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LETTER TO THE EDITOR

The reciprocal space properties of the electronic wave functions of the Penrose lattice

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Abstract. The spectral density of an electron in a Penrose lattice is investigated numerically. It is found that the profile of the spectral density of the energy versus the wavenumber plane exhibits a dispersion-relation-like pattern. The positions and the 'intensities' of the stationary points of the dispersion relation are accounted for by the ordinary structure factor, $S(\boldsymbol{Q})$, and the 'optical structure factor' $S_{\mathrm{opt}}(\boldsymbol{Q})$; the Penrose lattice is a 'non-Bravais type' quasi-lattice and the eigenstates near the top of the band are considered to be 'optical modes'.

A quasicrystal is an unusual type of matter with a quasi-periodic positional long range order together with a non-crystallographic point symmetry (Schechtman *et al* 1984, Steinhardt and Ostlund 1987). The present authors investigated the spectral density of an electron in an icosahedral quasicrystal (Niizeki and Akamatsu 1990: to be referred to as I). They found that the spectral density has several striking features: (i) it exhibits a dispersion-relation-like pattern, which is quasi-periodic in reciprocal space, and (ii) the positions and the intensities of the 'quasi-dispersion-relation' are well accounted for by the structure factor and its generalised versions, associated with the special wave vectors, which correspond to the zone-boundary wave vectors in the case of a periodic lattice.

In this letter, we report the results of a similar investigation to I but in this case we use the Penrose lattice, which is a representative decagonal quasi-lattice in two dimensions (2D). The purpose of the investigation is to answer the questions: (i) do the properties of the electronic wave functions of a quasicrystal depend on the dimensionality of the system (note that the dimensionality is crucial in the localisation properties of the wave functions in a disordered system (Abrahams *et al* 1979)), and (ii) do some differences in the structure between the Penrose lattice and the icosahedral quasi-lattice result in any qualitative difference in the spectral density between them.

The electronic structure of condensed matter is strongly dependent on the atomic structure. Therefore, we begin by investigating the real space and the reciprocal space properties of the Penrose lattice (de Bruijn 1981 and Jaric 1986). A Penrose lattice L is the set of all the vertices of the Penrose tiling, i.e., a quasi-periodic tiling of the plane in terms of two kinds of rhombic tiles whose inner angles are multiples of $\pi/5$. L has a decagonal macroscopic point symmetry whose point group is D_{10}, the dihedral group of order 20. A side of a tile represents a 'bond' between the two relevant sites. We shall call the bond length a the lattice constant of L. The average coordination number

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$\bar{z}$ of sites of L is four and the area per site is given by $S_0 = a^2\sqrt{5}\tau^{-2}\sin(\pi/5)$, with $\tau = (1+\sqrt{5})/2$.

Let $\boldsymbol{e}_i = (\cos(i\theta), \sin(i\theta))$, where $i = 0$–4 with $\theta = 2\pi/5$, be the unit vectors pointing to the vertices of a regular pentagon. Then the basis vectors of L are given by $\boldsymbol{a}_i = a\boldsymbol{e}_i$, $i = 0$–4. Since $\Sigma_i \boldsymbol{e}_i = 0$, only four of the five basis vectors are linearly independent over $\boldsymbol{Z}$; $\boldsymbol{a}_i$ form an overcomplete set of basis vectors. A lattice point of L is represented as $\boldsymbol{l} = \Sigma_i n_i \boldsymbol{a}_i$ with $n_i \in \boldsymbol{Z}$. n_i are determined up to an arbitrary common additive integer, so that they are determined uniquely if we impose the condition $0 \leqslant p(\boldsymbol{l}) \leqslant 4$, where $p(\boldsymbol{l}) \equiv \Sigma_i n_i$ is called the level of $\boldsymbol{l}$. L has, in fact, no lattice points on level 0.

A bond can be formed only between two sites whose levels differ by ± 1. Therefore, L is divided into four interpenetrating sublattices L_p, $p = 1$–4. L is considered, in fact, to be a 'non-Bravais type' quasi-lattice. It is derived by the cut-and-projection method from a 4D non-Bravais type decagonal lattice which has four lattice points per one unit cell corresponding to the four sublattices of L (Janssen 1986, Niizeki 1989). L is bipartite because it is decomposed into two interpenetrating sublattices $L^{(1)} = L_1 \cup L_3$ and $L^{(2)} = L_2 \cup L_4$. It can be shown that $L^{(1)}$ and $L^{(2)}$ have pentagonal point symmetry (D_5).

The basis vectors of the reciprocal lattice L^* to L are given by $\boldsymbol{a}_i^* = a^*\boldsymbol{e}_i$ with $a^* = 4\pi/(5a)$. The conjugate basis vectors to $\boldsymbol{a}_i^*$ are defined by $\tilde{\boldsymbol{a}}_i^* = a^*\boldsymbol{e}_{2i}$, where the subscript $2i$ is assumed to be reduced in modulo 5 to an integer between 0 and 4. A reciprocal lattice vector (RLV), $\boldsymbol{G}\,(\in L^*)$, and its conjugate counterpart, $\tilde{\boldsymbol{G}}$, are represented, respectively, as $\boldsymbol{G} = \Sigma_i n_i \boldsymbol{a}_i^*$ and $\tilde{\boldsymbol{G}} = \Sigma_i n_i \tilde{\boldsymbol{a}}_i^*$ with $n_i \in \boldsymbol{Z}$ and $0 \leqslant q(\boldsymbol{G}) \leqslant 4$, where $q(\boldsymbol{G})$ $(= q(\tilde{\boldsymbol{G}})) \equiv \Sigma_i n_i$. The pair of RLVs form a 4D RLV which belongs to a 4D decagonal Bravais lattice in the 4D reciprocal space. The 4D vector is near the real (reciprocal) space if $|\tilde{\boldsymbol{G}}| < 1/a$. $\boldsymbol{G}$ is indexed with the basis vectors as $(n_0 n_1 n_2 n_3 n_4)$.

The ten vectors $\pm\boldsymbol{e}_i$, $i = 0$–4, represent the vertices of the unit regular decagon centred on the origin of the reciprocal space. We shall denote by Δ (or Σ) the ten equivalent directions parallel to $\pm\boldsymbol{e}_i$ (or $\pm(\boldsymbol{e}_{i+1} - \boldsymbol{e}_i)$). An RLV on a Δ axis is indexed as $\boldsymbol{G} = (n_0 n_1 n_2 n_2 n_1)$ and its level $q(\boldsymbol{G}) = n_0 + 2n_1 + 2n_2$ can take any value between 0 and 4. On the other hand, an RLV on a Σ axis is indexed as $\boldsymbol{G} = (0 n_1 n_2 \bar{n}_2 \bar{n}_1)$ and $q(\boldsymbol{G}) = 0$.

The structure factor, $S(\boldsymbol{Q})$, of L is given (Jarić 1986) by

$$S(\boldsymbol{Q}) = \sum_{\boldsymbol{G}\in L^*} |\sigma(\tilde{\boldsymbol{G}})|^2 (2\pi)^2 \delta(\boldsymbol{Q} - \boldsymbol{G})/S_0 \tag{1}$$

$$\sigma(\tilde{\boldsymbol{G}}) = \Omega^{-1} \sum_{p=1}^{4} \hat{V}_p(-\tilde{\boldsymbol{G}}) \zeta^{-pq(\tilde{\boldsymbol{G}})} \tag{2}$$

where $\zeta = \exp(2\pi i/5)$, $\hat{V}_p(\boldsymbol{Q})$ are the Fourier transforms of the Bruijn's pentagons, V_p, $p = 1$–4, and $\Omega = \Sigma_p A_p\,(= 5\tau^3 S_0)$ with $A_p\,(= \hat{V}_p(0))$ being the area of V_p. $\sigma(\tilde{\boldsymbol{G}})$ is divided as $\sigma(\tilde{\boldsymbol{G}}) = \sigma^{(1)}(\tilde{\boldsymbol{G}}) + \sigma^{(2)}(\tilde{\boldsymbol{G}})$, where $\sigma^{(1)}(\tilde{\boldsymbol{G}})$ and $\sigma^{(2)}(\tilde{\boldsymbol{G}})$ are the contributions from the two sublattices $L^{(1)}$ and $L^{(2)}$.

Since the Penrose lattice is bipartite, we can define the 'optical structure factor', $S_{\text{opt}}(\boldsymbol{Q})$, into which the two sublattices contribute in opposite phases. $S_{\text{opt}}(\boldsymbol{Q})$ is given by a similar expression to the one for $S(\boldsymbol{Q})$ but $\sigma(\tilde{\boldsymbol{G}})$ is replaced by $\sigma_{\text{opt}}(\tilde{\boldsymbol{G}}) = \sigma^{(1)}(\tilde{\boldsymbol{G}}) - \sigma^{(2)}(\tilde{\boldsymbol{G}})$. It is important that $S(\boldsymbol{Q})$ and $S_{\text{opt}}(\boldsymbol{Q})$ have delta-function peaks at common positions and only the intensities are different.

$\hat{V}_p(\boldsymbol{Q})$ becomes vanishingly small when $|\boldsymbol{Q}|$ increases beyond $1/a$, so that $\sigma(\tilde{\boldsymbol{G}})$ (or $\sigma_{\text{opt}}(\tilde{\boldsymbol{G}})$) becomes small when $|\tilde{\boldsymbol{G}}| \gg 1/a$. We consider, then, the limit of $\sigma(\tilde{\boldsymbol{Q}})$ (or $\sigma_{\text{opt}}(\tilde{\boldsymbol{G}})$) when $|\tilde{\boldsymbol{G}}|$ tends to 0. Since $A_1 = A_4$, $A_2 = A_3$ and $A_{2(3)} = \tau^2 A_{1(4)}$, we can conclude that $\sigma(\tilde{\boldsymbol{G}}) \simeq 1$, $-1/2$ or 0 and $\sigma_{\text{opt}}(\tilde{\boldsymbol{G}}) \simeq 0$, $(4\tau\sin(2\pi/5))^{-1}$ or $(2\sin(\pi/5))^{-1}$ according to whether $q \equiv 0$, ± 1 or ± 2 mod 5, respectively. If $\sigma^{(1)}(\tilde{\boldsymbol{G}})$ and $\sigma^{(2)}(\tilde{\boldsymbol{G}})$ are constructive in

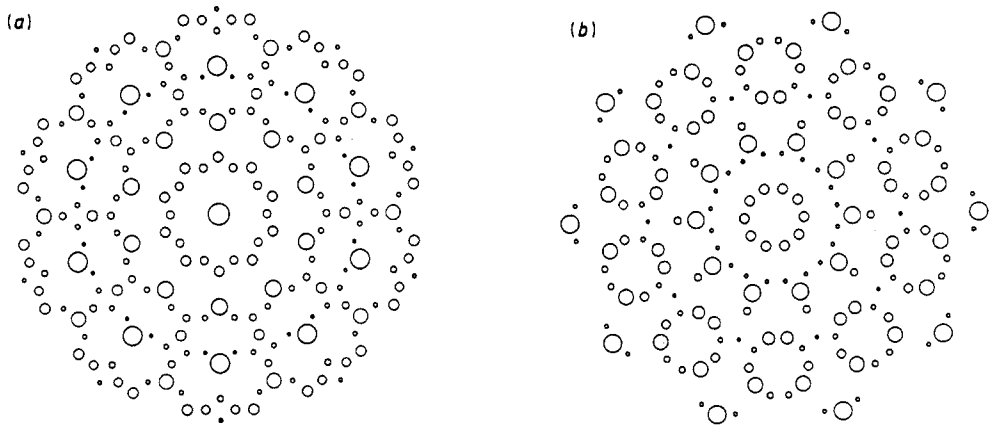

Figure 1. The structure factor $S(\boldsymbol{Q})$ (*a*) and the optical structure factor $S_{\rm opt}(\boldsymbol{Q})$ (*b*) of the Penrose lattice. The area of a circle is proportional to the intensity. A circle with an intensity lower than 2% of the full intensity is neglected. The centre is the origin of the reciprocal space. The horizontal axis is parallel to a Δ axis and the vertical one to a Σ axis. The strongest spot of $S(\boldsymbol{Q})$ on a Δ (or Σ) axis is indexed as $(41\bar{3}\bar{3}1)$ (or $(032\bar{2}\bar{3})$). On the other hand, the innermost (or outermost) spot of $S_{\rm opt}(\boldsymbol{Q})$ on a Δ axis is indexed as (11001) (or $(52\bar{3}\bar{3}2)$).

$\sigma(\tilde{\boldsymbol{G}})$, they are destructive in $\sigma_{\rm opt}(\tilde{\boldsymbol{G}})$ and vice versa, so that the magnitudes of $\sigma(\tilde{\boldsymbol{G}})$ and $\sigma_{\rm opt}(\tilde{\boldsymbol{G}})$ are complementary.

We show $S(\boldsymbol{Q})$ and $S_{\rm opt}(\boldsymbol{Q})$ in figures 1(*a*) and (*b*), respectively. We can see quasi-periodic distributions of Bragg spots with point symmetry D_{10}. The high-intensity Bragg spots and the medium-intensity ones are located on RLVs whose levels are 0 or ± 1 mod 5 for $S(\boldsymbol{Q})$ but ± 1 or ± 2 mod 5 for $S_{\rm opt}(\boldsymbol{Q})$. A high-intensity Bragg spot of $S(\boldsymbol{Q})$ is located in a region where Bragg spots of $S_{\rm opt}(\boldsymbol{Q})$ are weak and vice versa. $S(\boldsymbol{Q})$ has high-intensity spots on both the Δ and Σ axes but $S_{\rm opt}(\boldsymbol{Q})$ only has them on the Δ axis.

Each Bragg spot of $S(\boldsymbol{Q})$ corresponds to a Γ-point in the reciprocal space in the extended-zone scheme of a periodic Bravais lattice. The Γ-points of a quasi-lattice differ from those of a periodic lattice in that different Γ-points have different intensities and that they are distributed densely, though most of them have vanishingly small intensities.

We now turn our attention to the one-electron states of a Penrose lattice. We take a finite but macroscopic piece of the Penrose lattice, whose lattice points are numbered arbitrarily from 1 to N. We assume that the Hamiltonian is given in the tight-binding approximation as

$$H = -\sum_{\langle i,j\rangle} t(|i\rangle\langle j| + |j\rangle\langle i|) \tag{3}$$

where t stands for the transfer integral between two sites i, j connected by a 'bond' and $|i\rangle$ an s-orbital on the site i.

Let us denote the eigen energies of H by $E_1, E_2, \ldots, E_N$ and the corresponding normalised eigenvectors by $\varphi^{(1)}, \varphi^{(2)}, \ldots, \varphi^{(N)}$. Then, the spectral density is represented as

$$\rho(\boldsymbol{Q}, E) = \sum_{\nu} |\langle \boldsymbol{Q}|\varphi^{(\nu)}\rangle|^2 \delta(E - E_\nu) \tag{4}$$

where

$$|\mathrm{Q}\rangle = N^{-1/2} \sum_i \exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{l}_i)|i\rangle$$

stands for a normalised plane-wave state. The dependence of $|\boldsymbol{Q}\rangle$ on $\boldsymbol{Q}$ is not periodic

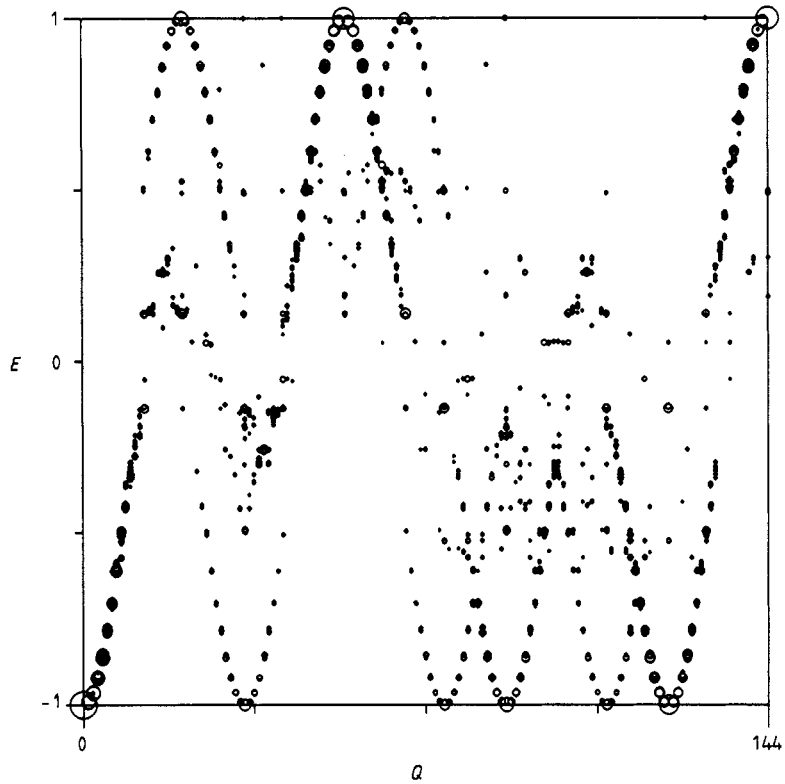

Figure 2. The spectral density along a Δ axis. The area of a circle is proportional to the Fourier intensity $|\langle \boldsymbol{Q}|\varphi^{(\nu)}\rangle|^2$. Low-intensity signals are cut-off at 0.004. The wavenumber is quantised to multiples of $\Delta Q = 2\pi/(D\sin(2\pi/5))$. The ordinate is scaled in units of W ($\simeq 4.23\,t$), half of the band width. The wavenumber at the right hand end of the abscissa is equal to $144\Delta Q$ ($\simeq 11.1\,(2\pi/a)$).

but quasi-periodic in contrast to the case of a periodic lattice. Note that $|\boldsymbol{Q}\rangle \simeq |\boldsymbol{Q}+\boldsymbol{G}\rangle$ if $\boldsymbol{G}$ is an RLV satisfying the conditions $|\tilde{G}| \ll 1/a$ and $q(\boldsymbol{G}) = 0$.

We investigate $\rho(\boldsymbol{Q}, E)$ by the numerical method. In order to supress the surface effects, we take a unit cell of a 'periodic Penrose lattice' and employ the cyclic boundary condition (Tsunetsugu *et al* 1986, Okabe and Niizeki 1988). The size N of our sample is 1364. The unit cell is a rhombus similar to the fat tile and the length of the side is given by $D = 2a\tau^7\sin(\pi/5)$ ($\simeq 34.1a$). On account of the cyclic boundary condition, $\boldsymbol{Q}$ in (4) can only take discrete values determined by the unit cell.

We do not present the figure of the density of states (Choy 1985), whose shape is similar to an inverted funnel. Half the band width W is about $4.23\,t$, which is slightly larger than $\bar{z}t$ ($=4\,t$), the value in the quasicrystalline approximation.

We show in figure 2 the spectral density along a Δ axis (exactly speaking, the figure shows a pseudo-spectral-density because the width of the delta functions is chosen to be smaller than the average level distance). We can clearly observe a dispersion-relation-like pattern, which we shall call a quasi-dispersion-relation (QDR). The parabolic dispersion minimum located on the origin recurs quasi-periodically with different intensities. The positions and the intensities agree well with those of the Bragg spots of $S(\boldsymbol{Q})$ as given in figure 1(*a*).

We find that parabolic dispersion maxima derived from the top of the band also appear quasi-periodically. The positions and the intensities agree well with those of the 'Bragg spots' of $S_{opt}(\boldsymbol{Q})$ as given in figure 1(b). This is a reasonable result because the eigenstates near the top of the band are antibonding-like with respect to the nearest-neighbour interactions. The fact that the dispersion maxima derived from the top of the band appear at Γ-points is in sharp contrast to the case of the 3D icosahedral quasi-lattice where they appear at special wave vectors corresponding to zone-boundary wave vectors in the case of a periodic lattice (see I). Since the Penrose lattice is a non-Bravais type quasi-lattice, the QDR near the top of the band can be considered to be due to 'optical modes'.

We see that the QDR is disordered in a region around the centre of the band ($E \simeq 0$). A close investigation of the real-space wave functions in that region revealed that they have a strong tendency towards localisation. In particular, there exist localised states called 'confined states', which are degenerate at $E = 0$; a confined state is strictly confined to a region with a particular structure and the ratio of the number of confined states to the total number of states is finite (Semba 1985, Kohmoto and Sutherland 1986). Therefore, the apparent gaps of the QDR are due to the localised states and almost localised states but not to any zone-boundary wave vector; the low intensity signals are lost on account of the cut-off.

We have also investigated $\rho(\boldsymbol{Q}, E)$ along a Σ axis and confirmed that parabolic dispersion minima appear at appropriate positions and intensities in agreement with the distribution of Γ-points along the same axis (see figure 1(a)). On the other hand, the dispersion maxima along this axis are not due to Γ-points associated with the top of the band but to other kinds of special points; this is because the optical structure factor, $S_{opt}(\boldsymbol{Q})$, has no intensities on the Σ axis.

In conclusion, the electronic spectral density of the Penrose lattice exhibits a similar dispersion-relation-like pattern to that of the icosahedral quasi-lattice but the former has dispersion maxima derived from 'optical modes' because the Penrose lattice is a non-Bravais type quasi-lattice composed of four Bravais sublattices.

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