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Lattice dynamics of three-dimensional quasi-crystals

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Abstract. The density of states (DOS) is calculated for a three-dimensional Penrose tiling with icosahedral symmetry by taking two different approximations, the cluster approximation and the commensurate approximation. It is compared with the DOS for a model of the icosahedral phase of Al–Mn–Si (i-ALMnSi) in the cluster approximation. At low frequencies the DOS contains pseudo-gaps. The spectrum possesses scaling properties. The global contours of the DOS for i-ALMnSi are in reasonable agreement with the experiments.

1. Introduction

In 1984 Shechtman *et al* [1] found a diffraction pattern with sharp spots in combination with icosahedral point group symmetry by doing measurements on a rapidly cooled Al–Mn alloy. Since then other compounds with similar properties have been found.

This amazing fact implied a new kind of problem for solid state physicists: to determine the structure as well as to deal with the physical properties of these structures, such as the dynamics and the electronic behaviour which, although ordered, are not lattice periodic. Here we will consider the lattice dynamics.

Concerning the structure, most people working on the subject seem to agree that the structure of i-ALMnSi is related to a three-dimensional icosahedral quasi-lattice, and therefore this structure is called a quasi-crystal. A quasi-lattice is not periodic, but so-called quasi-periodic. Connecting the vertices of this quasi-lattice in a suitable way one gets a non-periodic packing of a finite number of cells or ‘tiles’, which is called a Penrose tiling (PT) [2–4]. There are several methods to construct Penrose patterns: the deflation rule method [5, 6], the projection method [7, 8], the section method [9, 10] and the general dual method [11]. In this paper we will use the section method, which consists of taking the intersection of a periodic structure in a higher-dimensional space (superspace) with the normal space of the PT we are looking at.

The problem we are faced with when dealing with the lattice dynamics of quasi-periodic structures is that we have an infinite number of coupled equations of motion. Although it is possible to make a Bloch *ansatz* by making use of the superspace translational symmetry in a similar way as was done by Janssen [12] for modulated structures, this does not reduce the number of coupled equations to a finite number, as is the case in ordinary crystals, because in superspace we have instead of point atoms ‘atomic surfaces’, which in fact contain an infinite number of point atoms. In other words, the unit cell in superspace contains an infinite number of atoms. Still a PT is very well ordered, but until now no one has succeeded in using this order to

simplify drastically the problem of finding the lattice vibrations. We will have to make approximations. One possibility is to make the number of equations of motion finite. This can be done in two different ways.

(i) The commensurate approximation, i.e. deformation to a periodic structure. In general one can make successive approximations which are better and better having more and more atoms in the unit cell. By comparing successive approximations we can look for the limit of the density of states (DOS) or the integrated density of states (IDOS).

(ii) The cluster approximation. Here also we can look to the convergence of the DOS by comparing the DOS for clusters of different size, i.e. with more and more atoms.

Of course comparison of the results of both approximations might give information about how accurate they are.

The outline of this paper is as follows. In section 2 we discuss briefly the way how the three-dimensional PT (3DPT) is constructed by using the section method. Then we use this PT to construct a simple dynamical model taking a spring potential. In subsection 2.1 the cluster approximation is discussed and the DOS is presented for different sizes of the cluster, different boundary conditions and different choices of the spring constants. In subsection 2.2 we show how commensurate approximations can be made by making use of the superspace description. The DOS is given for three successive approximations. Next we analyse the fractal properties of the spectrum by a method that was formulated by Kohmoto [13], who introduced an entropy function describing the behaviour of the bandwidths for successive periodic approximations. In section 3 we say something about the structure of *i*-AlMnSi as proposed by Janot *et al* [14] and we use this structure to calculate the DOS in the cluster approximation using a Lennard-Jones potential. Finally, we give some concluding remarks.

2. Structure and dynamics of an icosahedral PT

The icosahedral 3DPT can be found by taking the intersection of a periodic structure in a six-dimensional space V_s with a three-dimensional subspace V_E (external space). The basis in V_s can be chosen as hypercubic:

$$\begin{aligned} a_1 &= a(1, \phi, 0, 1, \phi, 0) & a_3 &= a(0, 1, \phi, -\phi, 0, -1) & a_5 &= a(\phi, 0, -1, 0, -1, -\phi) \\ a_2 &= a(-1, \phi, 0, 1, -\phi, 0) & a_4 &= a(\phi, 0, 1, 0, -1, -\phi) & a_6 &= a(0, 1, -\phi, -\phi, 0, 1) \end{aligned} \quad (1)$$

where a is a lattice constant, which we choose to be equal to 1 for simplicity, and ϕ the golden rule, i.e. $\phi = (\sqrt{5} + 1)/2$.

The first three components of these vectors are in the normal space V_E , the last three in the internal space V_I , which is perpendicular to V_E . So we have:

$$V_s = V_E \oplus V_I.$$

When we project the six-dimensional hypercubic unit cell on V_I we get a three-dimensional 'surface', the triacontahedron. A six-dimensional periodic structure is obtained by attaching such a triacontahedron to each lattice point of the six-dimensional lattice perpendicular to V_E , the centre of the triacontahedron coinciding with the lattice point.

The intersection of this structure with a three-dimensional subspace parallel to V_E is a 3DPT, containing two types of tiles, a prolate rhombohedron and an oblate rhombohedron (see figure 1 (a), (b)). When the three-dimensional subspace parallel to V_E contains a lattice point of the six-dimensional lattice, the PT has almost icosahedral point group symmetry, this lattice point being the centre of symmetry. That the icosahedral symmetry is not complete is due to the fact that one of two opposite boundaries of the triacontahedron is excluded in the six-dimensional structure.

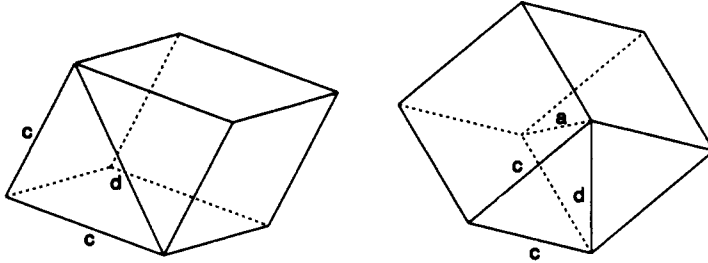


Figure 1. The ‘tiles’ of the 3DPT: the prolate rhombohedron (a) and the oblate rhombohedron (b). The distances are $a = 1.070$, $c = 1.902$ and $d = 2.000$. The other distance, ie $b = 1.236$, which occurs in the 3DPT comes from placing the ‘tiles’ together in the right way.

Once we have the quasi-lattice we place an atom with mass $m=1$ in each vertex. Connecting neighbouring atoms by harmonic springs we get the following expression for the total potential energy:

$$\Phi = \frac{1}{4} \sum_i \sum_{i'(i)} \alpha_{ii'} [(\mathbf{u}_i - \mathbf{u}_{i'}) \hat{\mathbf{r}}_{ii'}]^2 \tag{2}$$

where $\sum_{i'(i)}$ means summation over the neighbours of i , $\alpha_{ii'}$ the spring constant of the spring between atom i and i' , \mathbf{u}_i the displacement of atom i from its equilibrium position and $\hat{\mathbf{r}}_{ii'}$ a unit vector in the direction of the line connecting the equilibrium positions of both atoms.

As neighbours we have taken all pairs of atoms with an equilibrium distance equal to 1.070, 1.236, 1.902 or 2.000, which are the four shortest distances occurring in the 3DPT. The interaction between other pairs is taken to be zero. Figure 1 shows where those distances occur with respect to both rhombohedra.

The relevant quadratic term of Φ is given by:

$$\text{quadratic term} = \frac{1}{2} \sum_{j'\alpha'} \sum_{j\alpha} u_{j'\alpha'} \Phi^{(2)} \begin{pmatrix} j' & j \\ \alpha' & \alpha \end{pmatrix} u_{j\alpha} \tag{3}$$

where $u_{j\alpha}$ is the displacement of the j th atom in the α th direction and

$$\Phi^{(2)} \begin{pmatrix} j' & j \\ \alpha' & \alpha \end{pmatrix} = \frac{\partial^2 \Phi}{\partial u_{j'\alpha'} \partial u_{j\alpha}} = \sum_{i(j)} \alpha_{ij} \hat{\mathbf{r}}_{ij\alpha'} \hat{\mathbf{r}}_{ij\alpha} \delta_{jj'} - \sum_{i(j)} \alpha_{jj'} \hat{\mathbf{r}}_{jj'\alpha'} \hat{\mathbf{r}}_{jj'\alpha} \delta_{ij'} \tag{4}$$

The equation of motion is given by

$$\ddot{u}_{j\alpha} = - \sum_{j'\alpha'} \Phi^{(2)} \begin{pmatrix} j & j' \\ \alpha & \alpha' \end{pmatrix} u_{j'\alpha'} \tag{5}$$

Substituting $u_{j\alpha} = c_{j\alpha} e^{i\omega t}$ we get the following infinite eigenvalue problem:

$$\omega^2 c_{j\alpha} = \sum_{j'\alpha'} \Phi^{(2)} \begin{pmatrix} j & j' \\ \alpha & \alpha' \end{pmatrix} c_{j'\alpha'}. \quad (6)$$

2.1. Cluster approximation

To reduce the number of coupled equations to a finite number, so that we can solve the eigenvalue problem (6), one possibility is to take a cluster of the 3DPT with a finite number of atoms. We can do this either by taking free boundary conditions or fixed boundary conditions. A free boundary means that there is no interaction between the atoms at the boundary and anything outside the cluster. A fixed boundary means that the cluster is embedded in the infinite system, but in that case the displacements of atoms outside the cluster are just equal to zero.

Furthermore, we enforce the cluster to have icosahedral symmetry just by including all boundaries of the triacontahedron in the six-dimensional structure. This hardly violates the original 3DPT and it has been checked that it does not produce too small neighbour distances. Then we know that the eigenstates transform according to the irreducible representations of the icosahedral group. By using a symmetrized basis we can uncouple the set of equations, leaving us to solve an eigenvalue problem for each irrep. The order of these eigenvalue problems are of course much smaller than the order of the dynamical matrix for the total system. Regarding the finiteness of the computer storage capacity this is a very useful fact.

Another useful fact is that the irreducible components of the dynamical matrix, apart from being real and symmetric, are also band matrices, the bandwidth being about one quarter of the order of the matrix blocks. This is due to the fact that there is no interaction between atoms with an equilibrium distance bigger than 2.0. Although the matrix elements of these irreducible blocks do not describe the coupling between atoms, but the coupling between orbits of atoms, it is still true that 2 orbits for which the difference in distance to the centre of the cluster, which is the symmetry centre, is bigger than 2.0 do not couple.

Figures 2(a), (b) give the DOS for clusters of, respectively, 7895 and 16009 atoms with free boundary conditions and all spring constants equal to one. Figure 3 gives the DOS for a cluster of 7895 atoms with fixed boundary conditions. (All $\alpha_{ii'} = 1$.) Figures 4(a), (b) give the DOS for clusters of 7895 atoms with free boundary conditions where the spring constants for the two smallest neighbour distances are taken to be 2 and 3 respectively. The other two spring constants are taken to be equal to one.

In these figures the units on the frequency axis are arbitrary.

From figure 2 one can conclude that, although the global contours are about the same for both clusters, there is a lot of difference in the fine structure, so that one cannot decide which peak will occur for the infinite PT. The same remark holds when we compare the figures 2 and 3. We also remark that the left shoulder in the DOS in the case of free boundary conditions is somewhat higher than in the other case. Comparing figures 4(a) and 4(b) we can say that some peaks remain while others disappear or are moved when we vary some of the spring constants.

Another interesting feature is the behaviour at low frequencies. Will there be gaps for an infinite system? Or will the behaviour become smoother and smoother, converging to a normal ω^2 behaviour when we take bigger and bigger clusters? We will come back to this point when we discuss the results of the commensurate approximation.

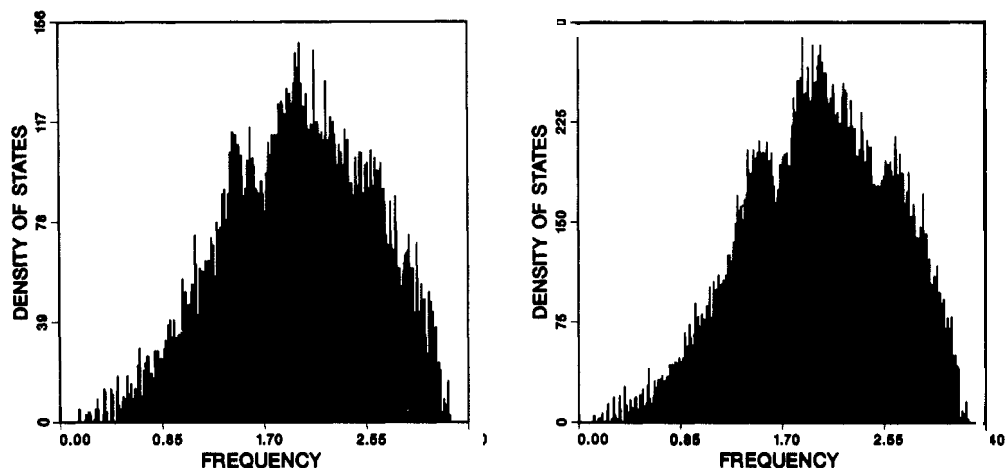


Figure 2. The DOS for clusters of the 3DPT with 7895 (a) and 16009 (b) atoms for free boundary conditions and all spring constants equal to one.

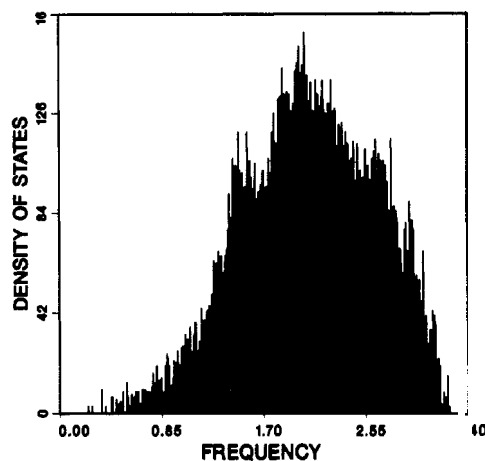


Figure 3. The DOS for a cluster of the 3DPT with 7895 atoms for fixed boundary conditions and all spring constants equal to one.

2.2. Commensurate approximation

A commensurate approximation of the 3DPT can be obtained by taking for ϕ in the set of basis vectors (1) a rational approximant ϕ_n . This can be done by taking two successive numbers of the Fibonacci-sequence:

$$\phi_n = f_n / f_{n-1} \quad (7)$$

where $f_0 = f_1 = 1$ and $f_{n+1} = f_n + f_{n-1}$.

As in the former case the six basis vectors with ϕ replaced by ϕ_n span a six-dimensional space V_s which again is the orthogonal sum of two three-dimensional spaces, V_E and V_I , attached to respectively the first and the last three components of those basis vectors. When we take a three-dimensional subspace of V_s parallel to V_E passing through a lattice point of the six-dimensional lattice it automatically will

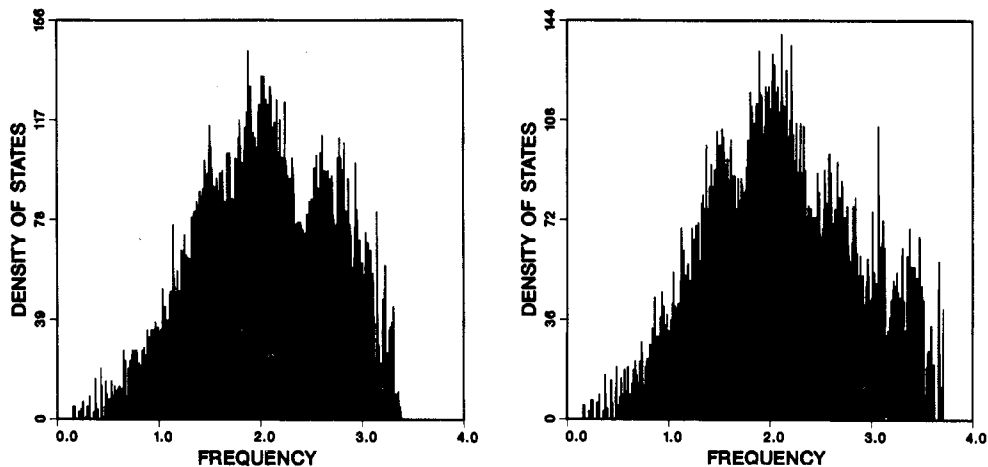


Figure 4. The DOS for a cluster of the 3DPT with 7895 atoms for free boundary conditions. The spring constants for both biggest neighbour distances are taken equal to one, and those for both smallest neighbour distances are taken equal to two (a) and three (b).

contain other lattice points occurring periodically in three independent directions. This defines a periodic lattice in three dimensions. A basis of this lattice depends on n and is given by

$$\begin{aligned}
 a_1^{(n)} &= (2/f_{n-1})(f_n^2 + f_{n-1}^2, 0, 0) \\
 a_2^{(n)} &= (2/f_{n-1})(0, f_n^2 + f_{n-1}^2, 0) \\
 a_3^{(n)} &= (2/f_{n-1})(0, 0, f_n^2 + f_{n-1}^2)
 \end{aligned} \tag{8}$$

showing that the commensurate approximation has cubic lattice periodicity.

To find the positions of the atoms in the unit cell we might proceed in the same way as we did to find the original structure, i.e. attach to each lattice point of the changed lattice the projection of the unit cell of this lattice on V_I and take the intersection with V_E . However we want the periodic approximation to be a deformation of the original PT, and therefore we determine the positions of the atoms as follows.

The original positions of the atoms are given by integral (not all!) linear combinations of the following six vectors:

$$\begin{aligned}
 a_{1E} &= (1, \phi, 0) & a_{3E} &= (0, 1, \phi) & a_{5E} &= (\phi, 0, -1) \\
 a_{2E} &= (-1, \phi, 0) & a_{4E} &= (\phi, 0, 1) & a_{6E} &= (0, 1, -\phi)
 \end{aligned} \tag{9}$$

The positions in the commensurate approximation are found by taking the same integral linear combination but with ϕ replaced by ϕ_n . Of course we only need to know the positions inside the unit cell, for which the edges are given by $a_1^{(n)}$, $a_2^{(n)}$ and $a_3^{(n)}$. We remark that both methods of determining the atomic positions are not equivalent. The number of atoms inside the unit cell $N_0(n)$ as a function of the approximation, using this method, is given in table 1.

Table 1.

ϕ_n	2/1	3/2	5/3	8/5	13/8
$N_0(n)$	135	565	2506	10 313	44 359
$N_1(n)$	136	576	2440	10 336	43 784
$N_2(n)$	136	576	2440	10 336	43 785

Analytically the number of atoms inside the unit cell as a function of the approximation is given by

$$N_1(n) = \frac{V_{\text{cell}}(n)}{V_{\text{at}}(n)} \tag{10}$$

where $V_{\text{cell}}(n)$ is the volume of the unit cell and $V_{\text{at}}(n)$ the mean volume per atom.

For the section method one can derive that

$$V_{\text{at}}(n) = \frac{V_{s\text{ cell}}(n)}{V_{\text{tria}}(n)} \tag{11}$$

where $V_{s\text{ cell}}(n)$ is the volume of the unit cell in superspace and $V_{\text{tria}}(n)$ the volume of the deformed triacontahedron both as function of the approximation we are considering. Expressing these quantities in terms of f_n and f_{n-1} one finds

$$N_1(n) = 4f_n(3f_{n-1}^2 + 3f_n f_{n-1} + 2f_n^2). \tag{12}$$

An approximation for the number of atoms per unit cell is given by

$$N_2(n) = N_0 c^n \tag{13}$$

where $c = \phi^3$ and N_0 is a constant to be fitted. That this is a rather good approximation can be understood by realising that the original structure scales with scaling factor ϕ^3 .

In table 1 $N_1(n)$ and $N_2(n)$ are given as a function of the approximation.

In the commensurate approximation the icosahedral point group symmetry is lost, but there is still symmetry left which is the tetrahedral group plus inversion, T_h . Here again we have to include all the boundaries of the deformed triacontahedron, otherwise we have no symmetry at all. For the total symmetry group we distinguish between two cases.

(i) When $f_n + f_{n-1}$ is odd, the total symmetry group consists of lattice translations $\mathbf{R} = m_1 \mathbf{a}_1^{(n)} + m_2 \mathbf{a}_2^{(n)} + m_3 \mathbf{a}_3^{(n)}$ (m_i integer) and elements of the point group T_h .

(ii) When $f_n + f_{n-1}$ is even, there is an additional symmetry element, which is the translation $\mathbf{t} = 1/2(\mathbf{a}_1^{(n)} + \mathbf{a}_2^{(n)} + \mathbf{a}_3^{(n)})$.

Whereas in the original tiling only two tiles occur, in the periodic approximation more than two tiles occur, due to the deformation. Remark that the rhombohedra are the projections of the three-dimensional boundaries of the six-dimensional hypercube. These projections will in general not all be equal to one another. This depends on the orientation of the subspace with respect to the hypercube. For the original tiling the orientation is such that only two tiles occur, but for the commensurate approximation

the orientation is slightly different. This means that more neighbour distances occur. For the commensurate approximations up to $\phi = \frac{5}{3}$ these distances are:

$$\begin{aligned}\phi_n &= 2/1 : 2.000; 2.236; 2.449 \\ \phi_n &= 3/2 : 0.866; 1.118; 1.803; 1.871; 2.000; 2.062 \\ \phi_n &= 5/3 : 1.054; 1.158; 1.333; 1.945; 2.000; 2.054.\end{aligned}$$

In the limit of $n \rightarrow \infty$ these distances converge to the four distances occurring in the original tiling.

For the displacement of the atoms we can now make a Bloch *ansatz*:

$$u_{n\mathbf{i}\alpha} = c_{i\alpha} \exp[i(\mathbf{k}\mathbf{n} - \omega t)] \quad (14)$$

where $u_{n\mathbf{i}\alpha}$ is the displacement in the α direction of the i th atom in the n th unit cell.

Substituting this *ansatz* in (5) leads to

$$\omega^2 c_{j\alpha} = \sum_{j'\alpha'} D_{\alpha\alpha'}(\mathbf{k}|jj') c_{j'\alpha'} \quad (15)$$

where

$$D_{\alpha\alpha'}(\mathbf{k}|jj') = \sum_{\mathbf{n}} \Phi^{(2)} \begin{pmatrix} n_j & 0_{j'} \\ \alpha & \alpha' \end{pmatrix} e^{-i\mathbf{k}\mathbf{n}} \quad (16)$$

is \mathbf{k} -dependent, but finite dimensional.

To find all eigenstates we can restrict ourselves to \mathbf{k} -vectors inside the first Brillouin zone. We have determined the eigenvalues for commensurate approximations up to $\phi_n = 5/3$ for special \mathbf{k} -points, namely those for which the symmetry of the dynamical matrix is T_h , i.e. $\mathbf{k}_1 = \mathbf{o}$ and $\mathbf{k}_2 = (\pi/a)(1, 1, 1)$, or D_{2h} (order 8), i.e. $\mathbf{k}_3 = (\pi/a)(1, 0, 0)$ and $\mathbf{k}_4 = (\pi/a)(1, 1, 0)$ and symmetry related \mathbf{k} -points. For other \mathbf{k} -points the symmetry group has order smaller than eight and, at least in the case of $\phi = 5/3$, the irreducible matrix blocks are too large to handle.

Figures 5 (a)–(c) show the DOS for respectively $\phi = 2/1$, $\phi = 3/2$ and $\phi = 5/3$. All spring constants $\alpha_{ii'}$ were taken to be one. Figure 6 gives the integrated density of states (IDOS) for the cluster approximation (7895 atoms) and the commensurate approximation ($\phi = 5/3$). All $\alpha_{ii'} = 1$.

Comparing the results of the cluster approximation with those of the commensurate approximation it seems that the DOS is converging, but it is clear that the limit has not been reached yet. The fine structure of the spectrum for the infinite system remains uncertain. Another remarkable feature is the relative high left shoulder in the DOS of the cluster approximation with respect to the commensurate approximation. This difference also comes out quite clearly in the IDOS.

Another result is that all branches which occur in the commensurate approximations do have overlap with one or more other branches. In other words there are no gaps.

To investigate the low-frequency behaviour we can take some further steps. We approximate each branch by a hyperplane in the four-dimensional (ω, \mathbf{k}) -space passing through the four $(\omega_s(\mathbf{k}_i), \mathbf{k}_i)$ -points ($i = 1 \dots 4$) belonging to the same branch. Having done this we can determine the density of states $D(\omega)$ by analytic integration:

$$D(\omega) = \sum_s \frac{1}{(2\pi)^3} \int_{\text{Brz}} d\mathbf{k} \delta(\omega - \omega_s(\mathbf{k})) = \sum_s \frac{1}{(2\pi)^3} \int_{dS} \frac{1}{|\hat{\mathbf{n}} \cdot \nabla \omega_s(\mathbf{k})|} \quad (17)$$

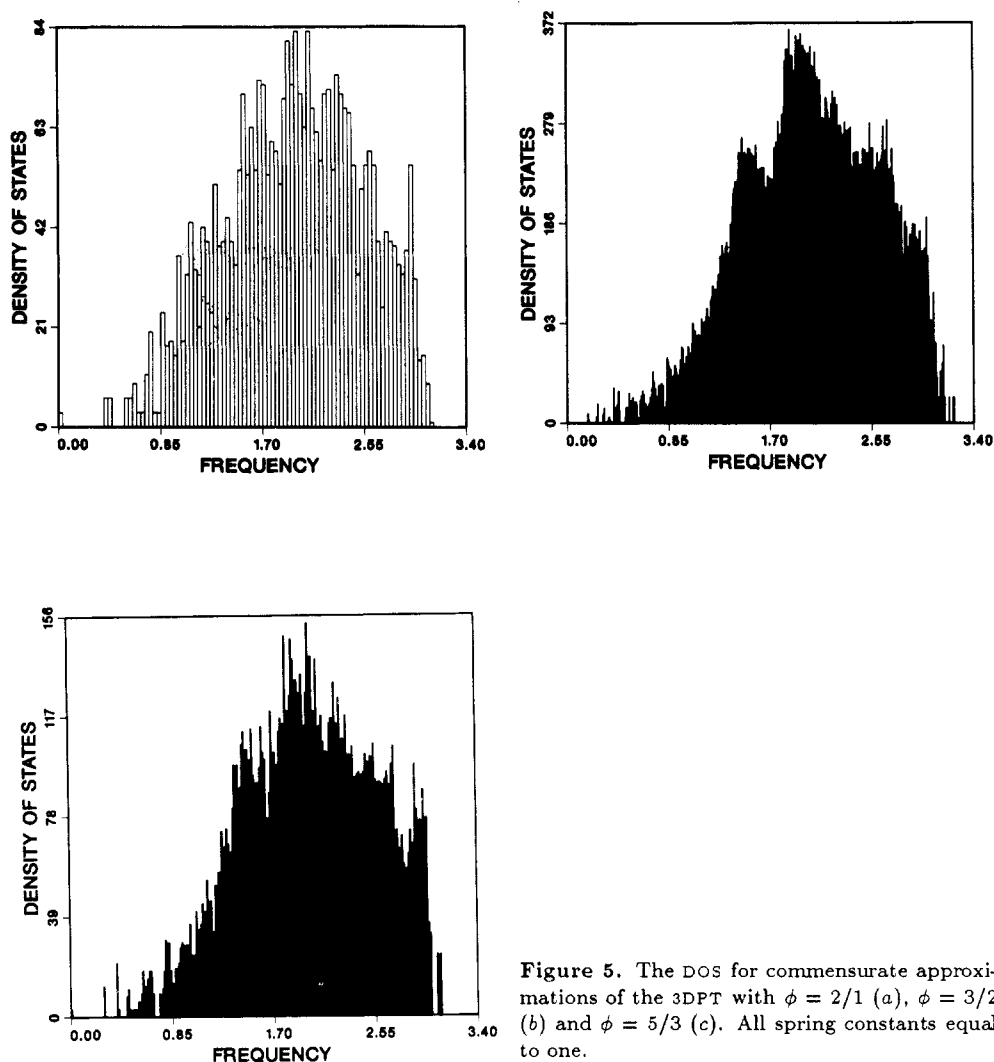


Figure 5. The DOS for commensurate approximations of the 3DPT with $\phi = 2/1$ (a), $\phi = 3/2$ (b) and $\phi = 5/3$ (c). All spring constants equal to one.

where \sum_s means summation over all branches, \int_{dS} means integration over the surface of constant ω and \hat{n} a unit vector normal to this surface.

Figure 7 shows the DOS at low frequencies for the three commensurate approximations calculated using the above method.

We see a couple of deep minima occurring in the curves which are called pseudo-gaps.

For one-dimensional quasi-periodic structures it has been shown by several people for various models that the spectrum possesses scaling properties [15-18]. To investigate the scaling behaviour of our three-dimensional model we will use a pseudo-thermodynamical formalism, which was introduced by Kohmoto [13].

Let us say that for a certain commensurate approximation the spectrum contains N branches. We define the width Δ_i ($i = 1 \dots N$) of these branches as follows:

$$\Delta_i = \max\{\omega_i\} - \min\{\omega_i\} \tag{18}$$

where $\max\{\omega_i\}$ and $\min\{\omega_i\}$ are respectively the maximal and minimal frequency in

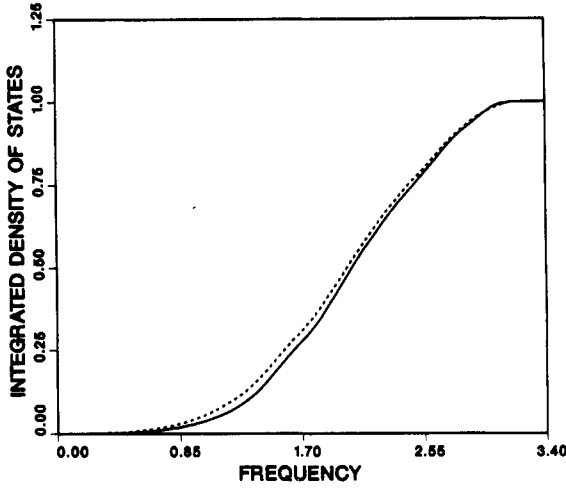


Figure 6. The integrated density of states (IDOS) for the 3DPT in the cluster approximation (broken curve) and the commensurate approximation with $\phi = 5/3$ (full curve). All spring constants equal to one.

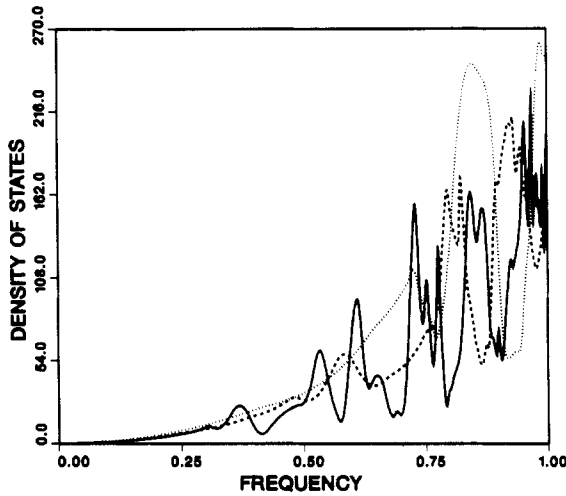


Figure 7. The DOS for low frequencies for three successive commensurate approximations using a linear approximation for the branches. Dotted curve: $\phi = 2/1$; broken curve: $\phi = 3/2$; full curve: $\phi = 5/3$.

the set of four frequencies belonging to the four k -points mentioned above. Remark that these frequencies are not necessarily the minimal and maximal frequencies of the whole branch.

Now suppose that these bandwidths scale for successive commensurate approximations and let us define a scaling index ϵ_i for Δ_i by

$$\epsilon_i = -(1/p) \ln \Delta_i \tag{19}$$

where p labels the successive commensurate approximations.

A suitable choice for p is

$$p = \frac{\ln 3N_p}{\ln c} \tag{20}$$

where N_p is the number of atoms in the unit cell, $3N_p$ the number of bands and $c = \phi^3$.

An entropy function $S(\epsilon)$ is defined by

$$S(\epsilon) = (1/p) \ln \Omega(\epsilon) \quad (21)$$

where $\Omega(\epsilon)d\epsilon$ is the number of bands whose scaling index lies between ϵ and $d\epsilon$.

From equation (21) we can see that p indeed has to be proportional to $\ln 3N_n$ to make that $S(\epsilon)$ is a function which might converge when we take successive approximations. If so, this is an indication that the spectrum has scaling properties. If in the limit of p tending to infinity the support of the S function is just one point this means that the spectrum is either absolute continuous corresponding to extended states or a point spectrum corresponding to localized states.

Furthermore, as in the formalism of statistical mechanics, a 'partition function' and a 'free energy' are introduced as follows:

$$Z_p(\beta) = \sum_i e^{-\beta p \epsilon_i} = \sum_i \Delta_i^\beta \quad (22)$$

$$F(\beta) = \lim_{p \rightarrow \infty} (1/p) \ln Z_p(\beta). \quad (23)$$

The functions $S(\epsilon)$ and $F(\beta)$ are related by the following Legendre transformation:

$$S(\epsilon) = F(\beta) + \beta\epsilon \quad (24)$$

with

$$\epsilon = -\frac{dF(\beta)}{d\beta}. \quad (25)$$

By numerically differentiating $F(\beta)$ one can pick up an ϵ and calculate the corresponding $S(\epsilon)$.

Figure 8 shows this entropy as a function of ϵ for the commensurate approximations with $\phi = 2/1$, $\phi = 3/2$ and $\phi = 5/3$.

Comparing the entropy functions for the three commensurate approximations it seems that convergence takes place, which means that the spectrum indeed possesses scaling properties. Furthermore we see that the support of the function is not just one point but an interval, which is an indication that the spectrum is so-called singular continuous. In that case the eigenstates are neither extended nor localized but something in between. However, we only have three approximations and it might be early to draw any conclusions.

3. The DOS of i-AlMnSi

The structure of i-Al₇₄Si₅Mn₂₁ may be possibly seen as a decorated icosahedral 3DPT. As decoration various propositions have been made. Here we will take the structure as proposed by Janot *et al* [14].

In this structure the atoms occur at the vertices (merely Mn atoms), the long diagonals of the faces (Al atoms) and only for the prolate rhombohedra at one of the body diagonals (Al atoms). Some of the positions have an occupation probability less

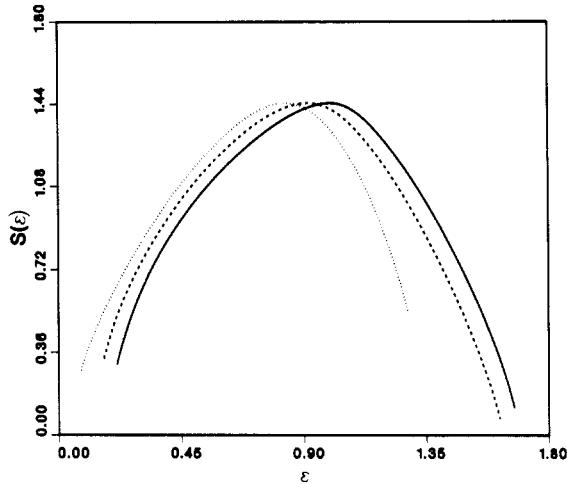


Figure 8. The entropy function $S(\epsilon)$, describing the distribution of scaling indices ϵ for the spectrum of the 3DPT in the commensurate approximations with $\phi = 2/1$ (dotted curve), $\phi = 3/2$ (broken curve) and $\phi = 5/3$ (full curve).

than one. So to calculate the DOS one has to average over all configurations. This however would take too much computer time and, realising that not all configurations do have icosahedral point group symmetry, too much storage space. However, only a small number of the positions do have an occupation probability less than one and therefore we just do the calculation for one cluster with a ‘reasonable’ configuration, having icosahedral symmetry.

As neighbours we take atoms with an equilibrium distance less than 4.85 \AA . The shortest neighbour distance is 1.594 \AA .

Instead of a spring potential we used a Lennard-Jones potential, which is more realistic in the sense that differences in neighbour distances are taken into account in a natural way. Such a potential has been successfully applied to amorphous alloys by Hafner [19].

$$\Phi(\dots \mathbf{r}_{ii'} \dots) = \sum_i \sum_{i'(i)} \left(\frac{A_{ii'}}{|\mathbf{r}_{ii'}|^{12}} - \frac{B_{ii'}}{|\mathbf{r}_{ii'}|^6} \right) \equiv \sum_i \sum_{i'(i)} \Phi_{ii'}(\mathbf{r}_{ii'}) \quad (26)$$

where $\mathbf{r}_{ii'} = \mathbf{r}_i + \mathbf{u}_i - \mathbf{r}_{i'} - \mathbf{u}_{i'}$.

It can easily be shown that the minimum of the pair potential $\Phi_{ii'}$ is equal to $-B_{ii'}^2/4A_{ii'}$, occurring at $|\mathbf{r}_{ii'}| = (2A_{ii'}/B_{ii'})^{1/6}$. In our model the well depth was taken to be 4.2 mRy for each pair occurring at the equilibrium distance and this determines the values of $A_{ii'}$ and $B_{ii'}$.

The value of the well depth was chosen such that the range of the calculated energies was in good agreement with the results of neutron scattering experiments. See for example the neutron scattering study of the vibrational density of states in icosahedral and crystalline AlMn by Miceli *et al* [20].

Figure 9 shows the DOS for a cluster with 1489 Mn and 5990 Al atoms.

It should be interesting to compare this result with the result of the same calculation for the crystalline phase, which still has to be done.

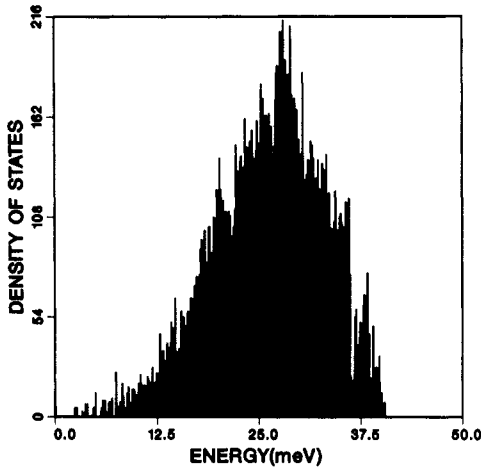


Figure 9. The DOS for an icosahedral cluster (7479 atoms) of *i*-ALMnSi using a Lennard-Jones potential with well depth equal to 4.2 mRy for each neighbouring pair.

4. Concluding remarks

We have investigated the lattice dynamics of models for icosahedral quasi-crystals. Several approaches to this problem were compared.

The cluster and commensurate approximations to models with harmonic springs give essentially the same density of states. In the cluster approximation the effect of boundary conditions seems to vanish for increasing clusters. No sensitive dependence in these has been found. There is a clear dependence on the choice of the spring constants. Therefore the density of states was determined for a model structure for ALMnSi found in the literature using a Lennard-Jones potential. The result is in qualitative agreement with experiments.

For low frequencies a global ω^2 dependence of the density of states is found, but with a complicated structure in top of that. A further investigation of these low-frequency properties is in progress.

A multifractal analysis does not show the typical behaviour of simple extended states. The entropy function seems to converge taking successive commensurate approximations. The precise character of the modes still has to be studied.

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