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Special points in the reciprocal space of an icosahedral quasi-crystal and the quasi-dispersion relation of electrons

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Abstract. It is shown that there exist special points in the reciprocal space of an icosahedral quasi-lattice; they correspond to high-symmetry points in the Brillouin zone of a periodic lattice. The translationally equivalent special points are distributed quasi-periodically with different intensities in the reciprocal space. On the other hand, electronic wavefunctions of the icosahedral quasi-lattice are investigated using a numerical method based on the tight-binding model. Their Fourier spectra are mapped in the energy versus wavenumber plane along several axes in reciprocal space. Dispersion-relation-like patterns are observed. It is found that critical points (stationary points) of the quasi-dispersion relation appear at the special points. The quasi-dispersion relation recurs quasi-periodically all over reciprocal space.

1. Introduction

A quasi-crystal is a novel kind of matter with quasi-periodic positional long-range order together with non-crystallographic point symmetry (see Schechtman *et al* (1984), Levine and Steinhardt (1986) and, for a review, Henley (1987)). Most familiar quasi-crystals are icosahedral. Since the structure of a quasi-crystal is not periodic but quasi-periodic, electronic states in it will be very different from those in a (periodic) crystal or an amorphous system.

An idealised model of the structure of a quasi-crystal is a quasi-lattice; an icosahedral quasi-lattice (IQL) is constructed by the cut-and-project method from a six-dimensional (6D) periodic lattice (Elser 1986, Katz and Duneau 1986). The Fibonacci lattice is a 1D analogue of the IQL; the former is similar to an array of lattice planes along a twofold axis of the latter. Electronic states on the Fibonacci lattice have been studied extensively by many authors (for a review, see Kohmoto (1987)). These investigations revealed that the energy spectrum is of the Cantor type and the wavefunctions are critical with respect to localisation, i.e. they are not extended nor localised exponentially.

The Penrose lattice is a 2D analogue of the IQL. Several analytical or numerical investigations of electronic states on the lattice have been reported. It has been conjectured that the energy spectrum is singular continuous (but not of Cantor type) and the wavefunctions are critical (Tsunetsugu *et al* 1986). Also, novel states called 'confined states' are found (Semba 1985, Kohmoto and Sutherland 1986); a confined state is a special localised state that is strictly confined to a region of a particular local structure.

Since a quasi-lattice has definite reciprocal-lattice vectors that are discrete, it will be important to investigate the electronic wavefunctions on it in reciprocal space (the wavenumber space). We have previously performed such an investigation on the Fibonacci lattice (Akamatsu and Niizeki 1987). We found that a dispersion-relation-like pattern is clearly observed in the energy versus wavenumber plane. We have recently performed similar investigations for the case of the Penrose lattice and the IQL, and obtained similar results. In this paper, we will report the results for the case of the IQL.

We will review in section 2 the real-space properties of the IQL and in section 3 the reciprocal-space properties. We present in section 3, also, an exact definition of the special points and discuss their properties. In section 4, we investigate the structure factor and its generalised versions. In section 5, we investigate plane-wave states (the Bloch sums) and similar states. We treat in section 6 the electronic states of the IQL with the quasi-crystalline approximation. In section 7 we report the results of the numerical investigation of the reciprocal-space properties of the wavefunctions. In the final section, section 8, we summarise the results of this paper. We also discuss related subjects.

2. The icosahedral quasi-lattice

An icosahedron has 6, 10 and 15 axes of five-, three- and twofold rotational symmetry, respectively. They are directed along the vertices, the face centres and the midpoints of the edges, respectively. The order of the icosahedral group, Y_h, is 120, i.e. $|Y_h| = 120$.

An IQL, L_i $(= L_{i,P})$, is constructed via the cut-and-project method from a 6D simple hypercubic lattice, $L_{6,P}$ (Elser 1986, Katz and Duneau 1986). A 3D subspace (the real space), E_3, of the 6D Euclidean space, E_6, embedding $L_{6,P}$ is chosen so that the six basis vectors $\boldsymbol{\varepsilon}_i$, $i = 1$–6, of $L_{6,P}$ are projected onto $\boldsymbol{a}_i$, $i = 1$–6, six of the 12 vertex vectors of an icosahedron in E_3. A window W of a rhombic triacontahedron is taken in the conjugate space, $\tilde{E}_3$, which is another subspace orthogonal to E_3. A strip in E_6 is defined by thickening E_3 with W. Then, L_i is given by the projections onto E_3 of all the lattice points of $L_{6,P}$ included in the strip.

Let $\boldsymbol{R} \in L_i$. Then, it is indexed with six integers as $\boldsymbol{R} = n_1\boldsymbol{a}_1 + \ldots + n_6\boldsymbol{a}_6 = [n_1 \ldots n_6]$. The common length of the basis vectors is denoted by a. For all $\boldsymbol{R} = [n_1 \ldots n_6] \in L_i$, there exists a unique companion $\tilde{\boldsymbol{R}} = n_1\tilde{\boldsymbol{a}}_1 + \ldots + n_6\tilde{\boldsymbol{a}}_6$ in $\tilde{E}_3$ such that the 6D vector $(\boldsymbol{R}, \tilde{\boldsymbol{R}}) = n_1\boldsymbol{\varepsilon}_1 + \ldots n_6\boldsymbol{\varepsilon}_6$ belongs to $L_{6,P}$ where $\boldsymbol{\varepsilon}_i = (\boldsymbol{a}_i, \tilde{\boldsymbol{a}}_i)$, $i = 1$–6, with $\boldsymbol{\varepsilon}_i \cdot \boldsymbol{\varepsilon}_j = 2a^2\delta_{i,j}$ are the basis vectors of $L_{i,P}$. $\tilde{\boldsymbol{R}}$ is called the conjugate vector to $\boldsymbol{R}$. By definition, $\tilde{\boldsymbol{R}} \in W$.

All the nearest-neighbour bonds of $L_{6,P}$ form a 6D network, which gives rise to a 3D network of bonds in L_i. Two sites connected by a bond in L_i are called an arithmetic neighbour pair, but they are not necessarily a geometrical nearest-neighbour pair. The coordination numbers of the sites in the network range from 4 to 12; the average is 6. Moreover, the network as well as the original 6D network contain only even-membered rings and give rise to a partition of E_3 into two types of rhombohedra. Thus, L_i has many common features to those of the simple cubic lattice in 3D.

$L_{6,P}$ is divided into two 6D face-centred hypercubic lattices $L_{6,F}$ and $L'_{6,F}$, which are translationally equivalent: $L'_{6,F} = \boldsymbol{\varepsilon}_1 + L_{6,F}$. The two sublattices are distinguished by the parity of the sum of the indices $n_1 + \ldots + n_6$. Correspondingly, L_i is divided into two sublattices, $L_{i,F}$ and $L'_{i,F}$, which are just the projections of the cuts of $L_{6,F}$ and $L'_{6,F}$, respectively. $L_{i,F}$ (or $L'_{i,F}$) is an icosahedral quasi-lattice belonging to a different Bravais class from that of $L_i = L_{i,P}$ (Rokhsar *et al* 1987). The network associated with L_i has bonds only between the sites in $L_{i,F}$ and those in $L'_{i,F}$.

The set of lattice vectors, $L_{6,I} = \{n_1\boldsymbol{\varepsilon}_1 + \ldots + n_6\boldsymbol{\varepsilon}_6 | n_i$ being all even or all odd$\}$ is a 6D body-centred hypercubic lattice. It is one of the 32 translationally equivalent sublattices into which $L_{6,P}$ is divided. $L_{6,I}$ gives rise to another icosahedral quasi-lattice $L_{i,I}$ ($\subset L_{i,P}$), which belongs to the third Bravais class (Rokhsar *et al* 1987).

3. The reciprocal lattice and special points of the icosahedral quasi-lattice

The reciprocal lattice, L_6^* $(= L_{6,P}^*)$, of L_6 is another simple hypercubic lattice whose basis vectors are given by $\boldsymbol{\varepsilon}_i^* = \pi\boldsymbol{\varepsilon}_i/a^2$. L_6^* is embedded in the 6D reciprocal space E_6^*. E_6^* is divided into two 3D spaces, $E_6^* = E_3^* \oplus \tilde{E}_3^*$, so that the projections of $\boldsymbol{\varepsilon}_i^*$ onto E_3^* (or $\tilde{E}_3^*$) coincide with $\boldsymbol{a}_i^* = \pi\boldsymbol{a}_i/a^2$ (or $\tilde{\boldsymbol{a}}_i^* = \pi\tilde{\boldsymbol{a}}_i/a^2$), $i = 1$–6. It follows that $\boldsymbol{\varepsilon}_i^* = (\boldsymbol{a}_i^*, \tilde{\boldsymbol{a}}_i^*)$, $i = 1$–6. We shall denote the relevant projection operators by π and $\tilde{\pi}$, respectively.

The reciprocal lattice of L_i is defined by $L_{i,P}^* = \pi(L_6^*)$ and its conjugate by $\tilde{L}_{i,P}^* = \tilde{\pi}(L_6^*)$. Let $\boldsymbol{G} \in L_{i,P}^*$ and $\tilde{\boldsymbol{G}} \in \tilde{L}_{i,P}^*$ be a conjugate pair of reciprocal-lattice vectors. Then, they are indexed with six integers as $\boldsymbol{G} = m_1\boldsymbol{a}_1^* + \ldots + m_6\boldsymbol{a}_6^* \equiv (m_1 \ldots m_6)$ and $\tilde{\boldsymbol{G}} = m_1\tilde{\boldsymbol{a}}_1^* + \ldots + m_6\tilde{\boldsymbol{a}}_6^*$. $L_{i,P}^*$ and $\tilde{L}_{i,P}^*$ are countable but dense sets in E_3^* and $\tilde{E}_3^*$, respectively. Note that $\sigma L_{i,P}^*$ $(= \{\sigma\boldsymbol{G} | \boldsymbol{G} \in L_{i,P}^*\}) = L_{i,P}^*$ for all $\sigma \in Y_h$. We shall denote the 6D reciprocal-lattice vector $(\boldsymbol{G}, \tilde{\boldsymbol{G}}) = m_1\boldsymbol{\varepsilon}_1^* + \ldots + m_6\boldsymbol{\varepsilon}_6^* \in L_{6,P}^*$ by the symbol $(m_1 \ldots m_6)_{6D}$.

In the reciprocal space of the usual periodic lattice, there exist special points (wavevectors) whose symmetries are larger than those of neighbouring points. We shall extend the definitions of special points to the case of a quasi-lattice. The point symmetry group of a wavevector $\boldsymbol{k}$ in the reciprocal space of an IQL is defined by $\mathscr{G}(\boldsymbol{k}) = \{\sigma | \sigma \in Y_h$ and $\sigma\boldsymbol{k} \equiv \boldsymbol{k} \bmod L_{i,P}^*\}$. $\mathscr{G}(\boldsymbol{k})$ is a subgroup of Y_h. We shall call a wavevector $\boldsymbol{k}_0$ a special point (wavevector) if $\mathscr{G}(\boldsymbol{k}_0)$ has no fixed planes nor fixed lines but a fixed point only. For example, C_{5v} ($\subset Y_h$) has a fixed line, while D_{5d} ($\subset Y_h$) has only a fixed point.

By definition, $\mathscr{G}(\boldsymbol{k}_0) = \mathscr{G}(\boldsymbol{k}_0 + \boldsymbol{G})$ for all $\boldsymbol{G} \in L_{i,P}^*$, so that translationally equivalent special points are distributed densely in the reciprocal space. Such a set of special points is denoted by $L_{i,P}^*(\boldsymbol{k}_0)$ $(= \boldsymbol{k}_0 + L_{i,P}^*)$ with $\boldsymbol{k}_0$ being a representative.

Let $\boldsymbol{k}_0$ be a special point. Then, the star of $\boldsymbol{k}_0$ is the set of wavevectors. $\mathscr{S}(\boldsymbol{k}_0)$, formed by translationally inequivalent wavevectors among $\{\sigma\boldsymbol{k}_0 \mid \sigma \in Y_h\}$. It follows that $|\mathscr{S}(\boldsymbol{k}_0)| = 120/|\mathscr{G}(\boldsymbol{k}_0)|$ $(|Y_h| = 120)$.

It can be shown easily that there exists eight types of special points. We denote them as Γ, R, X_5, M_5, X_3, M_3, X_2 and M_2, representative wavevectors of which are given with $h = \frac{1}{2}$ by (000000), $(hhhhhh)$, $(h00000)$, $(0hhhhh)$, $(hhh000)$, $(000hhh)$, $(hh0000)$ and $(00hhhh)$, respectively. Then $\mathscr{G}(\boldsymbol{k}_0) = Y_h$ and $|\mathscr{S}(\boldsymbol{k}_0)| = 1$ for Γ and R points. For other types of special points, $\mathscr{G}(\boldsymbol{k}_0)$ is isomorphic with D_{5d}, D_{3d} or D_{2h} and $|\mathscr{S}(\boldsymbol{k}_0)| = 6$, 10 and 15 according as the suffix is 5, 3 or 2, respectively.

A special point $\boldsymbol{k}_0 = (h_1 \ldots h_6)$ is the projection of $(h_1 \ldots h_6)_{6D} \in E_6^*$ onto E_3^*. The 6D vector is nothing but a special point of the 6D periodic lattice, L_6^*. Here, a special point in E_6^* should be defined in terms of the point group $Y_h' = \pi^{-1}(Y_h)$, which is a subgroup of $\Omega(6)$, the full point symmetry group of the 6D simple hypercubic lattice, L_6^*. If special points of $L_{i,P}$ are defined with respect to $\Omega(6)$†, X_3 and M_3 should not be distinguished from each other.

† The enumeration of special points in this case is simpler than in the case of the point group Y_h'. The special points in the latter case are sought from those in the former case.

The R points are the projections of $L_6^{*\prime} = (111111)_{6D}/2 + L_6^*$. L_6^* and $L_6^{*\prime}$ form $L_{6,I}^*$, the 6D body-centred hypercubic lattice, which is the reciprocal lattice of $L_{6,F}$, i.e. one of the two sublattices of L_6.

All the special points in E_6^* form another simple hypercubic lattice, $L_6^*/2$, whose lattice constant is half that of L_6^*. It follows that a necessary and sufficient condition for $\boldsymbol{k} \in E_3^*$ to be a special point is that $2\boldsymbol{k} \in L_i^*$. Let $\boldsymbol{G} \in L_i^*$ and let λ be the number of odd integers in the indices of $\boldsymbol{G}$. Then, to which type the special point $\boldsymbol{k}_0 = \boldsymbol{G}/2$ belongs is almost determined by λ; λ represents the number of half-integers in the indices of $\boldsymbol{k}_0$. Note that $|\mathcal{S}(\boldsymbol{k}_0)| = \binom{6}{\lambda}$, the binomial coefficient, unless $\lambda = 3$. We shall call λ the level of $\boldsymbol{k}_0$ and denote it as $\lambda(\boldsymbol{k}_0)$.

The definition of special point can be extended to that of special line (direction) or special plane. However, we shall not pursue it any further. We present only a few compatibility conditions: a special point $\boldsymbol{k}_0$ can be located on an n-fold axis in E_3^* with $n = 2, 3$ or 5 if and only if $\mathcal{G}(\boldsymbol{k}_0)$ includes the relevant n-fold rotation and, similarly, it can be located on a mirror plane if $\mathcal{G}(\boldsymbol{k}_0)$ includes the mirror.

4. The structure factor and its generalisations

Let $\boldsymbol{k}_0 = (h_1 \ldots h_6)$ be a special point. Then, the plane wave in E_6^* with wavevector $(\boldsymbol{k}_0, \tilde{\boldsymbol{k}}_0) = (h_1 \ldots h_6)_{6D}$ has phase factor $\exp[2\pi i(h_1 n_1 + \ldots + h_6 n_6)]$ at the lattice point $[n_1 \ldots n_6]_{6D} \in L_6^*$. The phase factor takes value 1 or -1 depending on the indices of the lattice point because h_i are integers and/or half-integers. Alternatively, the phase factor can be regarded as a function of $\boldsymbol{R} = [n_1 \ldots n_6] \in L_i$, which we shall denote as $\eta(\boldsymbol{k}_0; \boldsymbol{R})$ or, more simply, as $\eta_\Gamma(\boldsymbol{R})$ or $\eta_R(\boldsymbol{R})$ if $\boldsymbol{k}_0$ is a Γ point or R point, respectively.

Let us introduce a generalised structure factor by

$$S(\boldsymbol{k}_0; \boldsymbol{Q}) = \left| \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R} \in L_i} \eta(\boldsymbol{k}_0; \boldsymbol{R}) \exp(-i\boldsymbol{Q} \cdot \boldsymbol{R}) \right|^2 \tag{1}$$

where N is the total number of lattice sites and $\boldsymbol{Q} \in E_3^*$ the momentum transfer (in units of $\hbar$). Then $\eta_\Gamma(\boldsymbol{R})$ takes value 1 for all $\boldsymbol{R} \in L_i$ and $S_\Gamma(\boldsymbol{Q})$ ($= S(\boldsymbol{k}_0; \boldsymbol{Q})$ with $\boldsymbol{k}_0 = 0$) is reduced to the usual structure factor $S(\boldsymbol{Q})$. Structure factor $S(\boldsymbol{Q})$ can be easily calculated with the projection method (Katz and Duneau 1986, Elser 1986, Zia and Dallas 1985). Using a similar procedure, we can show that

$$S(\boldsymbol{k}_0; \boldsymbol{Q}) = \sum_{\boldsymbol{k} \in L_i^*(\boldsymbol{k}_0)} I(\boldsymbol{k})\delta(\boldsymbol{Q} - \boldsymbol{k}) = \sum_{\boldsymbol{G} \in L_i^*} I(\boldsymbol{k}_0 + \boldsymbol{G})\delta(\boldsymbol{Q} - \boldsymbol{k}_0 - \boldsymbol{G}) \tag{2}$$

where the intensity function is given in terms of the form factor (the Fourier transform) of the window function $\hat{W}(\boldsymbol{q})$ ($\hat{W}(0) = 1$) by $I(\boldsymbol{k}) = |\hat{W}(\tilde{\boldsymbol{k}})|^2$. Here $|\hat{W}(\hat{\boldsymbol{k}})|^2$ is a monotonically decreasing function of $0 < |\tilde{\boldsymbol{k}}| \leqslant 1/|W|$ with $|W|$ being the diameter of W, but an oscillatory function in $|\tilde{\boldsymbol{k}}| \geqslant 1/|W|$ whose envelope decreases rapidly as $\simeq \text{const.}/|\tilde{\boldsymbol{k}}|^{-6}$. Also $I(\boldsymbol{k})$ ($\boldsymbol{k} \in L_i^*(\boldsymbol{k}_0)$) tends to 1 as $\tilde{\boldsymbol{k}}$ tends to 0 or, in other words, the special point $(\boldsymbol{k}, \tilde{\boldsymbol{k}})$ in E_6^* comes near to E_3^*.

The structure factor is given by equation (2) with $\boldsymbol{k}_0 = 0$:

$$S(\boldsymbol{Q}) = \sum_{\boldsymbol{G} \in L_i^*} I(\boldsymbol{G})\delta(\boldsymbol{Q} - \boldsymbol{G}). \tag{3}$$

$S(\boldsymbol{k}_0; \boldsymbol{Q})$ is virtually translationally congruent with $S(\boldsymbol{Q})$ because $S(\boldsymbol{k}_0; \boldsymbol{Q}) \simeq S(\boldsymbol{Q} - \boldsymbol{k})$, for there is a $\boldsymbol{k} \in L_i^*(\boldsymbol{k}_0)$ such that $\tilde{\boldsymbol{k}} \simeq 0$.

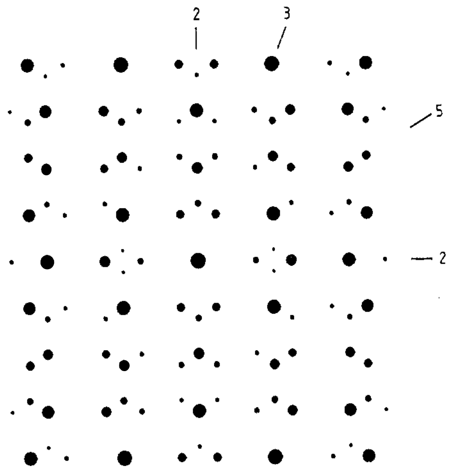

Figure 1. The structure factor of the IQL along a mirror plane perpendicular to a twofold axis in the reciprocal space. In the plane, two twofold axes are included; one of them is horizontal and the other vertical. Also, one threefold axis and one fivefold axis are included. The area of a spot (full circle) is proportional to the intensity. A spot with an intensity lower than 0.01 is ignored.

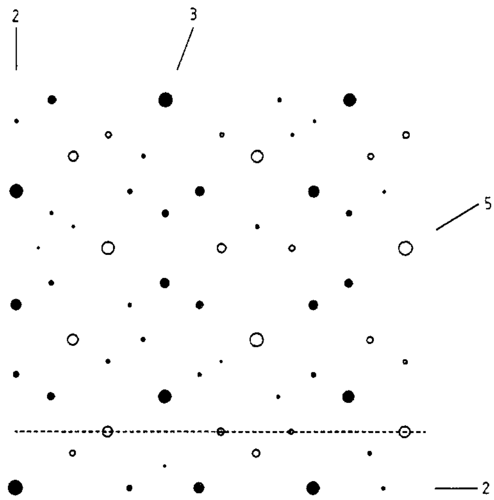

Figure 2. The generalised structure factor, $S_R(Q)$, along the same plane as in figure 1. Only the first quadrant is shown. The intensities are represented by (open) circles with appropriate areas. The structure factor $S(Q)$ represented by spots (full circles) is superimposed. If circles and spots are not distinguished, the resulting pattern represents the structure factor of $L_{i,F}$. A broken line is drawn for later use.

The point symmetry of $S(\boldsymbol{k}_0; Q)$ as a function of Q is given by $\mathscr{G}(\boldsymbol{k}_0)$. Therefore, $S_\Gamma(Q)$ and $S_R(Q)$ have Y_h, the full icosahedral symmetry, as their point symmetry. In the case where the type, T, of $\boldsymbol{k}_0$ is different from Γ and R, it is convenient to introduce the symmetrised version:

$$S_T(Q) = \sum_{\boldsymbol{k} \in \mathscr{S}(\boldsymbol{k}_0)} S(\boldsymbol{k}; Q) \tag{4}$$

which has the full icosahedral symmetry.

We show $S(Q)$ in figure 1 along a mirror plane that is perpendicular to a two-fold axis in E_3^*. On evaluating the intensities, we have approximated W, the rhombic triacontahedron, by a sphere with the same volume. A reciprocal-lattice vector with a strong or medium intensity satisfies $|\tilde{G}| \leqslant 1/W|$. Since the intensity function vanishes rapidly as $|\tilde{\boldsymbol{k}}|$ is increased beyond $1/|W|$, $S(Q)$ is virtually discrete notwithstanding that L_i^* is dense. $S(Q)$ is a quasi-periodic function in E_3^*, which is contrasted with the case of a periodic Bravais lattice, where it is periodic.

Figure 1 is considered to represent a weighted distribution of the Γ points in the reciprocal space. A remarkable feature of figure 1 in comparison with the case of a periodic lattice is that Γ points with partial intensities are present and, strictly speaking, only the Γ point at the origin has the full intensity.

The weighted distributions of other types of special points are given by the generalised structure factors; this is a generalisation of the case of a periodic Bravais lattice. We show $S_R(Q)$ in figure 2, together with $S(Q)$ superimposed. $S_R(Q)$ has intensities on the threefold and fivefold axes but not on the twofold ones. It can be shown

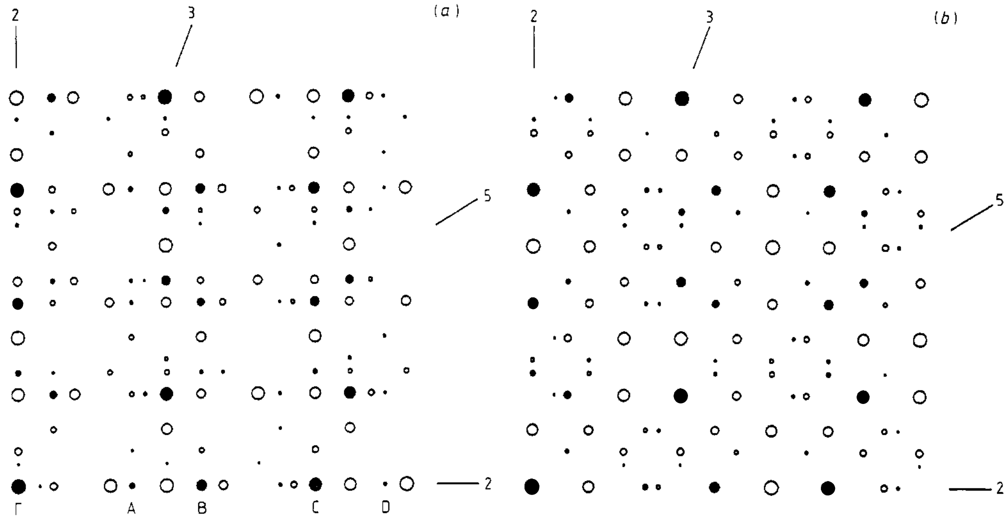

Figure 3. The symmetrised generalised structure factors for X_2 (a) and M_2 (b) along the same plane as in figure 1 (circles). The structure factor $S(\boldsymbol{Q})$ is superimposed (spots). Three of the 15 translationally inequivalent sets of X_2- (or M_2-) type special points are located on the plane in (a) (or (b)). Several Γ points on the horizontal twofold axis are indicated in (a) by symbols A–D for later use.

that the contributions of the two sublattices $L_{i,F}$ and $L'_{i,F}$ to $S(\boldsymbol{Q})$ at $\boldsymbol{Q} = \boldsymbol{k}$ are in phase if $\boldsymbol{k} \in L^*_{i,P}$ but in anti-phase if $\boldsymbol{k} \in L^*_{i,P}(\boldsymbol{k}_0)$ with $\boldsymbol{k}_0$ being R. Therefore, $S_\Gamma(\boldsymbol{Q}) + S_R(\boldsymbol{Q})$ is exactly equal to the structure factor of $L_{i,F}$.

An R point $\boldsymbol{k}$ is located at half the distance of a Γ point $\boldsymbol{G}$ ($\boldsymbol{k} = \boldsymbol{G}/2$) whose indices are all odd. Then, $I(\boldsymbol{k})$ is usually larger than $I(\boldsymbol{G})$ because $|\tilde{\boldsymbol{k}}|$ $(=|\tilde{\boldsymbol{G}}|/2) < |\tilde{\boldsymbol{G}}|$.

We show $S_T(\boldsymbol{Q})$ with $T = X_2$ and M_2 in figure 3. They have intensities on twofold axes but not on other symmetry axes. Only three of the 15 stars of X_2 (or M_2) have intensities on the plane shown in figure 3(a) (or 3(b)). Note that the sum of $S_T(\boldsymbol{Q})$ over $T = \Gamma$, R, X_2 and M_2 yields the structure factor of the sublattice $L_{i,I}$ of $L_{i,P}$; the special points of these types are on even levels.

We will not show $S_T(\boldsymbol{Q})$ for other types of special points. We mention only that it has intensities on the three- (or five-) fold axes if $T = X_3$ and M_3 (or X_5 and M_5). The sum of $S_T(\boldsymbol{Q})$ over all types of special points is equal to $S(\boldsymbol{Q}/2)$, which is the structure factor of $2L_{i,P}$.

5. The plane-wave states (Bloch sums) of the icosahedral quasi-lattice

We shall take a finite (but macroscopic) block of an IQL composed of N lattice sites and number the lattice sites arbitrarily. We will investigate the electronic structure of the block, which we shall denote by the same symbol L_i as that for the infinite lattice. We employ the tight-binding approximation with a single s orbital per site. A normalised orbital localised on the nth site is denoted by $|n\rangle$. We shall neglect non-orthogonality between different orbitals.

A normalised Bloch sum with wavevector $\boldsymbol{k}$ is given by

$$|\boldsymbol{k}\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_n)\, |n\rangle \tag{5}$$

where $\boldsymbol{R}_n$ stands for the nth lattice vector. Hereafter, we shall refer to this state as a plane wave.

Let $\boldsymbol{k}_0$ be a representative wavevector of type-T special points. Then, another plane-wave-like state is defined by

$$|\mathrm{T}; \boldsymbol{k}_0\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \eta(\boldsymbol{k}_0; \boldsymbol{R}_n)\, |n\rangle. \tag{6}$$

The state is determined independently of the particular choice of the representative. This state is nothing but a 'cut' of a 6D Bloch sum because $\eta(\boldsymbol{k}_0; \boldsymbol{R}_n) = \exp[\mathrm{i}(\boldsymbol{k}_0 \cdot \boldsymbol{R}_n + \tilde{\boldsymbol{k}}_0 \cdot \tilde{\boldsymbol{R}}_n)]$.

We shall write $|\mathrm{T};\, \boldsymbol{k}_0\rangle$ simply as $|\Gamma\rangle$ or $|\mathrm{R}\rangle$ if $\mathrm{T} = \Gamma$ or R, respectively. All the nearest-neighbour pairs in L_i are bonding in $|\Gamma\rangle$ (or antibonding in $|\mathrm{R}\rangle$) irrespective of the direction of the bonds.

In a case where $\mathrm{T} \neq \Gamma$, R, $|\mathrm{T};\, \boldsymbol{k}_0\rangle$ has both bonding and antibonding bonds. More exactly, a bond is bonding or antibonding if the relevant index in $\boldsymbol{k}_0 = (h_1 \ldots h_6)$ to the direction of the bond is an integer or half-integer, respectively. Accordingly, the direction of an antibonding bond can take values $2\lambda(\boldsymbol{k}_0)$ of the 12 possible directions. If a spherical coordinate system is introduced consistently with the main axis (or axes) of the point group $\mathscr{G}(\boldsymbol{k}_0)$, the antibonding (or bonding) bonds have high (or low) latitudes for the X-type special points, but the situation is converse for M-type ones.

Using equations (1), (2), (5) and (6) together with the assumption that $N \gg 1$, we can show that

$$|\langle \boldsymbol{k} | \mathrm{T}; \boldsymbol{k}_0\rangle|^2 = \begin{cases} I(\boldsymbol{k}) & \text{if } \boldsymbol{k} \in \mathrm{L}^*_{i,\mathrm{P}}(\boldsymbol{k}_0) \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

Accordingly, the weighted distribution of special points as given by $S(\boldsymbol{k}_0; \boldsymbol{Q})$ is considered, alternatively, to represent the distribution of the quantum probabilities by which $|\mathrm{T};\, \boldsymbol{k}_0\rangle$ is included in the plane waves. Note that $|\boldsymbol{k}\rangle$ with $\boldsymbol{k} \in \mathrm{L}^*_{i,\mathrm{P}}(\boldsymbol{k}_0)$ is almost equal to $|\mathrm{T};\, \boldsymbol{k}_0\rangle$ if $I(\boldsymbol{k}) \simeq 1$ or, equivalently, $\tilde{\boldsymbol{k}} \simeq 0$.

Using equation (7) for the case of $|\Gamma\rangle\, (= |0\rangle)$ together with the equality $\langle \boldsymbol{k} | \boldsymbol{k}'\rangle = \langle \boldsymbol{k} - \boldsymbol{k}' | 0\rangle$, we obtain

$$|\langle \boldsymbol{k} | \boldsymbol{k}'\rangle|^2 = \begin{cases} I(\boldsymbol{G}) & \text{if } \boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{G} \text{ for } \boldsymbol{G} \in \mathrm{L}^*_{i,\mathrm{P}}(\boldsymbol{k}_0) \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

Note here that the wavevectors are assumed to be discretised (quantised) in such a way that each one is given a share of the volume $(2\pi)^3/\Omega$ in E^*_3, with Ω being the volume of the block.

In the case of a periodic system, all the plane waves in the first Brillouin zone (or some irreducible zone) form an orthonormal complete set and they repeat periodically in the reciprocal space (the extended zone scheme). The situation is very different in the case of the quasi-lattice; it is impossible to choose an orthonormal complete set of plane waves. Nevertheless, equation (8) means that the plane waves recur quasi-periodically in the reciprocal space. This is very different also from the case of an amorphous system, where the plane waves (Bloch sums) are 'randomised' in a high-wavenumber region on account of the diffuseness of the structure factor.

Let $\boldsymbol{k}_0$ and $\boldsymbol{k}_0'$ be special points belonging to different types T and T'. Then, $\boldsymbol{k}_0'' = \boldsymbol{k}_0' - \boldsymbol{k}_0$ is a special point belonging to the third type T'' ($\neq \Gamma$) and we obtain $\langle \mathrm{T}; \boldsymbol{k}_0 | \mathrm{T}'; \boldsymbol{k}_0' \rangle = \langle \Gamma | \mathrm{T}''; \boldsymbol{k}_0'' \rangle = 0$, where the second equality follows from equation (7). Therefore, the plane-wave-like states associated with the 64 translationally inequivalent sets of special points form an orthonormal (but incomplete) set.

6. The electronic structure of the icosahedral quasi-crystal in the quasi-crystalline approximation

We assume the following expression for the Hamiltonian matrix on the electronic states of the system:

$$H = -t \sum_{\langle n, n' \rangle} (|n\rangle\langle n'| + |n'\rangle\langle n|) \tag{9}$$

where t (> 0) is the transfer integral and the summation is restricted to bonds in the network associated with L_i.

Since the system has no translational symmetries, the plane-wave states are not exact eigenstates of H. However, it may not be a bad approximation to assume them to be approximate eigenstates. Such an assumption is known as the quasi-crystalline approximation (QCA) and is sometimes used for an amorphous system or a liquid metal (Roth 1973). In this section we employ it. Then, the eigenenergy for $|\boldsymbol{k}\rangle$ is given by

$$E_{\mathrm{QCA}}(\boldsymbol{k}) = \langle \boldsymbol{k} | H | \boldsymbol{k} \rangle = -t \sum_{i=1}^{6} \cos(\boldsymbol{a}_i \cdot \boldsymbol{k}) \tag{10}$$

which follows from the fact that the average coordination number is 6. This represents a dispersion relation.

A wavevector $\boldsymbol{k}$ satisfying the condition $\boldsymbol{a}_i \cdot \boldsymbol{k} = \pi \times$ integer, $i = 1$–6, is a critical point (a stationary point) of $E_{\mathrm{QCA}}(\boldsymbol{k})$. This condition is virtually satisfied by a special point $\boldsymbol{k}_0$ such that $\tilde{\boldsymbol{k}}_0 \simeq 0$ (i.e. $I(\boldsymbol{k}_0) \simeq 1$). We shall take such a representative from each set of translationally equivalent special points. Then, we obtain $E_{\mathrm{QCA}}(\boldsymbol{k}_0) = -6t + 2t\lambda(\boldsymbol{k}_0)$. That is, we obtain $E_{\mathrm{QCA}}(\boldsymbol{k}_0) = -6t, -4t, -2t, 0, 0, 2t, 4t$ and $6t$ for $\boldsymbol{k}_0$ being representatives of Γ, X_5, X_2, X_3, M_3, M_2, M_5 and R, respectively. Note that in the case of a periodic system, a special point is always a critical point of the dispersion relation because it is an isolated point with a higher symmetry than those of neighbouring points.

We consider next the behaviour of $E_{\mathrm{QCA}}(\boldsymbol{k})$ in the neighbourhood of a special point $\boldsymbol{k}_0$. We expand $E_{\mathrm{QCA}}(\boldsymbol{k}_0 + \boldsymbol{k})$ to the second order in $\boldsymbol{k}$ as

$$E_{\mathrm{QCA}}(\boldsymbol{k}_0 + \boldsymbol{k}) = E_{\mathrm{QCA}}(\boldsymbol{k}_0) + \tfrac{1}{2} \sum_{i=1}^{6} s_i (\boldsymbol{a}_i \cdot \boldsymbol{k})^2 \tag{11}$$

where s_i takes value 1 or -1 depending on whether h_i in $\boldsymbol{k}_0 = (h_1 \ldots h_6)$ is an integer or a half-integer, respectively. The second term in equation (11) is equal to ta^2k^2 (or $-ta^2k^2$) for Γ (or R), respectively, so that Γ (or R) is an M_0- (or M_3-) type critical point of $E_{QCA}(\boldsymbol{k})$. We can conclude by a similar calculation that an X- (or M-) type special point is an M_1- (or M_2-) type critical point.

Before closing this section, we remark on the symmetry of the Hamiltonian matrix H. It connects sites in the sublattice $L_{i,F}$ of L_i only with those in the other one, $L'_{i,F}$, and vice versa. Then, $PHP = -H$, where P with $P^2 = 1$ is a diagonal matrix that inverts the signs of the amplitudes associated with the sites in $L'_{i,F}$ only. Therefore, the density of states has a line of mirror symmetry at $E = 0$. Moreover, since $P|\Gamma\rangle = |R\rangle$, the electronic structure in reciprocal space is symmetric against interchange of Γ and R (and between X_r and M_r, $r = 2$, 3 and 5) provided that the sign of the energy is inverted simultaneously. For example, $E_{QCA}(\boldsymbol{k}) = -E_{QCA}(\boldsymbol{k}_0 + \boldsymbol{k})$ with $\boldsymbol{k}_0$ being R. These results are similar to those of the case of the simple cubic lattice.

7. A numerical investigation of the wavefunctions in the reciprocal space

We investigate numerically the eigenstates of H. We have to treat a finite sample of size $N \sim 10^3$ sites on account of the limitation of the computer. Then, the boundary condition is important. In order to suppress surface effects, we adopt the periodic boundary condition (PBC). Though the PBC cannot strictly be reconciled with the quasi-periodicity of the IQL, it can be done approximately by a minor modification of the IQL (Elser and Henley 1985): by approximating the golden ratio, $\tau = (1 + \sqrt{5})/2$, with a series of its rational approximants, we obtain a series of 'periodic' IQL of size 32, 136, 576, 2440, 10336, . . ., which have cubic unit cells. We have used a sample of size 2440. Note that the wavevectors of the plane-wave states are quantised by the PBC as $(2\pi/L)(l_1, l_2, l_3)$ where L stands for the linear dimension of the cell and l_i are integers.

Let E_i, $i = 0, 1, \ldots, N-1$, be the eigenenergies of H and ψ_i the corresponding normalised eigenvectors. Then, the probability of the plane-wave state $|\boldsymbol{k}\rangle$ to have energy E_i is given by $P(E_i, \boldsymbol{k}) = |\langle\psi_i|\boldsymbol{k}\rangle|^2$. The probabilities of all the eigenstates sum to 1. We can represent $P(E_i, \boldsymbol{k})$ as a two-dimensional map in the E–k plane if $\boldsymbol{k}$ is restricted on an axis in reciprocal space; the magnitude of $P(E_i, \boldsymbol{k})$ is represented by a circle whose area is proportional to $P(E_i, \boldsymbol{k})$.

We show in figure 4 such a map in the case where the axis in reciprocal space coincides with a twofold axis. The pattern has mirror symmetry with respect to the vertical axis and the left half is not shown. We can clearly observe a parabolic dispersion relation in the neighbourhood of the origin. As the wavenumber is increased, it recurs with different intensities at other Γ points (A–D in figure 3(*a*)); the intensities agree well with the intensities of the Γ points in figure 3 (or figure 1).

The ground-state energy is $E_0 = -6.6t$. This is a reasonable result because of the variational inequality, $E_0 = \langle\psi_0|H|\psi_0\rangle \leqslant \langle\Gamma|H|\Gamma\rangle = -6t\ (= E_{QCA}(\Gamma))$; the true ground state ψ_0 will gain band energies by having larger amplitudes at sites with high coordination numbers.

We have estimated the effective mass at the Γ point from the curvature of the dispersion relation and found that it agrees with the QCA effective mass, $m^*_{QCA} = \hbar^2/(2ta^2)$, within 2%.

The dispersion relation is diffused at higher energies but we can clearly observe the three dispersion maxima at the level $E = 2.1t$. The abscissae (the wavenumbers) and the intensities of the maxima are well accounted for by ascribing them to the M_2 points as given in figure 3(*b*). Though the level energy is not determined sharply, it

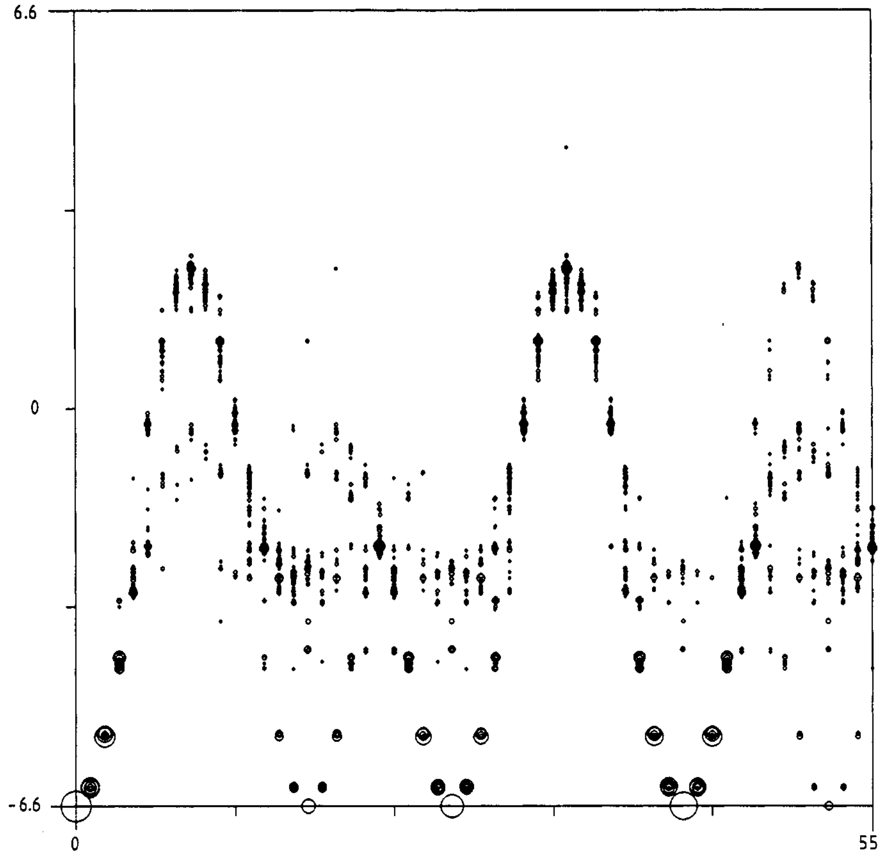

Figure 4. The map of the Fourier intensities of the wavefunctions along a twofold axis in the reciprocal space. The area of a circle is proportional to the intensity. A component with an intensity lower than 0.005 is ignored. Note that heavy overlappings among different intensities occur. The wavenumber is quantised to a multiple of $2\pi/L$, with L ($=11.66a$) being the linear dimension of the cubic cell. The abscissa is cut off at 55 units ($\simeq 5 \times (2\pi/a)$). The energy is scaled in units of t.

agrees well with $E_{\text{QCA}}(\text{M}_2)$ ($=2t$). We will sometimes call the dispersion-relation-like pattern in the map of $P(E_i, \boldsymbol{k})$ a quasi-dispersion relation.

The map in figure 4 is complicated in $-3.3t \leqslant E \leqslant 0$. However, if we inspect it closely, we can observe that a sharp maximum with $E = -2.1t$ is present in the dispersion between the second Γ point (A in figure 3(a)) and the third one (B); it is obscured partly on account of a large quantisation effect of the wavenumber because L ($=11.66a$) is not sufficiently large compared with a. A similar maximum can be seen between C and D. These maxima can be ascribed to X_2 points as given in figure 3(a). The QCA effective mass at the representative X_2 point is negative along the horizontal axis but has the same magnitude as the one at the Γ point. Note that the X_2 point on the left of the second Γ point (A) and the one on the right of the fourth (D) are not translationally equivalent to the previous two X_2 points.

We show in figure 5 a map along the axis represented by the broken line in figure 2. There exist five dispersion maxima originating from the R points and, also, three

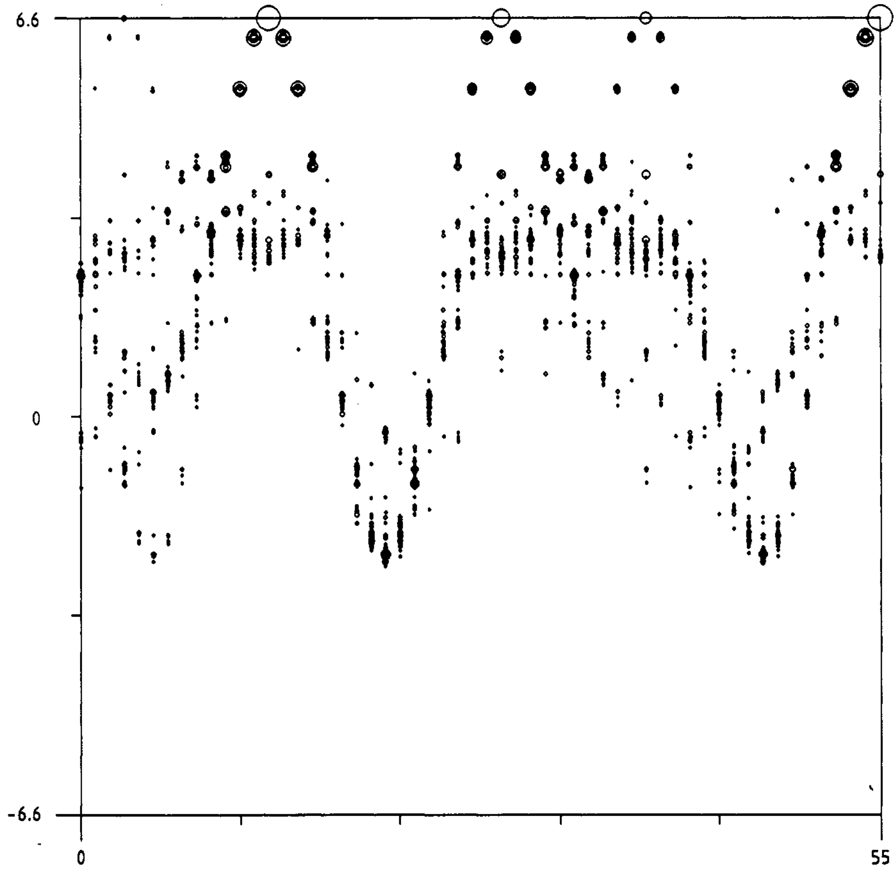

Figure 5. A similar map to figure 4 but along the broken line in figure 2, on which R points are located. The abscissa represents the component of the wavevector parallel to the horizontal axis in figure 2.

minima from X_2 points. The intensities of these critical points are in good agreement with those of R points in figure 2 and X_2 points in figure 3(*a*). If figure 5 is rotated by 180° around the centre of the box, a similar pattern to figure 4 is obtained, which is a consequence of the previously mentioned symmetry of H. The symmetry would be more perfect if figure 4 were compared with a map along the horizontal axis passing through the strongest R point on the fivefold axis in figure 2.

We have investigated similar maps along several other axes and confirmed that critical points of the quasi-dispersion relation also appear at X_5, M_5, X_3 and M_3 with appropriate intensities and energies.

8. Summary and discussion

We have shown that there exist several types of special points in the reciprocal space of the IQL. The translationally equivalent special points are distributed quasi-periodically in the reciprocal space with different intensities. On the other hand, the

Fourier spectra of electronic wavefunctions on the IQL are investigated in the tight-binding approximation. We have observed a quasi-dispersion relation in two-dimensional maps of the spectra along several axes in the reciprocal space. The positions of the critical points of the quasi-dispersion relation and their intensities are well accounted for by the weighted distributions of different types of special points in the reciprocal space.

We have calculated the density of states of H, which is, however, not presented here because it deteriorates on account of the size effect (a similar deterioration occurs for the density of states of the simple cubic lattice of a similar size). Nevertheless, we can observe several structures that appear to be bulk effects due to the critical points of the quasi-dispersion relation. We are now undertaking a calculation for the sample of size $N = 10336$, in order to confirm this observation.

We have investigated the energy dependence of $P(E_i, \boldsymbol{k})$ for several fixed wavevectors. The profiles in the E versus P plane indicate that the spectra are singular continuous but not of point spectra nor absolutely continuous; this is partly evidenced by the fact that heavy overlappings among different intensities are observed in figures 4 and 5. This observation indicates that the wavefunctions are critical with respect to localisation as in the case of the Fibonacci lattice (and, probably, the case of the Penrose lattice).

If the spectra were of point spectra, the quasi-dispersion relation would be as sharp as the case of a crystal (this is the case of the Harper model in the extended regime (Aubry and André 1979, Sokoloff 1985); the model is a 1D quasi-periodic system). On the other hand, absolutely continuous spectra are realised in the case of a disordered system and also the localised regime of the Harper model. If the conjecture that the electronic wavefunctions on the IQL are critical is true, the localisation property of a quasi-lattice is not sensitive to its dimensionality, in contrast to the case of a disordered system (Abrahams *et al* 1979). This subject will be discussed in the near future based on a more extensive calculation with larger samples.

We have investigated the electronic wavefunctions of the Penrose lattice by Fourier decompositions of them and obtained similar results to the case of the IQL. The results will be published elsewhere.

Special points are defined also for other icosahedral quasi-lattices belonging to different Bravais classes (Rokhsar *et al* 1987) and also for two-dimensional quasi-lattices (see, for example, Niizeki 1989a). A complete classification of the special points in these cases is published in Niizeki (1989b, c).

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