s3.m12.p5 **Periodic diffraction patterns for selected quasicrystals.**
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In this paper we consider a one-parameter family of 1D quasicrystals. Specifically, our model is a fixed (Fibonacci) sequence of two types of "atoms" with a varying amount of space around each type of atom, under assumption that the overall density is fixed. The control parameter κ is the ratio of the two allowed distances between nearest neighbors. In all cases, the diffraction pattern is discrete, and the locations of the Bragg peaks are independent of κ. However, the *intensities* of the peaks are κ-dependent. When κ is rational, the intensities form a periodic pattern, while when κ is irrational, the diffraction pattern is aperiodic. We compute this diffraction pattern in two independent but equivalent ways: a) by recovering periodicity going to higher dimension (the "cut and project method"); b) using the concept of the reference lattice (proposed in [1]), taking advantage of physical space properties of the set only. As a result we get that the amplitude of each peak is a continuous function of κ. In fact, it is infinitely differentiable. As κ is varied, there is no phase transition between commensurate and incommensurate diffraction patterns; the evolution is smooth. As such, with measurement apparatus of fixed accuracy, it is impossible to determine whether a given pattern is precisely periodic. These results are compared to the ergodic theory of tiling spaces. It is known that the Bragg peaks of a tiling *T* occur at eigenvalues of the generator of translations on the hull of *T* (i.e., the space of all tilings in the same local isomorphism class as *T*) [2]. It is also known [3] that the hulls of modified Fibonacci chains with the same average spacing are topologically conjugate, hence that their generators of translations have the same spectral decomposition. The question of when and how such a modification affects the dynamical spectrum was addressed for one dimensional patterns in [4]. (It should be noted that for a substitution tiling whose substitution matrix has two of more eigenvalues greater than 1, a generic change in tile length will destroy the Bragg peaks altogether, in sharp contrast to the behavior of modified Fibonacci chains, other Pisot substitutions, and other Sturmian sequences.) Ergodic theory says nothing, however, about the intensities of the Bragg peaks. Although the spectrum of the generator of translations is complicated, for special values of the control parameter some of the peaks may have intensity zero, resulting in a simpler diffraction pattern. The calculations in this paper demonstrate that this does in fact happen.

[1] Wolny, J. (1998). *Philos. Mag.* A**77**, 395-412.
[2] Dworkin, S. (1993). *J. Math. Phys.* **34**, 2965-7.
[3] Radin, C. & Sadun, L. (2001). *Ergodic Theory Dynam. Systems* **21**, 1239-48.
[4] Clark, A. & Sadun, L. (2003). *Ergodic Theory Dynam. Systems* **23**, 1043-57.

s3.m12.p6 **A new approach for solving quasicrystal structures.**
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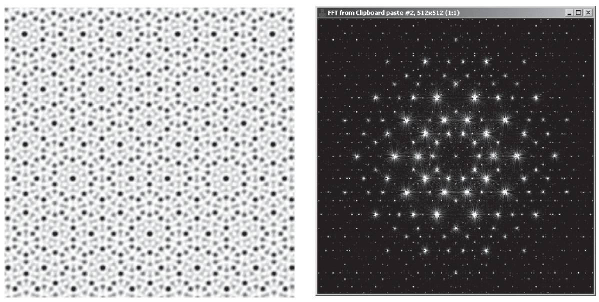
Keywords: Quasicrystal; Decagonal quasicrystal; Approximants

Since the first report of quasicrystals was reported 20 years ago, great efforts have been made to find out the nature of quasicrystals. Different approaches are made to determine the structures of quasicrystals. One approach of solving quasicrystal structures is from their approximants, since it was found by high resolution electron microscopy that quasicrystals and their approximants have very similar building clusters. In many cases, a series of approximants is related to a quasicrystal [1]. The unit cell dimensions of different approximants within the same series increase by the golden number τ, τ^2, τ^3… At the end of such a series, when the unit cell dimensions become infinite, a quasicrystal is formed. Based on this, a few structure models have been proposed for different quasicrystals. However, there is no general procedure for solving quasicrystal structures from their approximants. Recently we have derived a new general approach for solving quasicrystal structures from their approximants. By analysing the structure factor phases and amplitudes of the approximants within a series, we found the common features among those approximants. Those common features should also exist in the corresponding quasicrystal. In this way, we can generate the structure of a series of approximants with unit cells inflated by τ, and finally the perfect structures of quasicrystals. For example, the approximants starting with $Al_{13}Fe_4$ [2] (*C2/m*, *a* = 15.489, *b* = 8.083, *c* = 12.476 Å and β = 107.71°) approach the decagonal quasicrystal in the Al-Fe system (Fig. 1). This method is general and can be applied to all types of quasicrystals, including decagonal and icosahedral quasicrystals.



(a) (b)

Fig. 1 (a) Projection of the $Al_{13}Fe_4$ related quasicrystal deduced from the structure of $Al_{13}Fe_4$. (b) The corresponding Fourier transform of (a).

[1] Ma, X. L., Li, X. Z., Kuo, K. H., *Acta Cryst.* B**51**, 36-43 (1995).
[2] Freiburg, C., Grushko, B., Wittenberg, W., Reichert, W., *Mater. Sci. Forum*. **228-231**, 583-586 (1996).