Effects of quasiperiodic (Penrose tile) symmetry on the eigenvalues and eigenfunctions of the wave equation

by Shanjin He
J. D. Maynard

In addition to the basic crystalline and amorphous structures for solids, it is possible that solids may also form with a quasiperiodic, or Penrose tile, structure. A current problem in condensed-matter physics is to determine how this structure affects the various physical properties of a material. A fundamental question involves the consequences of quasiperiodic symmetry in the eigenvalue spectrum and eigenfunctions of a wave equation. While rigorous theorems have been derived for one-dimensional systems, there is currently no known "quasi-Bloch theorem" for two and three dimensions. To gain insight into this problem, an acoustic experiment has been used to study a two-dimensional wave system with a Penrose tile symmetry. The results show an eigenvalue spectrum containing bands and gaps with widths which are in the ratio of the Golden Mean, $(\sqrt{5} + 1)/2$.

Introduction

Until a few years ago it was believed that solid matter could exist in two basic forms: crystalline and amorphous (glassy). In an amorphous material the atoms are positioned randomly, and a macroscopic sample would be homogeneous and isotropic. Crystals are, of course, quite different; crystals are formed by taking a unit cell and periodically repeating it to fill three-dimensional space. In order to fill all space with long-range periodic order, only unit cells of particular shapes are allowed; only fourteen shapes fit together to fill space, and these form the bases for the fourteen Bravais lattices of crystallography (**Figure 1**). Since there are only fourteen possible unit cells, only certain rotational symmetries are allowed; in particular, fivefold rotational symmetry is forbidden. However, a few years ago Shechtman [1] at the National Bureau of Standards made an aluminum alloy whose X-ray diffraction pattern indicated fivefold rotational symmetry. While it is possible to have atoms in clusters with fivefold (icosahedral) order, the diffraction patterns had sharp spots, indicating long-range order. Furthermore, macroscopic samples of the aluminum alloy had facets indicating fivefold rotational symmetry [2]. At first the existence of such materials seemed impossible, but theorists pointed out that while it is impossible to have fivefold rotational symmetry and long-range periodic order, it is possible to have fivefold rotational symmetry and another type of long-range order which is quasiperiodic. Thus atoms may minimize their energy by arranging themselves quasiperiodically, forming quasicrystals.

In one dimension the notion of quasiperiodicity is relatively easy to understand, as illustrated in **Figure 2(a)**. For a line with periodic lattice sites at a spacing a, the Fourier transform (or diffraction pattern) has a sharp line at π/a. If a line has points positioned randomly, as shown in the lowest line in Figure 2(a), then the Fourier transform shows a broad spectrum. Now suppose one takes a line with periodic lattice spacing b and superimposes it on the line with periodic spacing a. The result may appear similar to the line with random spacing. However, if the two lattice constants a and b are commensurate (i.e., their a/b ratio is equal to the ratio of two integers), then the superposition will be periodic. The period may be much larger than a or b, but it will be exactly periodic, the powerful theorems pertaining to periodic systems (Bloch's theorem, group theory, etc.) will apply, and the properties of the system which follow from symmetry may be calculated exactly. On the other hand, if the two lattice constants a and b are not commensurate (i.e., their a/b ratio is equal to an irrational number), then the superposition is not periodic, and there is in general no easy way to calculate the properties. Nevertheless, the superposition does possess long-range order; it is constructed from simple rules, and its Fourier transform contains sharp peaks at π/a and π/b. The superposition of periodic lines with incommensurate lattice constants is an example of one-dimensional quasiperiodicity.

While quasiperiodicity in one dimension is fairly straightforward, in two and three dimensions the notion is considerably more interesting [3]. To show how to obtain quasiperiodicity in higher dimensions, a second method of obtaining one-dimensional quasiperiodicity is illustrated in **Figure 2(b)**. One begins with a periodic lattice in a higher dimension, e.g., a square lattice in two dimensions. The higher-dimensional lattice is traversed by a lower-dimensional surface, e.g., a straight line passing through the square lattice, making an angle θ with one of the lattice directions. Next a window width is defined, and lattice points falling within that window are projected onto the lower-dimensional surface. If the direction cosines describing the orientation of the lower-dimensional surface are irrational, then the sites projected onto the surface will form a quasiperiodic pattern. In the one-dimensional example, a particularly interesting case occurs when the slope of the line is such that $\tan\theta = (\sqrt{5} + 1)/2$, the Golden Mean (also known as the Divine Ratio), which is "the most irrational number." In this case the pattern of sites can be related to a Fibonacci sequence, and rigorous theorems describing the properties of this special quasiperiodic symmetry can be derived. General theories for one-dimensional systems have been reviewed by Simon [4], and renormalization-group and dynamic mapping techniques have been introduced by Kohmoto, Kadanoff, and Tang [5] and by Ostlund et al. [6]. Since the discovery of the aluminum alloy quasicrystals [1], there has been considerably more work with renormalization-group techniques and numerical calculations [7, 8]. Some special properties of 1D quasiperiodic systems are as follows:

1. The eigenvalue spectrum is a Cantor set.
2. There may exist a mobility edge and a metal–insulator transition.

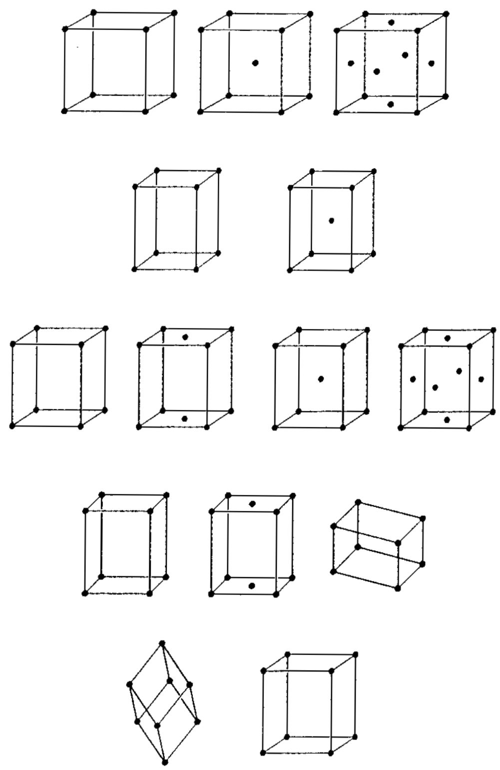

Figure 1

Unit cells for the fourteen Bravais lattices.

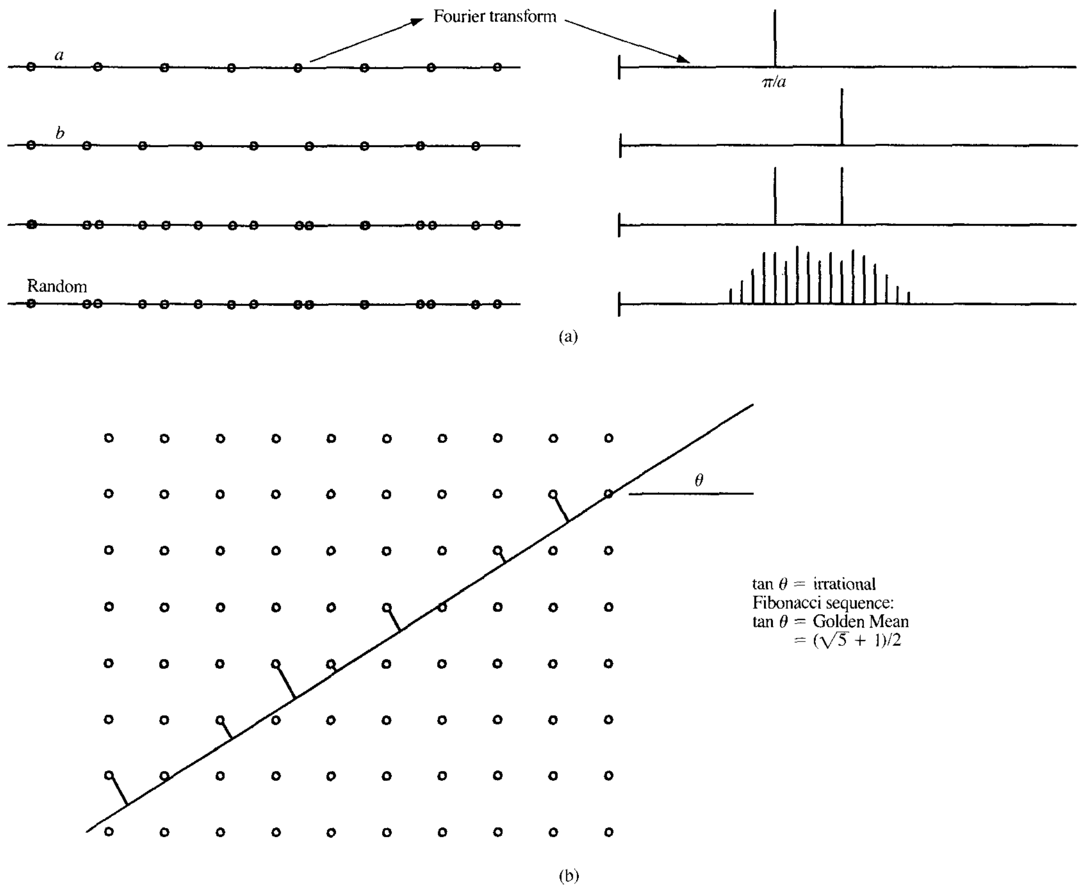

Figure 2

(a) Illustration of periodic, quasiperiodic, and random structures in one dimension. (b) Illustration of the projection technique for obtaining one-dimensional quasiperiodicity.

3. The eigenfunctions may be extended, localized, or critical.

One-dimensional quasiperiodic systems have received some experimental attention, through measurements of infrared reflectivity in quasiperiodic superlattices formed with molecular beam epitaxy [9].

If one begins with a six-dimensional periodic lattice (e.g., a hypercubic lattice) and intersects it with a three-dimensional surface, then one may obtain a three-dimensional quasiperiodic pattern; such patterns may describe the recently discovered aluminum alloy quasicrystals. If one begins with a five-dimensional periodic lattice and intersects it with a two-dimensional (plane) surface, one may obtain a two-dimensional quasiperiodic pattern, or Penrose tiling [10, 11]; one such pattern is illustrated in Figure 3(c). If one tries to tile a plane with only one tile shape (unit cell), then, as in three dimensions, only certain shapes and rotational symmetries are allowed. However, if one is allowed to use tiles of two or more shapes, fivefold and other symmetries are possible. Articles and cover stories on Penrose tiling have appeared in *Scientific American* [11], *American Scientist* [12], etc. There is even a company which makes bathroom tiles to be set in quasiperiodic Penrose patterns, and the patterns are also found on quilts.

Although Penrose tile patterns are not periodic, they do have some symmetry properties [11, 12]. Special patterns may have "inflation symmetry," so that a decoration of the tiles with certain lines will produce a replication of the original Penrose pattern, but with a reduced scale. There is also Conway's theorem, which states that given any local pattern (having some nominal diameter), an identical local

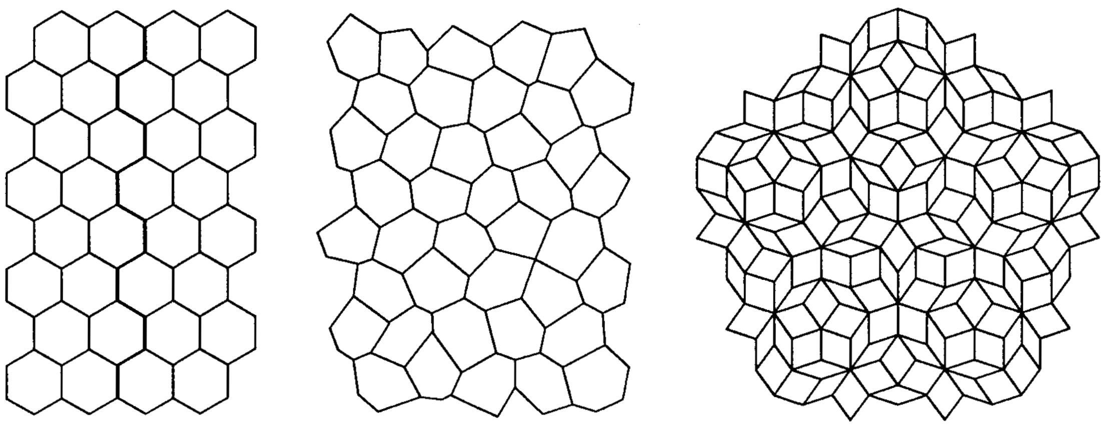

Figure 3

Three possible structures and the techniques which may be used to determine their properties: (a) Periodic (Bloch theorem); (b) Random (statistical methods); (c) Quasiperiodic (no known theoretical method).

pattern will be found within a distance of two diameters. The typical Penrose tiling shown in Figure 3(c) is formed with two different rhombuses, a fat one and a skinny one; the ratio of the areas is the Golden Mean, $(\sqrt{5} + 1)/2$.

Quasiperiodic patterns are a newly discovered symmetry of nature; it is important to understand how this new symmetry affects the properties of materials. For example, what is the density of states for phonons and for electrons in a quasicrystal? What is the heat capacity and electrical conductivity? How is a superconducting transition effected? A fundamental question is this: Given a wave equation (for Schrodinger waves or sound waves) with a potential field having quasiperiodic symmetry, what are the eigenvalues and eigenfunctions? Unlike the theorems for the quasiperiodic patterns in one dimension, theorems for two and three dimensions, if they exist, have not yet been discovered. For a pattern which is periodic **[Figure 3(a)]**, Bloch's theorem may be used to obtain exact solutions. For a pattern which is random **[Figure 3(b)]**, statistical methods may be used to make predictions about properties (e.g., Anderson localization). However, a quasiperiodic pattern **[Figure 3(c)]** is not periodic, so that Bloch's theorem cannot be used; and it is not random, so statistical methods cannot be used. In the absence of a quasi-Bloch theorem, progress in understanding the consequences of 2D quasiperiodic symmetry has relied mostly on numerical calculations. Early methods suggested the occurrence of a van Hove singularity [13], but nothing significantly unique to quasiperiodic symmetry [14]. More precise numerical studies indicated that there was no van Hove singularity, but rather a highly degenerate eigenvalue (at the center of a symmetric spectrum) with a gap on each side [15]. The states corresponding to the degenerate eigenvalue have been shown to be completely localized, and the surrounding gap is the result of the depletion of the nearby states into the central peak. There have been a few exact eigenfunctions discovered for 2D quasiperiodic systems [16, 17], but these only apply to certain eigenvalues or special Hamiltonians.

Despite the notable efforts described above in searching for unique consequences of 2D quasiperiodic symmetry, existing studies do not treat the problem of a wave equation with a quasiperiodic potential. All of the current theoretical research has dealt with a hopping Hamiltonian involving a matrix reflecting quasiperiodic topology, but having all nonzero matrix elements identical. For an actual wave equation, the problem can be reduced to a similar matrix, but the nonzero matrix elements would be complex functions of the eigenvalue, whose determination would involve solving a complicated transcendental equation. It is likely that the resulting eigenvalue spectrum would be quite different from the ones found with the existing theoretical models, because now one must contend with the possibility of phase coherence effects in a system of scatters with a quasiperiodic pattern. Another way of viewing the situation is to note that another length, the wavelength, has entered the problem. The relation between the wavelength and the

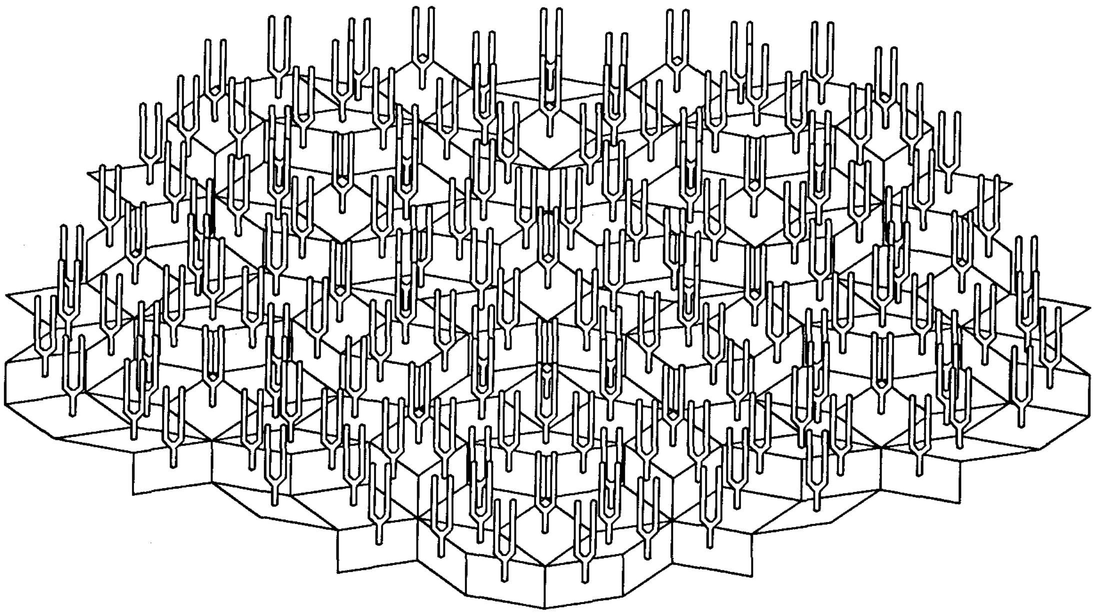

Figure 4

Schematic drawing of tuning fork quasicrystal. The tuning forks are mounted at the center of the rhombuses in the Penrose tile, with the two tines oriented in line with the shorter diagonal (for the sake of drafting simplicity, the tuning forks are not drawn with the correct orientation). For the nearest-neighboring coupling, arcs of steel wire (not shown) are spot-welded from one tine of a tuning fork to that of a nearest neighbor.

inflation and pattern-repetition properties of the quasiperiodic pattern may result in new features in the density of the states. Such effects have already been observed in other 2D quasiperiodic systems where a characteristic length has been introduced [18, 19], but these systems have not involved wave-mechanical effects.

At The Pennsylvania State University an acoustic model is being used to answer the fundamental question concerning the eigenvalues and eigenfunctions of the wave equation with a quasiperiodic potential [the fivefold Penrose tiling pattern of Figure 3(c)]. It is anticipated that once actual solutions can be observed, then theorems may be more readily developed, and further properties and applications may be revealed. The study of energy eigenstates of the Schrodinger equation through the use of acoustic wave analogs is discussed in the literature [20]. The wave function ψ may be energy eigenstates with time dependence exp $(iEt/\hbar)$ for quantum particles or monotonal waves with time dependence exp $(i\omega t)$ for sound waves. In either case the wave equation may be written

$$\nabla^2\psi + [q^2 - V(r)]\psi = 0, \qquad (1)$$

where for particles $q^2 = 2mE/\hbar^2$ (with m the particle mass), and for sound waves $q = \omega/C$ (with C the characteristic speed of sound). $V(r)$ is the potential (normalized with $2m/\hbar^2$) for particles and a combination of a stiffness operator and mass density for an acoustic medium. Using a suitably constructed acoustic system, the salient features of the quantum system and the acoustic system can be made mathematically identical.

A convenient model for developing theorems and computer simulations is the tight-binding model. In this model lattice sites are occupied by local oscillators which, if isolated, would have one or more sharp eigenfrequencies (such as the quantized energy levels of an isolated atom). These local oscillators are allowed to interact through some coupling mechanism to nearest-neighbor lattice sites; the local oscillator eigenfrequencies then broaden out into bands of eigenfrequencies. The symmetry of the coupling, i.e., the quasiperiodic Penrose pattern, should have some manifestation in the resulting eigenvalue spectrum and band structure.

For the ideal case, the system should have little or no damping; i.e., the local oscillators and the coupling mechanism should have a high quality factor (Q). Ordinary commercial tuning forks (440 Hz) were used for the local oscillators in the acoustic simulation. These have the advantage that they can be mounted by the stem and still maintain a high Q oscillation. The tuning forks are epoxied into a heavy aluminum plate in the Penrose pattern at the centers of the rhombuses (a schematic of the tuning fork quasicrystal is shown in **Figure 4**). For the nearest-neighbor coupling, arcs of 1-mm-diameter steel wire are spot-welded from one tine of a tuning fork to that of a nearest neighbor. Other coupling schemes were tested and found to be either too weak or too lossy, or they had too low a coupling wave velocity. Using the four sides of each rhombus, four nearest neighbors are identified, and each tine of a tuning fork is coupled to the two nearest tines of the adjacent tuning forks. With this coupling pattern each local oscillator has four nearest neighbors, but the nearest-neighbor length varies in a quasiperiodic pattern. There are four different lengths: 3.7, 5.8, 7.26, and 7.77 cm. From a separate measurement of the fundamental resonance in an isolated arc of the coupling wire, the nominal wavelength in the coupling wire system at 440 Hz was determined to be ~20 cm, or approximately 3 to 5 nearest-neighbor lengths. With a wavelength of this size, it is possible for the coupling wire system to interact with the quasiperiodic pattern in interesting ways and produce structure in the eigenvalue spectrum. Another method of coupling would have the local oscillators positioned at the vertices of the rhombuses in the Penrose pattern; the coupling lengths would then be the same, but the number of nearest neighbors would vary.

In order to drive the oscillations of the coupled tuning fork system, an electromagnet is positioned near one tine of the array, and an ac current is passed through the electromagnet. The response of the system is monitored with four electrodynamic transducers (electric guitar pickups) positioned next to random tines in the array. By sweeping the frequency of the drive electromagnet, the resonant response of the system is detected with the pickup transducers; the resonant frequencies, in bands near 440 Hz, correspond to the eigenvalues of the quasiperiodic system. The eigenvalue spectrum, determined as a composite of the resonant spectra from twenty different positions in the Penrose pattern, is presented in **Figure 5(a)**. This spectrum shows gaps and bands whose widths are in the ratio of the Golden Mean, $\tau = (\sqrt{5} + 1)/2$. Referring to Figure 5(a), $\gamma/\alpha = \tau$, $\delta/\beta = \tau$, $(\gamma + \delta)/(\alpha + \beta) = \tau$, and $\alpha/\epsilon = \tau^3$, with an average deviation of $\pm 5\%$. The density of states, determined as the inverse of the difference in frequency for neighboring eigenvalues, is shown in **Figure 5(b)**.

Measuring the eigenfunction involves driving the tuning fork array at one of its eigenfrequencies and recording the motion of each of the 300 tines. It would have been a prohibitive task to instrument and calibrate each tine (including two-dimensional movement). Instead, a very small mirror is placed at the end of each tine, and the tuning fork array is mounted on one wall of a dark room, with a

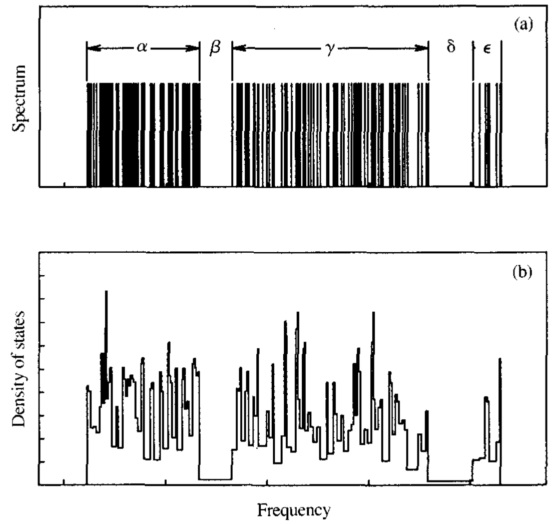

Figure 5

(a) Eigenvalue spectrum of the tuning fork quasicrystal. It is determined as a composite of the resonant spectra from twenty different positions in the Penrose pattern, and shows the gaps and bands whose widths are in the ratio of the Golden Mean, $(\sqrt{5} + 1)/2$. (b) The density of states, as the inverse of the difference in frequency for neighboring eigenvalues.

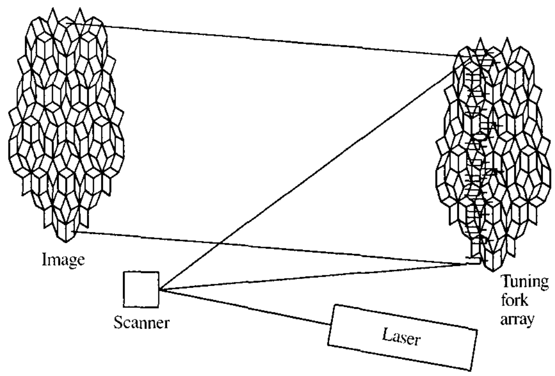

Figure 6

Schematic drawing of the system used to photograph the eigenfunctions of the tuning fork quasiperiodic system.

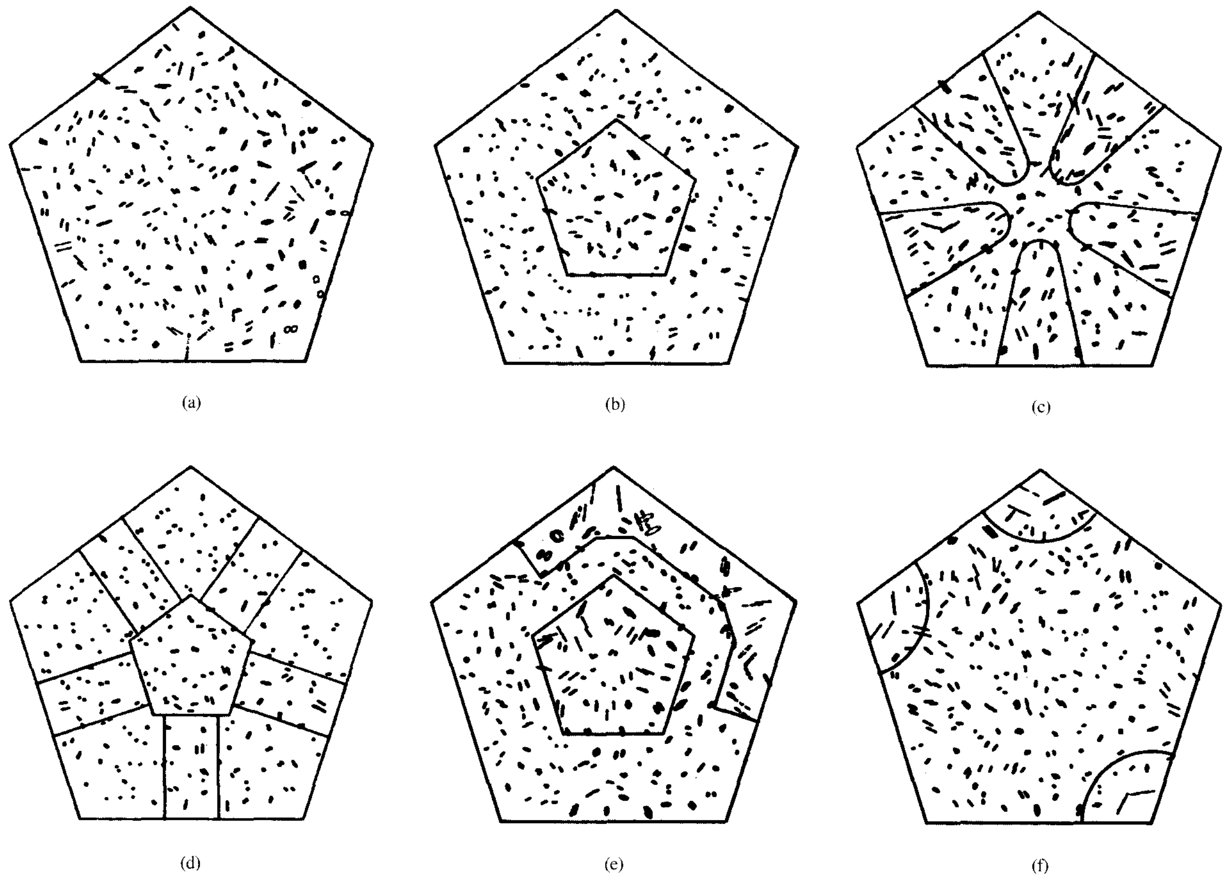

Figure 7

Several eigenfunctions of the tuning fork quasiperiodic system. They show the motion (both amplitude and polarization) of the system (note that the longer the laser spot, the larger the amplitude). In (a), (b), (c), and (d) energy distributions have fivefold rotational symmetry; in (e) and (f) the distributions have the symmetry of a mirror plane.

drawing depicting the mirror image of the Penrose pattern mounted on the opposite wall, as shown in **Figure 6**. The mirrors are adjusted so that a laser beam directed to one of the tines is reflected to the corresponding position of the tine in the image drawing. If a tine is vibrating, its motion (amplitude and polarization) will be reproduced in the motion of the laser spot in the image drawing, but with an amplified displacement resulting from the optical lever arm provided by the laser beam traversing the room. By scanning the laser beam over the entire tuning fork array, the motion of the tines may be observed in the motion of the laser spots in the image drawing. A time-exposed photograph of the moving laser spots taken during the scan records lines, ellipses, or circles of various amplitudes indicating the motion of each of the tuning forks; this is essentially a photograph of the eigenfunction at that particular eigenfrequency.

Several eigenfunctions are shown in **Figure 7**. It should be noted that the tuning fork quasicrystal is not perfect; there are defects arising primarily from unavoidable variations in the spot welds between the tines and the coupling wires. As a consequence of the adiabatic theorem for small perturbations, the defects have a minor effect on the eigenvalue spectrum, so that the observations concerning the gaps and bands are still valid. However, the defects may have a much greater effect on the eigenfunctions; furthermore, it was not possible to align the mirrors and identify the individual tines exactly in the eigenfunction photographs. As a consequence, the photographs are used only to obtain a qualitative idea of the nature of the eigenfunctions. Figure 7 illustrates some of the basic patterns which were found; lines have been drawn indicating the general areas containing the larger amplitudes. In (a) energy is uniformly distributed; in (b) energy is concentrated in the center; in (c) energy is concentrated in the five symmetric arms; in (d) energy is concentrated both in the center and in the arms; in (e) energy is localized in the center and partly at the edges; and in (f) energy is localized in three of the five corners. The lack of fivefold symmetry in (e) and (f) may be due to a combination of degenerate eigenstates.

Conclusion

As already mentioned, including the effects of a finite wavelength in a system coupled in a quasiperiodic pattern significantly increases the complexity of the eigenvalue problem. However, for a system with a few hundred scattering sites, a numerical computation should be possible. It is hoped that the acoustic "analog computer" results will stimulate further studies of waves in quasiperiodic systems and aid progress in finding theorems dealing with the consequences of quasiperiodic symmetry in two dimensions.

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Shanjin He *Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802.* Mr. He is a Ph.D. student at The Pennsylvania State University currently engaged in the study of Anderson localization and quasiperiodic systems in acoustics. He received his B.Sc. in physics from the University of Nanjing, People's Republic of China, in 1982. In 1982–1983 Mr. He was a member of the faculty of the Institute of Acoustics and Department of Physics, University of Nanjing.

Julian D. Maynard *Department of Physics, The Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802.* Professor Maynard received his B.S. degree from the University of Virginia in 1967 and his Ph.D. from Princeton University in 1974. He continued in a postdoctoral position working for Isadore Rudnick at UCLA, where he learned a good deal about experimental acoustics. In 1977 he joined the physics faculty at Penn State as an Alfred P. Sloan Fellow, and in 1988 became a Professor of Physics. His research interests include the acoustic properties of random and quasiperiodic systems and various applications of acoustics in superfluid helium, including thermodynamic measurements, the measurement of "fifth sound," the Kosterlitz–Thouless–Nelson transition and the wetting transition for liquid films, and the critical behavior of solid films. Professor Maynard's current research involves the measurement of ultrasound velocity and attenuation in single crystals of high-temperature superconductors.