Energy-level statistics of electrons in a two-dimensional quasicrystal

Frédéric Piéchon and A. Jagannathan
Laboratoire de Physique des Solides, Université Paris–Sud, 91405 Orsay, France
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Spectra of a tight-binding model on square approximants of the quasiperiodic octagonal tiling are calculated for both perfect and phason-randomized tilings. Level statistics for the randomized tilings are given by random matrix theory, while for the perfect tilings a new type of level statistics is found. Their level-spacing distributions are lognormal with power-law tails for large spacings. The spectral measure is seen to be multifractal.

Since the discovery of quasicrystalline alloys, many geometrical models have been built that are consistent with observed diffraction patterns. Tilings may have perfect quasiperiodic long range order with local symmetries that are not allowed for ordinary periodic structures, and which give rise to the 8-fold, 10-fold, or 12-fold symmetries of the diffraction patterns. Alternatively, one may consider randomized versions of perfect tilings, where geometric disorder is introduced through "phason flips" (*local* tile permutation operations). The perfect tiling has exact symmetries such as its self-similarity property under inflation or deflation operations that random tilings do not have. The constraint imposed by the fixed shape of the tiles of the random tiling are sufficient, however, to give rise to sharp peaks in its diffraction pattern, similar to the Bragg peaks of the perfect tiling.[1] Many existing phenomenological models to explain quasicrystal electronic properties are based on the construction of a pseudo-Brillouin-zone taking into account the brightest spots of the diffraction pattern, and at this level they would thus not distinguish between the perfect and random tiling models. The effect of phason disorder on electronic properties can, however, be very profound, as will be shown below.

In this paper we make a numerical study of statistical properties of the eigenvalue spectrum of a tight-binding Hamiltonian describing the hopping of electrons on vertices of a two-dimensional tiling. The tilings considered are square periodic approximants of the quasiperiodic octagonal tiling, containing up to 8119 sites. The hopping parameter is taken to be constant so that the resulting spectra are a pure consequence of the geometry, or site connectivity, of the tilings. The Hamiltonian is diagonalized numerically and the energy levels are used to compute the distribution $P^{(n)}(s)$ of spacings of nth-nearest-neighbor energy levels $s = E_{i+n} - E_i$. To place the current study in perspective, we begin by mentioning some previous work on electronic levels of tight-binding models, namely, studies of disordered *periodic* lattices on both sides of the metal-insulator transition.[2] These show that in the metallic regime, the first-neighbor level-spacing distributions $P(s)$ have the forms of the Wigner distributions, obtained for Gaussian random matrices.[3] In other words the energy levels of a crystalline hopping Hamiltonian with random distributed on-site energies have the statistics of levels of matrices belonging to the Gaussian orthogonal ensemble (GOE), $P(s) \sim s^{\beta} \exp(-c_{\beta} s^2)$, where c_{β} is a known constant and $\beta = 1$. In the case of an added magnetic flux traversing the lattice, the Hamiltonian belongs in the unitary class and levels obey Gaussian unitary ensemble (GUE) statistics, with $\beta = 2$. Finally, in the insulating regime (strong disorder) $P(s)$ has the Poisson form for large spacings, $P(s) \sim \exp(-s)$. A second quantity of interest calculated for these crystalline models is the spectral rigidity $\Sigma^2(E)$, which measures the fluctuation of the number of levels in an energy window of width E. In the metallic regime,[2] $\Sigma^2(E)$ grows logarithmically with E at small E just as for the random matrix ensembles. This behavior arises from correlations between levels due to the wave functions being extended on the scale of the sample size. These result in level fluctuations which are smaller compared to that of uncorrelated levels [as occurs in the insulating regime, where $\Sigma^2(E)$ depends linearly on E].

In our present work, we find that the randomized quasiperiodic tiling has level statistics of the GOE or GUE type, depending on the applied flux. The statistics of energy levels are thus similar to those of disordered tight-binding models on crystals in the diffusive regime, even though in our case the disorder is purely geometric.[4] In addition the energy dependence of $\Sigma^2(E)$ suggests diffusive propagation in the tiling, with a diffusion exponent that is in good accordance with results of a study of dynamics by Passaro *et al.*[5]

For the perfect approximants, we find a new type of level statistics. The perfect octagonal approximant has been studied previously by Benza and Sire[6] who presented results on level statistics. They did not propose a fit to any functional form, noting principally that level repulsion occurs in the perfect quasicrystal, since $P(s)$ drops to zero at small values of s. This is certainly true of the distribution that we propose in this paper. The physical significance of this level repulsion is that it indicates that wave functions are sufficiently extended, in real space, and that electrons in different states can "see" each other, leading to correlations and repulsion between ener-

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gies. For the perfect case, the calculations show that the density of states (DOS) has huge fluctuations at all energy scales, indicating multifractal properties of the spectral measure. We have calculated the effective $f(\alpha)$ function of the local singularity exponents α. It has the maximum value $f_{\max} = D_F \sim 1$ (the fractal dimension), indicating that the spectrum is gapless, in accordance with the finding of Ref. 6. The calculated first-neighbor distribution $P(s)$ and the second- and third-neighbor spacing distributions $P^{(2)}(s)$ and $P^{(3)}(s)$ are well described by log-normal laws with power-law tails at large spacings. To complicate matters, however, the low moments of the spacing distributions apparently do not have the size dependence that would be indicated by the calculated $f(\alpha)$, while the high moments have a size dependence that is characteristic of a power-law behavior $s^{-\gamma}$ in the large s tail of $P(s)$. It should be noted that the systems studied are comparatively small, and studying the next size of approximant will help in determining better the size dependence of these distributions.

We now describe more precisely our calculations. The perfect periodic approximant is generated using the method described by Duneau *et al.*[7] The perfect tilings can then be disordered by carrying out random phason flips. The Hamiltonian for either kind of tiling is defined by the following site-projected form

$$(H\psi)_i = \sum_{\langle ij \rangle} \psi_j = E\psi_i, \tag{1}$$

where the sum is taken over sites j linked to site i. The

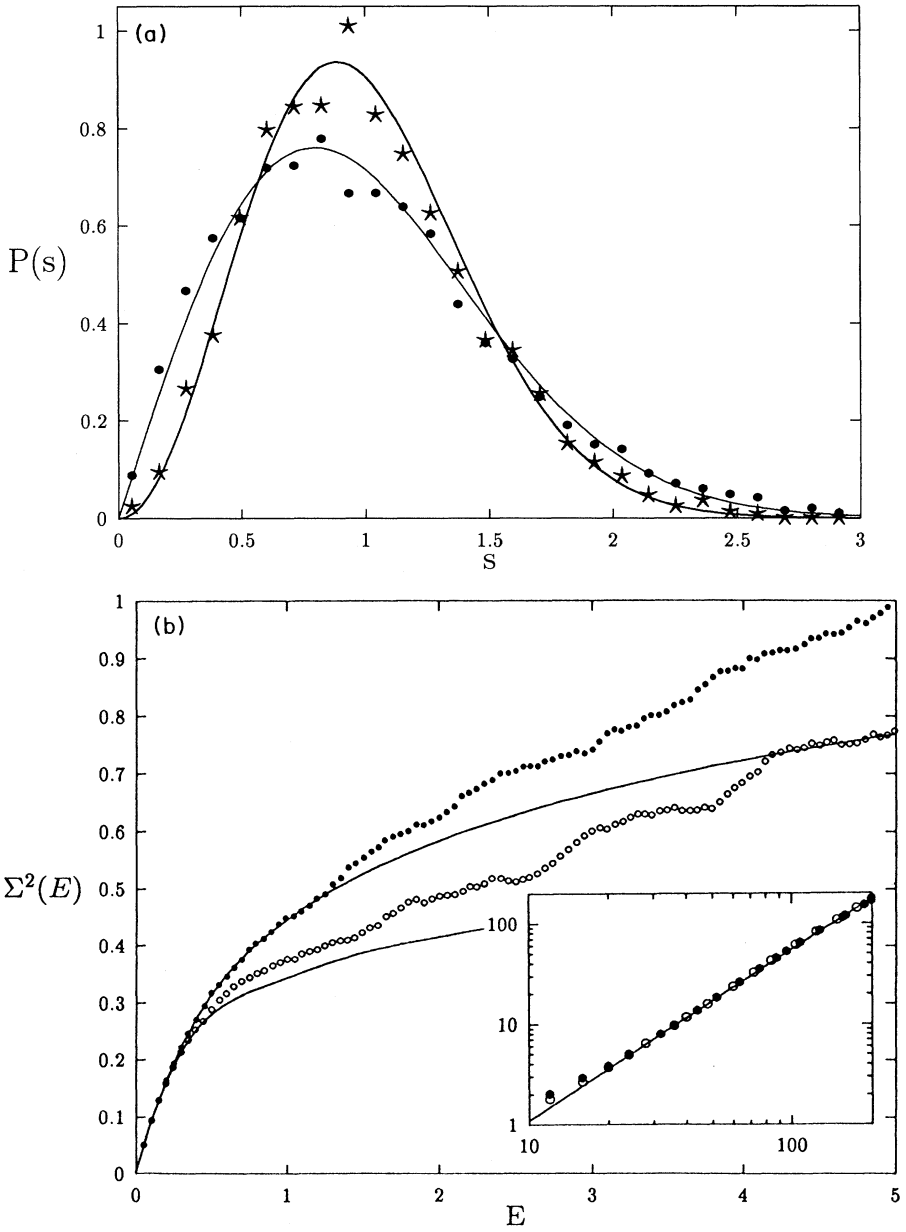

FIG. 1. (a) Level-spacing distribution for the randomized approximants, in the GOE case ($\phi = 0$ circles) and GUE ($\phi = 1/2$ stars). Solid lines show the corresponding Wigner distributions. (b) $\Sigma^2(E)$ (solid circles, GOE; open circles, GUE) and the corresponding RMT curves. The inset is a log-log plot of the power-law region.

number of links emanating from a given site i varies between 3 and 8 in the perfect case, corresponding to the six local environments[8] of the octagonal tiling. In the randomized case new local configurations appear, although the mean coordination is $\bar{z} = 4$ in both tilings. To reiterate, in this model the quasiperiodicity and the disorder are present purely in the connectivity and are of purely geometric nature. This may be compared with models in which one takes an explicit parameter in the Hamiltonian to generate the quasiperiodicity or disorder, such as a site-dependent potential. This distinction is not possible in one dimension, where the quasiperiodic nature of connections between sites must be coded by introducing for example two kinds of bonds, as in the Fibonacci chain.[9] Periodic continuation of the $L \times L$ square tilings allows one to impose boundary conditions of the form $\psi(x + L, y) = e^{i\pi\phi}\psi(x, y)$, $\psi(x, y + L) = \psi(x, y)$. This is equivalent to adding a magnetic flux ϕ along the y or z axis. One can eventually induce a GOE to GUE transition by varying ϕ.

We discuss first the results for the geometrically disordered case since their analysis and interpretation are relatively straightforward. The results obtained for $P(s)$ [taking a normalized spacing $s = (E_{i+1} - E_i)/(W/N)$, where W is the band width and N the number of levels] are shown in Fig. 1(a).

Figure 1(b) shows the spectral stiffness defined in terms of the number $N(E)$ of levels contained within an interval of energy E, by

$$\Sigma^2(E) = \langle [N(E) - \langle N(E) \rangle]^2 \rangle, \tag{2}$$

where the averages are taken over the entire energy band. It can be seen that the randomized tilings follow the RMT laws at low energy, crossing over to a power-law behavior that could imply a diffusive dynamics at intermediate time scales. For comparison, in disordered crystals, we note that for that case the RMT law for spectral stiffness can be derived, both in perturbation theory,[10] and by means of a semiclassical model[11] by *assuming* a diffusive motion for the particle. Both calculations obtain that the spectral stiffness follows the RMT logarithmic law $\Sigma^{(2)}(E) \propto \frac{2}{\beta\pi^2} \ln(E) + cst$ for low energies, crossing over to a power law. We obtain $\Sigma^2(E) \propto E^{1.7}$ for the random tiling. Using the semiclassical argument of Ref. 11, the value of the exponent ν [the root mean square distance covered by the particle in time t, $d_{\rm rms}(t) \propto t^{\nu}$] is 0.85 which implies a superdiffusive dynamics. Passaro *et al.*[5] have studied wave-packet evolution for a class of Hamiltonians including that of Eq. (1). They find anomalous diffusion in both perfect and randomized tilings with $\nu = 0.815$ for the latter.

We note that we have not been able to disorder (in the geometric sense) the tilings sufficiently to see a crossover to strong localization. Such a crossover *can* be seen in tilings that have a strong *energetic* disorder (see note in Ref. 4) wherein $H_{ij} = t_{ij} + \epsilon_i \delta_{ij}$, where the t_{ij} are those of a perfect tiling while the ϵ_i are random on-site energies chosen randomly in an interval of width comparable to the bandwidth of the perfect tiling. In the strongly localized regime, $P(s)$ tends to the exponentially decaying Poisson form.[3]

In contrast to the random case where the fluctuations of the DOS are small (compared to Poissonian, for example) the perfect approximant, like the one-dimensional Fibonacci systems,[12] has a self-similar DOS with huge fluctuations at all energy scales. This behavior can be expressed in terms of generalized fractal dimensions $D(q)$. To find these we consider a partition of the bandwidth W into M distinct boxes S_i of probability p_i and size l_i where $p_i = \frac{n_i}{N}$ and n_i is the number of levels in the box of size l_i. The dimensions $D(q)$ satisfy the condition[13]

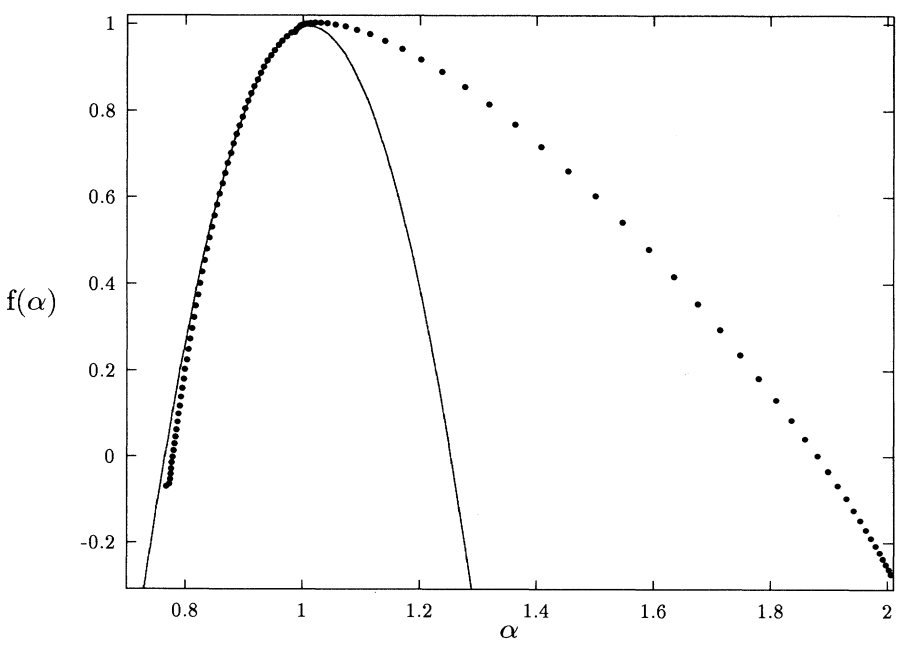

FIG. 2. $f(\alpha)$ distribution of singularity exponents α along with a fit to a parabolic shape.

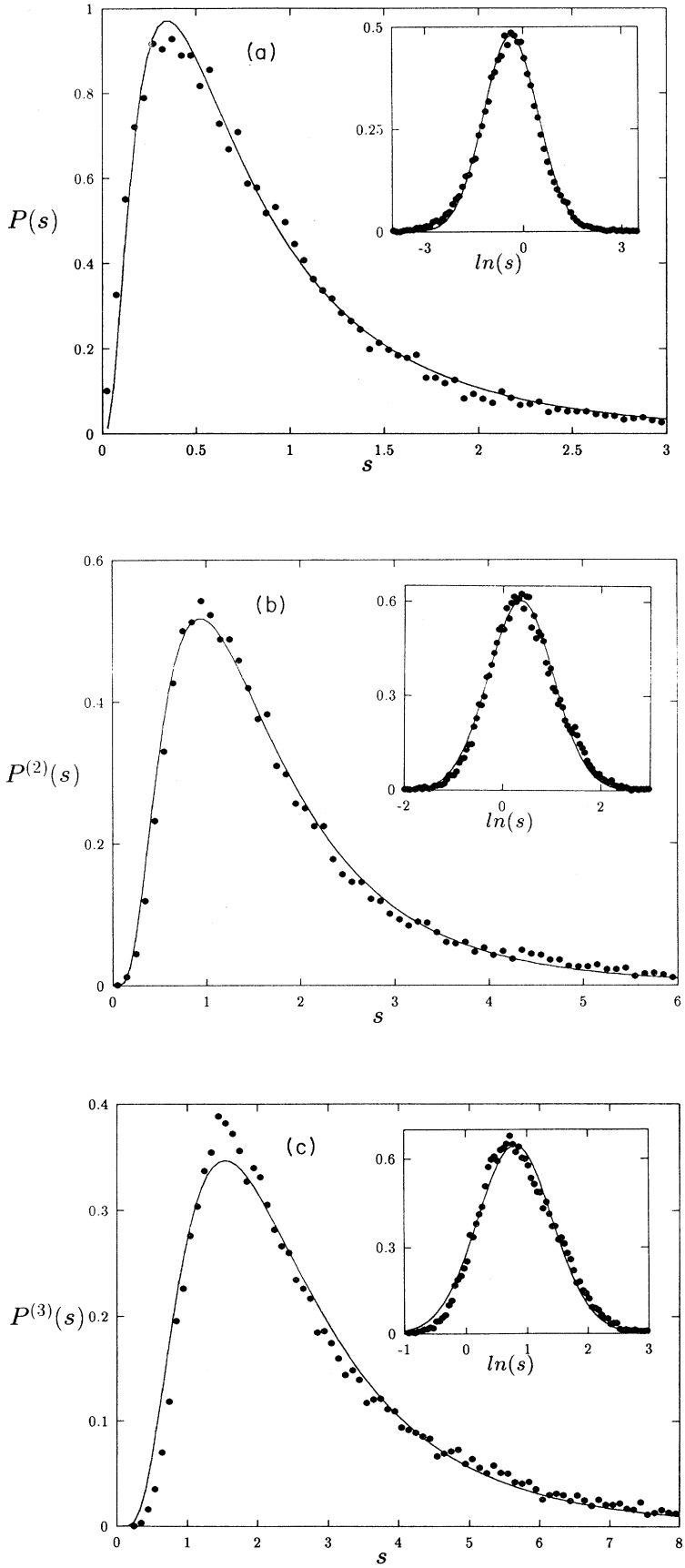

FIG. 3. (a) Level-spacing distribution for the perfect approximant fit to a log-normal form. In the inset the distribution of the logarithm of s is fit to a Gaussian. (b) and (c) Same as (a) for the next-nearest- and third-neighbor spacing distributions.

$$\sum_{i=1}^{M} \frac{p_i^{q-1}}{l_i^{\tau}} \approx 1, \tag{3}$$

with $\max_i(l_i) \to 0$ and $\tau(q) = (q-1)D(q)$. One may make a partition of boxes with equal size $l = W/M$. In that case, the measure p_i is assumed to scale as $p_i \sim l^{\alpha_i}$ when l tends to zero and the number of α_i between α and $\alpha+d\alpha$ is assumed to vary as $N_l(\alpha) \sim l^{-f(\alpha)}d\alpha$. The function $\tau(q)$ vs q and the effective $f(\alpha)$ vs α are then related by a Legendre transform. Conversely, one can fix the weights of the boxes to be identical, allowing their widths to fluctuate, and calculate $q(\tau)$. This is tantamount to calculating moments of spacings with respect to the underlying distributions $P^{(n)}(s)$. The nth-neighbor level-spacing moments $l_i = s_i^n = (E_{i+n} - E_i)/W$, $i = 1, N$, are obtained by taking the partition of fixed probability $p = n/N$.

We have computed the $f(\alpha)$ function using the two methods described above (Fig. 2). As already mentioned, the fractal dimension $D_F \sim 1$ indicating the spectrum is gapless. Another numerical argument in favor of a spectrum with no (finite measure) gap is our finding that the biggest spacing $s_{\max}$ scales as $\sim N^{-1/2}$ ($s_{\max} \to 0$ for increasing N is a necessary condition to apply the second of the two methods described above). The information dimension defined by $D_I = f(D_I)$ is $D_I = 0.98$. A fit to a parabolic form of $f(\alpha)$ close to its maximum gives its curvature $1/\mu$, $\mu = 0.03$. Now a parabolic shape for $f(\alpha)$ can be shown to lead to lognormal spacing distributions for each of the nth-nearest-neighbor spacings s^n (for $n \ll N$). The parameters of these distributions are related to D_I and μ. The distributions depend, as well, upon the system size. We have found, however, that when the distribution $P(s)$ of rescaled variables $s = N(E_{i+1} - E_i/W)$ is plotted, a single curve is obtained for the three sizes studied: N =239, 1393, and 8119 sites. The same remark applies to the two other distributions calculated, $P^{(2),(3)}$. A comment on the calculation of $P(s)$: It is well known that before computing any statistical spectral properties, the spectrum has to be unfolded.[3] Within a semiclassical scheme this is equivalent to considering the fluctuating part of the integrated density of states, where one keeps only the quantum interference corrections around the Thomas-Fermi zeroth $\hbar$ order term. However, to have an efficient unfolding, the fluctuating part has to be a small perturbation around the zeroth $\hbar$ order term which is not itself strongly fluctuating. In weakly disordered crystalline systems this is so, but in contrast the density of states of our quasiperiodic system has huge fluctuations at all energy scales. One may consider that in this case at least one of the hypotheses breaks down, and that the unfolding procedure is not well defined for our spectrum. We have therefore computed $P(s)$ without any unfolding.

The distribution of the logarithm of s is well fitted by a Gaussian [Fig. 3(a), inset], so that $P(s)$ is a log-normal function of the form

$$P(s) = \frac{1}{\sqrt{\pi B}s} \exp\left(-\frac{[\ln(s) - \ln(s_0)]^2}{2B}\right), \tag{4}$$

with $\ln(s_0) = -B/2$ for variables normalized to unity so that $\int_0^\infty sP(s)ds = 1$. Level repulsion clearly occurs, as $P(s)$ tends to zero with diminishing s at small s. The log-normal form is obeyed for spacings around the most probable value. At small s the repulsion seems *linear* rather than *exponential* as given by the log-normal, while at large spacings, $s \geq 3W/N$, the error function $\int_s^\infty P(s)ds$ behaves as $\sim s^{-2}$ implying $P(s) \sim s^{-3}$ [this agrees with the observed variation in the largest spacing as a function of the system size and with $P(s) \sim s^{-(1+\alpha_{\max})}$]. A final observation on the dependence of $P(s)$ on the flux traversing the tiling: We have done a separate calculation for each value of the flux ϕ. In the perfect approximants we find $P(s)$ to be independent of the flux, unlike the case of the random tilings and weakly localized metallic systems.[2]

In conclusion, we have numerical evidence for fundamental differences underlying spectra of perfect and random quasicrystal approximants, the latter resembling disordered crystalline systems insofar as their level statistics are concerned. The perfect approximants have log-normal distributions for the level spacings crossing over to a power law in the tails. Results for different sample sizes can be made to coincide by plotting distributions of suitably scaled variables. This result seems inconsistent with the size dependence expected of a straightforward multifractal energy spectrum and calculations on bigger systems should help resolve the issue.

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