 1$. Thus, $\phi_n(m,t) = \langle m|e^{iHt}|n\rangle = (e^{iHt})_{mn}$. The choice of phase for the corner elements of the Hamiltonian matrix determines the Bloch wavenumbers of the representative eigenfunctions from each of the F_N bands in the spectrum. The results shown below are for periodic boundary conditions, but different choices of wavenumber yield similar results.

We characterize the dynamics of wavepackets by monitoring two typical quantities: (a) the *survival probability* of the nth wavepacket, defined as the probability of finding the electron at its initial position at time t, which is given by

$$S_n(t) = |\phi_n(n,t)|^2 = \left|(e^{iHt})_{nn}\right|^2; \tag{2}$$

and (b) the *inverse participation ratio* of the nth wavepacket, which measures the spatial extent of the wavepacket, and is given by

$$I_n(t) = \frac{\sum_m |\phi_n(m,t)|^4}{\left(\sum_m |\phi_n(m,t)|^2\right)^2} = \sum_m \left|(e^{iHt})_{mn}\right|^4, \tag{3}$$

where the last equality holds because the wavepackets are normalized. Both of these quantities are often used to examine the dynamics of wavepackets. In particular, the manner in which they decay as the wavepackets spread with time is associated with different regimes of the quantum dynamics. The actual calculation is performed numerically by applying the discrete time-evolution operator $e^{iH\Delta t}$ successively to the initial conditions. The time-step Δt is kept sufficiently small to satisfy the Nyquist criterion by noting that the largest eigenvalue of H is bounded by $1+T$, thus requiring Δt to be smaller than $1/(2+2T)$.

If a function $F(t)$ asymptotically decays with some power law $F(t) \sim t^{-\beta}$, then the exponent β can be found by

$$\beta = \lim_{t\to\infty} -\frac{\ln F(t)}{\ln t}, \tag{4}$$

but in general the exponent β is not guaranteed to exist. The bounds $\beta_\pm$ on β, which always exist, are given by

$$\beta_+ = -\limsup_{t\to\infty} \frac{\ln F(t)}{\ln t}; \quad \beta_- = -\liminf_{t\to\infty} \frac{\ln F(t)}{\ln t}; \tag{5}$$

and if $\beta_+ = \beta_-$ then β exists. Furthermore, if an exponent $0 < \beta < 1$ characterizes the power-law decay of a function $F(t)$, then the same exponent also characterizes the decay of the time-averaged function

$$\langle F \rangle_t = \frac{1}{t}\int_0^t F(t')\mathrm{d}t'; \tag{6}$$

for exponents $\beta > 1$, characterizing the decay of $F(t)$, the exponent describing the decay of the time-averaged function (6) is always equal to 1, owing to the $1/t$ prefactor, and the constant contribution to the integral from early times. We use the definition of Equation (5) to study the long-time asymptotic values of the exponents β_S related to the survival probability of a wavepacket and β_I related to the inverse participation ratio of the wavepacket. In what follows, we are mostly concerned with the early-time behavior of these exponents, in which the log-periodic oscillations appear, and the behavior is not yet affected by the finite size of the system.

Damanik et al. [14,23] recently used the second moment of the position operator for the diagonal tight-binding Hamiltonian, to show that far from the periodic limit, or very close to it, the dynamics of wavepackets is independent of the initial site.

However, since we are interested in intermediate values of T as well – equivalent in the diagonal model to intermediate values of the difference $|V_L - V_S|$ between the different on-site energies – we expect to find different dynamical behavior depending on the choice of the initial site. Thus, we typically examine the maximal, the minimal, and the site-averaged survival probabilities and inverse participation ratios, all of which display similar qualitative behavior. In [8] we study the different exponents in detail, in one, two, and three dimensions. Here we concentrate on the $1d$ results for the maximal – with respect to the initial site – survival probability exponent $\beta_S^{\max}$.

3. Asymptotic behavior of the maximal survival probability

We look at the wavepacket whose time-averaged survival probability is maximal. Figure 1 shows the time-averaged maximal survival probability $\langle S_{\max}\rangle_t$ on a log-log scale for a 233-site $1d$ approximant, with periodic boundary conditions, for different values of T. The exponents extracted from the slopes of the curves in Figure 1 for four orders of approximants are shown in Figure 2, as functions of T.

Convergence of the exponent $\beta_S^{\max}$ is evident for values of $T > 2$ even for relatively small approximants. Convergence is not obtained for smaller values of T that approach the periodic limit $T \to 1$, where the dynamics is expected to become ballistic. In this limit the wavepackets quickly spread out and the finite size of the approximant has a stronger influence on the dynamics. Despite this limitation,

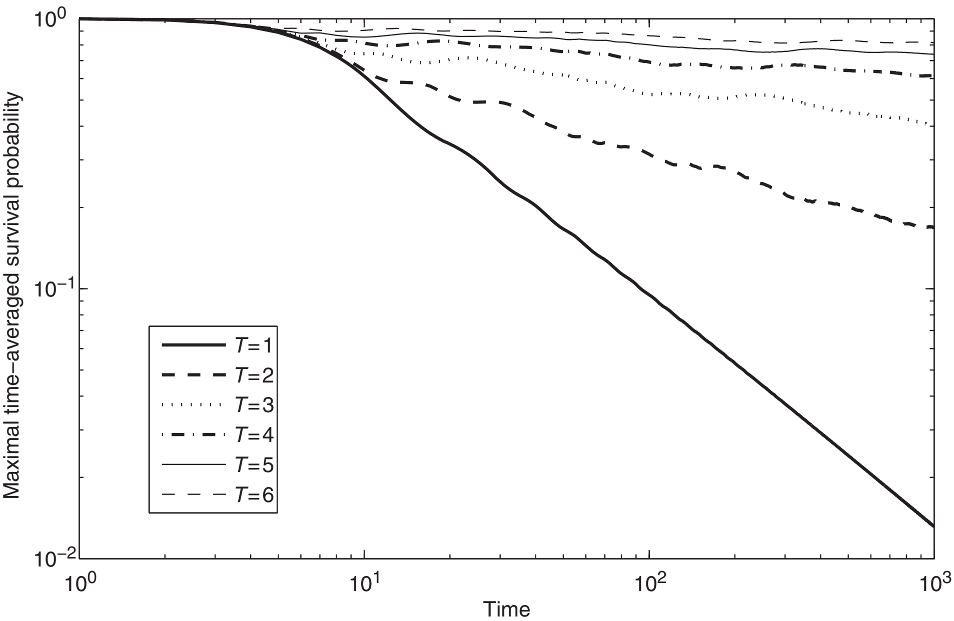

Figure 1. The time-averaged maximal survival probability for a 233-site $1d$ approximant, with periodic boundary conditions, calculated for different values of T. The asymptotic behavior of the slopes allows us to extract the diffusion exponent $\beta_S^{\max}$ as a function of T, which is displayed in Figure 2.

detailed studies of the slopes, for increasing orders of approximants and for varying time-ranges clearly show that the extracted exponents converge, as the order of the approximant increases, and longer averaging times are possible. Similar curves are obtained for the minimal and the site-averaged survival probabilities, as well as for the minimal, maximal, and site-averaged inverse participation ratios [8].

4. Log-periodic oscillations and the Fourier transform of the density of states

A closer inspection of the temporal decay of the survival probabilities in Figure 1 reveals a small oscillating behavior on top of the overall leading power-law. In order to better describe this behavior, we divide out the leading asymptotic power-law $t^{-\beta}$ that was found earlier, and obtain the curves shown in Figure 3. Similar results are observed in the study of the inverse participation ratio, but are not presented here owing to space limitations. The curves clearly exhibit log-periodic oscillations – oscillation that are periodic in log(t) – around the mean value of 1, especially for the larger values of T. These oscillations contain a basic frequency ω that seems to decrease with increasing T, as well as a sequence of higher-frequency oscillations with decreasing amplitudes that seem to develop with time. The fundamental oscillations can be described empirically by a temporal decay with a complex exponent of the form

$$f(t) \propto t^{-\beta} + \alpha t^{-\beta \pm i\omega} + (\text{corrections} \ll \alpha), \tag{7}$$

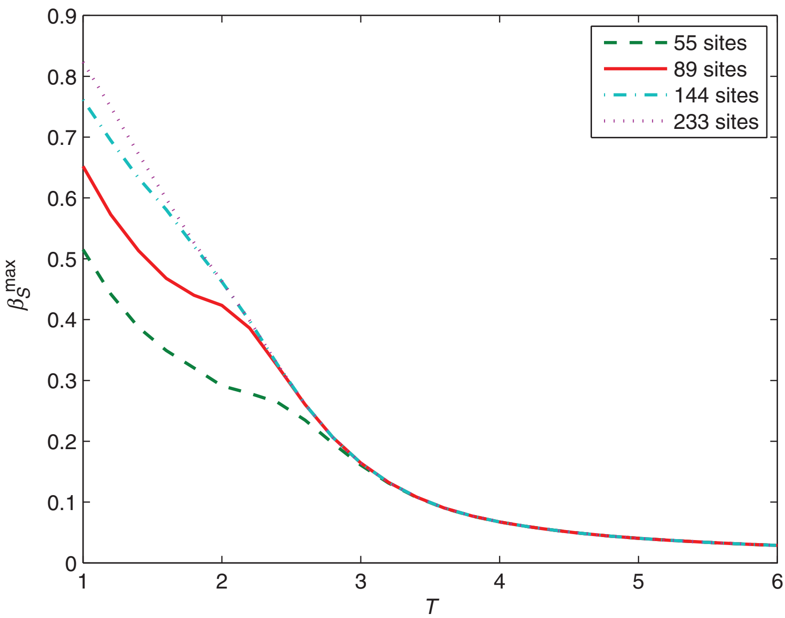

Figure 2. The exponent $\beta_S^{\max}$ as a function of T for increasing orders of approximants. Convergence is improved for decreasing values of T as the order of the approximant is increased.

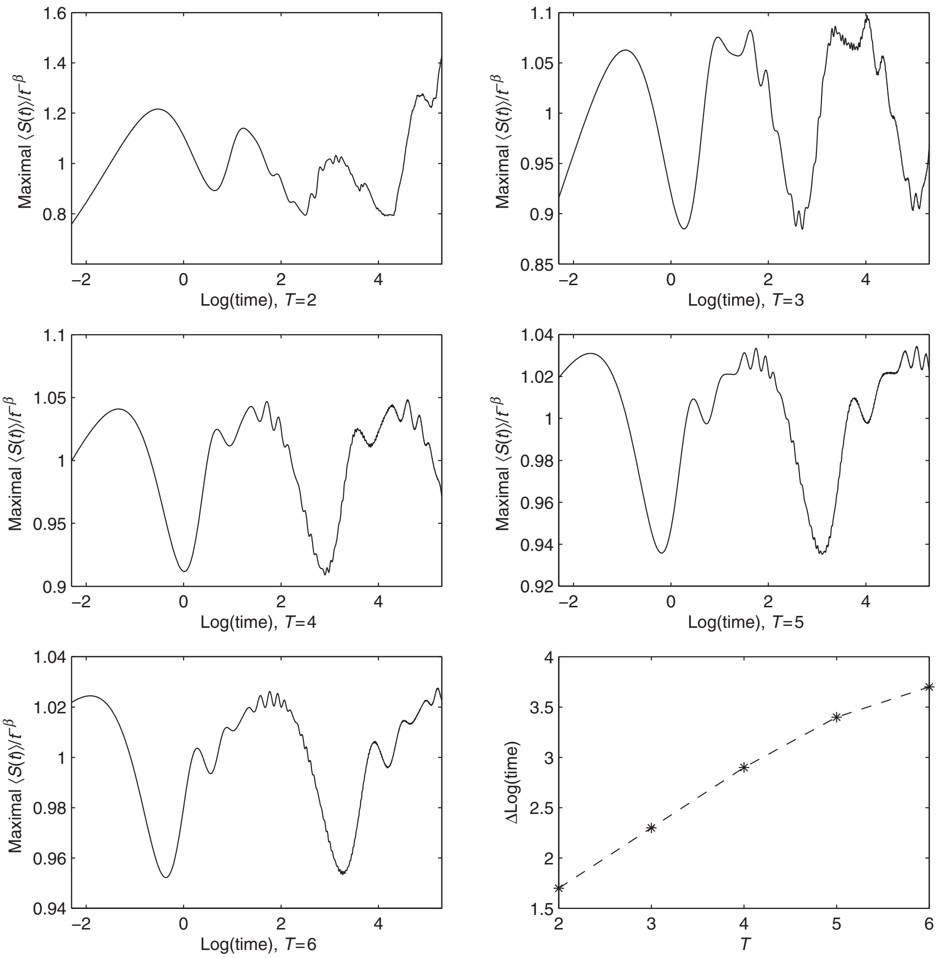

Figure 3. Log-periodic oscillations in the maximal survival probability, after dividing out the leading power-law decay, for an 89-site approximant with five different values of T. In addition to the basic periodic oscillation one observes the emergence of higher-frequency oscillations as time advances. The final panel shows the logarithmic period of the fundamental oscillations as a function of T.

which after dividing out the leading power-law term becomes

$$\frac{f(t)}{t^{-\beta}} \propto 1 + \alpha t^{\pm i\omega} = 1 + \alpha e^{\pm i\omega \log(t)}, \tag{8}$$

yielding oscillations of amplitude α around 1 that are periodic in $\log(t)$ with frequency ω.

Log-periodic oscillations are not as uncommon in physics as one may think. They appear in critical phenomena [24–26], where renormalization-group calculations yield power-law behavior near phase transitions with complex exponents; they also appear quite generally in problems related to random walks or classical diffusion on self-similar systems or fractals where the fractal dimension turns out to be complex [27–31]. As such, they naturally occur in quasiperiodic systems like the Fibonacci quasicrystal, where the spectrum of energies is multifractal. This has been observed in quasiperiodic Ising models [32], in specific heat studies of the tight-binding Fibonacci model [33–37], and in studies of the Harper model [38] and of the Octonacci quasicrystal [39].

The appearance of log-periodic oscillations in our particular model can be naturally explained by the self-similarity that is inherent to the Fibonacci quasicrystal. Assuming the wavepackets spread in a self-similar manner, one can expect to observe oscillations each time the spatial extent of the wavepacket increases by a factor of the golden ratio. While this description gives a qualitative explanation for the existence of log-periodic oscillations it should be noted that the values obtained for the real part β of the exponents and the imaginary part ω do not satisfy the expected relation for systems with discrete scaling [40]. Hence it is possible that the wavepacket does not spread in a self-similar fashion. Further study of this, as well as of the relation between the different exponents, will be pursued elsewhere.

In specific heat studies, where log-periodic oscillations appear in temperature, the object of calculation is the partition function

$$Z(\beta_T) = \sum_k e^{-\beta_T E_k}, \tag{9}$$

where β_T is the inverse temperature; whereas in problems of diffusion [31], the object of calculation is the so-called heat kernel of the diffusion equation

$$Z(t) = \sum_k e^{-E_k t}. \tag{10}$$

In both cases, when expressed in integral form, these are *Laplace transforms of the density of states*. To see the relation to the present problem of quantum dynamics, we expand the expression for the survival probability (2) in eigenstates of the Hamiltonian,

$$S_n(t) = \left| \sum_k \langle n | e^{iHt} | \psi_k \rangle \langle \psi_k | n \rangle \right|^2 = \left| \sum_k \left| \psi_k(n) \right|^2 e^{iE_k t} \right|^2. \tag{11}$$

Thus, what we are calculating is the magnitude-squared of the *Fourier transform of the density of states*, weighted by the overlap of each eigenstate with the initial state $|n\rangle$.

Equation (11) is easily calculated in the periodic limit $T \to 1$ of our model, where the eigenstates are Bloch functions, with $\left|\psi_k(n)\right|^2 = 1/N$ independent of n, and the eigenvalues form a single band with dispersion $E_k = \cos(k)$. This yields

$$S_{T=1}(t) \propto \left| \int_{-\pi}^{\pi} \mathrm{d}k e^{it\cos k} \right|^2 \propto J_0^2(t), \tag{12}$$

where $J_0(t)$ is the zeroth-order Bessel function of the first kind, which is known to decay asymptotically as $t^{-1/2}$. This is consistent with the expected ballistic dynamics of Bloch electrons in a periodic crystal. The time average of Equation (12) is approximately the behavior calculated numerically for $T = 1$ on a 233-site approximant, and shown in Figure 1. Note that the fine wiggles that are barely seen at very early times are associated with the first few zeros of the Bessel function, and are not log-periodic oscillations. Log-periodic oscillations appear for $T > 1$ as a result of the multifractal nature of the Fibonacci spectrum, for similar reasons as in the calculation of the partition function (9) [36,37]. A more detailed analysis of Equation (11) for $T > 1$ is required to quantitatively characterize the spectral properties of the log-periodic oscillations, which we have discovered here by numerical means.

Log-periodic oscillations in the specific heat of Fibonacci quasicrystals near zero temperature are difficult to observe experimentally. The discovery of log-periodic oscillations in the quantum dynamics of wavepackets in Fibonacci quasicrystals should open new possibilities for the actual experimental observation of this unique phenomenon. A particular realization could be in optical experiments that allow one to observe the dynamics of wavepackets within one-dimensional [41], as well as two-dimensional [42], photonic quasicrystals. Thus, we hope that our numerical observations here will stimulate further studies, analytical and experimental alike.

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