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# Average unit cell for Penrose tiling and its Gaussian approximation

**Janusz Wolny* and Bartłomiej Kozakowski**

Faculty of Physics and Nuclear Techniques, The University of Mining and Metallurgy, al. Mickiewicza 30, PL-30-059 Kraków, Poland. Correspondence e-mail: wolny@novell.ftj.agh.edu.pl

In this paper, the average unit cell for a quasicrystal is constructed by a statistical approach. For the Penrose tiling, it is shown that such a unit cell is fully equivalent to the oblique projection of the atomic surface onto physical space. The obtained statistical distributions can be easily extended to imperfect structures by using a Gaussian approximation. This leads to simple analytical expressions for diffraction intensities, which can be very useful in structure refinement.

## 1. Introduction

The concept of the average unit cell was first introduced in the theory of incommensurately modulated structures (Janner & Janssen, 1977). It has already been shown (Duneau & Oguey, 1990; Wolny, 1998; Xu & Mai, 1998; Steurer & Haibach, 1999; Steurer & Cervellino, 2001; Wolny & Kozakowski, 2001; Argon *et al*., 2002; Cervellino & Steurer, 2002; Wolny *et al*., 2002) that for quasicrystals one can also construct the average unit cell in physical space (for Penrose tiling see also Fig. 2). In Duneau & Oguey (1990), the property of quasiperiodic structures built by the cut-and-project method or any equivalent method is related to a periodic lattice with a bounded deformation of the atomic surface. The maximum repeated frequency of local close-packed structures in space, which has been considered by Xu & Mai (1998), gives the lowest energy for the quasicrystalline phase. A general method to find average lattices based on the so-called generalized dual method to generate quasiperiodic lattices has been discussed in Argon *et al*. (2002). To construct an average unit cell, Steurer *et al*. (Steurer & Haibach, 1999; Steurer & Cervellino, 2001; Cervellino & Steurer, 2002) have used an oblique projection of the atomic surface onto physical space. A probabilistic approach based on a concept of reference lattices has been formulated by Wolny (1998). Using two reference lattices, one can reconstruct the diffraction pattern (*i.e.* the main reflections and their satellites) in any direction of the scattering vector. Recently (Wolny & Kozakowski, 2001; Wolny *et al*., 2002), we have proved that for Penrose tiling the probabilistic approach for the single reference lattice is similar, except for inversion, to the oblique projection used by Steurer *et al*.

There are two properties of the structure factor that are very important for the presented concept of the average unit cell. The first one is the scalar product between the wave vector **k** and positional vector **r**, which means that for a chosen scattering vector the whole structure is then projected onto the direction pointed out by that particular wave vector. The second property is that these scalar products determine the phase shifts of the individual components and the information concerning the atomic positions can be significantly reduced to a single unit cell, *i.e.* modulo the corresponding wavelength. In the present approach, the diffraction intensity measures the quality of the adjustment of the reference lattice to the real structure. The diffraction peaks indicate a kind of *similarity resonance* between the reference lattice (linked to the scattering vector) and the real structure. For example, for the majority of wave vectors, the reference lattice fits improperly to the entire periodic structure, leading to the uniform distributions of occupational positions in the corresponding average unit cells. Fourier components of such distributions are equal to zero and no diffraction peaks are observed for such scattering vectors. Only for a certain set of wave vectors, *i.e.* for points of the reciprocal lattice, is there a resonant adjustment of the reference lattice to the real structure, leading to the Bragg reflections. One should remember that the concept of the average unit cell based on the reference lattice is not an approximation and so the unit cell can be constructed for an arbitrarily chosen scattering vector. However, more appropriate are those wave vectors corresponding to significantly non-zero intensities of diffraction patterns. For them, the similarity resonance of the reference lattice and the real structure are really observed as well developed diffraction peaks.

For the random tiling model, the most commonly used theory is the phason Debye–Waller theory (Elser, 1985; Widom *et al*., 1987; Tang & Jaric, 1990; Henley, 1991), which operates in the perpendicular space. On the other hand, the average unit-cell theory used in this paper operates in physical space only and it goes *beyond the tiling*. This theory requires no assumptions about the periodicity of the structure itself, both in real space and in higher dimensions. The only periodicity used in the calculations is the periodicity of a purely mathematical object, which is the reference lattice. In the

present theory, there is no possibility of distinguishing between phasons and phonons, and all of them are considered as fluctuations. It has already been proved (Wolny & Kozakowski, 2001; Wolny *et al.*, 2002) that for tilings (*i.e.* structures that can be described in higher dimensions) the results obtained from these two approaches are similar.

In the present paper, the theory of the average unit cell has been applied to the Penrose tiling, as an example of a 2D quasicrystal. The corresponding average unit cell consists of four pentagons where the probability distributions of distances from the lines of the reference lattices are non-zero. We decided to approximate the obtained distributions by a Gaussian to reduce the number of fitted parameters, which can drastically increase for decorated tilings. Although other approximations (like elliptical approximation) give better results, the Gaussian approximation seems to be the unique one to include any kind of imperfections usually present in the analysed structure.

There are infinitely many average unit cells, similar to normal crystals, which depend on the chosen scattering vectors. For Penrose tiling, the average unit cell can be, for example, obtained in two different ways, and the final results are fully equivalent. The first way is just an oblique projection of the perpendicular space atomic surface onto the physical space (Wolny, 1998; Steurer & Haibach, 1999; Steurer & Cervellino, 2001; Wolny & Kozakowski, 2001; Cervellino & Steurer, 2002; Wolny *et al.*, 2002). The projection, however, is not orthogonal to the physical space but to the plane embedded in 5D and spanned by two appropriately chosen scattering vectors. The projection consists of four pentagons: two big and two small (Fig. 2*a*).

The second method of constructing the average unit cell is based on the reference lattice concept using the statistical approach (Wolny, 1998). For two arbitrary chosen scattering vectors, $\mathbf{k}_1$ and $\mathbf{k}_2$, which do not need to be orthogonal, two reference lattices are constructed. The reference lattice is a set of parallel lines periodically arranged in 2D and perpendicular to the corresponding scattering vector. The periodicity of the lattice grid is equal to $\lambda_i = 2\pi/k_i$, $i = 1, 2$, for the first and second scattering vector, respectively. The position of any node (2D atom) with respect to the reference lattices is given by two coordinates, $(u_1, u_2)$, with the probability $P(u_1, u_2)$ defined for the whole structure. The Fourier transform of such a probability describes the structure factor not only for the given scattering vectors, $\mathbf{k}_1$ and $\mathbf{k}_2$, but also for all higher harmonics of those vectors, *i.e.*

$$\mathbf{k} = n_1\mathbf{k}_1 + n_2\mathbf{k}_2, \tag{1}$$

where $n_1$, $n_2$ are integers. The structure factor then reads:

$$F(k) = f_0 \int_0^{\lambda_1}\int_0^{\lambda_2} P(u_1, u_2)\exp[i(n_1k_1u_1 + n_2k_2u_2)]\,\mathrm{d}u_1\,\mathrm{d}u_2. \tag{2}$$

For further calculations, it will be assumed that the atomic form factor $f_0$ is equal to 1.

Fig. 2(*a*) shows the average unit cell calculated for two reference lattices associated with two wave vectors, $\mathbf{k}_1$ and $\mathbf{k}_2$, of the same lengths:

$$k_1 = k_2 = k_0 = (2\pi/5)2\tau \approx 4.067, \tag{3}$$

where $\tau$ is the golden mean value defined as $\tau = 1 + 5^{1/2}/2 \approx 1.618$.

Vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are directed at the angles of $\pm\alpha$ to the $x$ axis, respectively, where $\alpha = 2\pi/5$ (Fig. 1). When increased to 5D, the corresponding vectors, $\mathbf{K}_1$ and $\mathbf{K}_2$, have the following coordinates:

$$\begin{aligned}\mathbf{k}_1 &= k_0[\cos(\alpha), +\sin(\alpha)] \longrightarrow \mathbf{K}_1 = [0, 0, -1, -1, 0]\\ \mathbf{k}_2 &= k_0[\cos(\alpha), -\sin(\alpha)] \longrightarrow \mathbf{K}_2 = [-1, -1, 0, 0, 0].\end{aligned} \tag{4}$$

The calculations were performed for a cluster of Penrose tilings consisting of about 160000 nodes placed at the corners of the two types of rhombuses: thick and thin ones with edge length equal to 1. The boundaries of the obtained average unit cell are marked as dashed lines (Fig. 2*a*). One can easily notice that the probability distribution of atomic positions in the average unit cell fits very well to the oblique projection of the atomic surface onto physical space. It has already been shown analytically (Wolny & Kozakowski, 2001; Wolny *et al.*, 2002) that for the infinite structure the probability distribution consists of four pentagons shifted to a single unit cell as is shown in Fig. 2(*a*). The extended average unit cell for such wave vectors is shown in Fig. 2(*b*), where periodical arrangement of projected pentagons can easily be noticed. Dashed lines also mark the single average unit cell. To reconstruct the diffraction pattern (Fig. 1), two additional vectors are needed, namely the modulation vectors describing the satellite positions. The modulation vectors were chosen as following:

$$\begin{aligned}\mathbf{q}_1 &= \mathbf{k}_1/\tau \longrightarrow \mathbf{Q}_1 = [1, 0, 0, 0, 0]\\ \mathbf{q}_2 &= \mathbf{k}_2/\tau \longrightarrow \mathbf{Q}_2 = [0, 0, 0, 1, 0].\end{aligned} \tag{5}$$

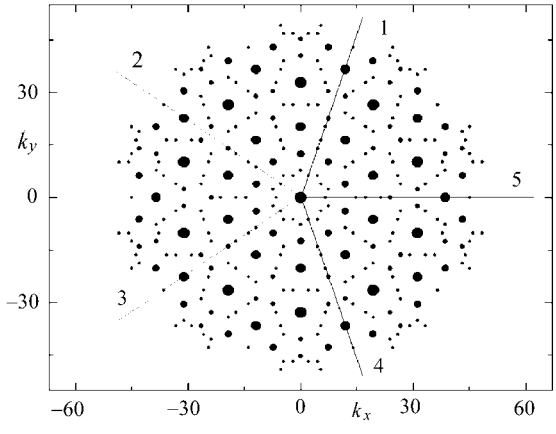


**Figure 1**
Diffraction pattern of Penrose tiling obtained by Fourier transform of an average unit cell defined in physical space by a statistical approach. The average unit cell has been constructed for scattering vectors $k_1 = k_2 \approx 4.07$ and the corresponding modulation vectors $q_1 = q_2 \approx 2.51$, *i.e.* $\tau$ times smaller than the previous ones. The pair of vectors $\mathbf{k}_1$ and $\mathbf{q}_1$ (and also $\mathbf{k}_2$ and $\mathbf{q}_2$) are parallel and directed at angles of $\pm 72^\circ$ (directions 1 and 4) to the $x$ axis, respectively. Five symmetry-equivalent directions are also marked. Intensities of the diffraction peaks are more or less proportional to the symbol size.

The position of any diffraction peak can then be described by a linear combination of four vectors: $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{q}_1$, $\mathbf{q}_2$, *i.e.*

$$\mathbf{k} = n_1\mathbf{k}_1 + n_2\mathbf{k}_2 + m_1\mathbf{q}_1 + m_2\mathbf{q}_2, \tag{6}$$

where $n_1$, $n_2$, $m_1$, $m_2$ are integers. Usually we call such a reflection the $m$th satellite to the $n$th main diffraction peak. The structure factor of the diffraction peak is then given by

$$F(\mathbf{k}) = f_0 \int\int\int\int_{\mathrm{AUC}} P(u_1, u_2, v_1, v_2) \exp[i(n_1k_1u_1 + n_2k_2u_2 + m_1q_1v_1 + m_2q_2v_2)]\,\mathrm{d}u_1\mathrm{d}u_2\mathrm{d}v_1\mathrm{d}v_2, \tag{7}$$

where AUC stands for the average unit cell and the integral bounds are $\pm\pi/k_1$, $\pm\pi/k_2$, $\pm\pi/q_1$, $\pm\pi/q_2$, for $u_1, u_2, v_1, v_2$, respectively (in the integrals below, these bounds will be omitted). Variables $v_1$ and $v_2$ describe the shortest distances between the node and the corresponding reference lattices of lines associated with the modulation vectors $q_1$ and $q_2$. In principle, one has to know the probability distribution $P(u_1, u_2, v_1, v_2)$ in 4D parameter space. This space is different from the 4D orthogonal space used for the usual description of Penrose tiling, with a completely different metric. All the distances are calculated in physical space and also the distribution density is defined in such a real space. The probability distribution depends on four variables, however, as has already been shown (Wolny & Kozakowski, 2001; Wolny *et al.*, 2002); the distribution is non-zero only along the lines given by

$$v_i = -\tau^2 u_i + \delta_{ij} \quad (i = 1, 2,\ j = 1, \ldots, 4), \tag{8}$$

where $\delta_{ij}$ are some constant parameters depending on the sequence of pentagons after projection onto the physical space. Knowing the distribution $P(u_1, u_2)$ and the set of appropriate parameters, one can reconstruct the whole diffraction pattern of Penrose tiling, including the intensities of the individual peaks. Such an approach as discussed above will be published separately. In this paper, however, the diffraction pattern is calculated in a slightly different way, as is described below. Similarly to what was done previously (Wolny & Kozakowski, 2001; Wolny *et al.*, 2002), the four pentagons $\{H_1, H_2, H_3, H_4\}$ and the two additional points $\{H_0, H_5\}$ of the projected atomic surface have been shifted to the centre of the unit cell and the appropriate phases have been added. $H_0$ and $H_5$ are equal to zero and they do not contribute to the value of the structure factor.

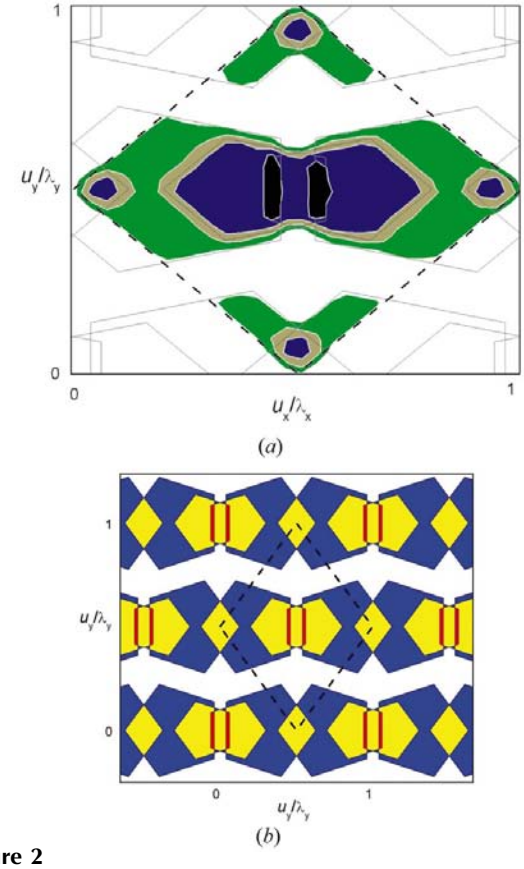


**Figure 2**
(*a*) Average unit cell calculated for the cluster of Penrose tiling of about 160 000 atoms by a statistical approach for two scattering vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ given in the text. The shape of the statistical distribution fits very well to the four pentagons of the atomic surface when projected onto the physical space. It was proved analytically that the shapes obtained from the projection method and the statistical approach are similar. (*b*) Average unit cell in the extended scale. Four pentagons of the atomic surface periodically fill the plane with the periodicity of the average unit cell. Dashed lines mark a single unit cell.

## 2. Diffraction pattern along the *x* direction

The two vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ when added give a scattering vector along the $x$ axis. The same holds also for $\mathbf{q}_1$, $\mathbf{q}_2$. Assuming that $n = n_1 = n_2$ and $m = m_1 = m_2$, one obtains the following expression for the structure factor along the $x$ direction:

$$F(k_x, 0) = \sum_{j=0}^{5} \int P_j(u_x) \exp\{i[(k_x - 2k_{1x}m5^{1/2})u_x + (2\pi j/5)(nr_1 + mr_2)]\}\,\mathrm{d}u_x, \tag{9}$$

where

$$k_x = 2(nk_{1x} + mq_{1x}) = 2k_{1x}(n + m/\tau) \tag{10}$$

points out all the diffraction peaks along the $x$ axis. Variables $k_{1x}$ and $q_{1x}$ are the $x$ components of $\mathbf{k}_1$ and $\mathbf{q}_1$; $r_1$ and $r_2$ are the sums of the corresponding 5D coordinates of scattering vectors ($\mathbf{k}_1$ and $\mathbf{q}_1$) modulo 5. $P_j(u_x)$ are components of the probability distribution calculated for the scattering vector $\mathbf{k}_x$ associated with the $j$th pentagon. Equation (9) fully describes the structure factor along the $x$ direction for all the main reflections and the satellites. To simplify (9), it is convenient to introduce a new variable $k_{xr}$, the reduced scattering vector along the $x$ direction, defined as

$$k_{xr} = k_x - 2k_{1x}m5^{1/2}. \tag{11}$$

The structure factor then reads

$$F_a(k_{xr}, 0) = \sum_{j=0}^{5} \int P_j(u_x) \exp\{i[k_{xr}u_x + (2\pi j/5)a]\}\,\mathrm{d}u_x, \tag{12}$$

where $a$ stands for $(nr_1 + mr_2)$ mod 5, with only three values of $a$ ($a$ = 0, 1, 2) required in the calculations. $F_a$ is the structure factor for a group of peaks associated with a certain value. From the symmetry point of view, the two probability distri-

butions for small pentagons are equal and will be described by $P_S(u_x)$, *i.e.* $P_1(u_x) = P_4(u_x) = P_S(u_x)$. The same holds for two big pentagons: $P_2(u_x) = P_3(u_x) = P_B(u_x)$. Equation (12) can then be written as

$$F_a(k_{xr}, 0) = 2\int[P_S(u_x)\cos(2\pi a/5) + P_B(u_x)\cos(4\pi a/5)] \times \exp(ik_{xr}u_x)\mathrm{d}u_x. \quad (13)$$

For $k_{xr} = 0$ (*i.e.* when $k_x = 2k_{1x}m5^{1/2}$),

$$F_a(0, 0) = 2\int[P_S(u_x)\cos(2\pi a/5) + P_B(u_x)\cos(4\pi a/5)]\,\mathrm{d}u_x. \quad (14)$$

Defining $P_S = \int_H P_S(u_x)\,\mathrm{d}u_x$ and $P_B = \int_H P_B(u_x)\,\mathrm{d}u_x$, one can also write: $2(P_S + P_B) = 1$ (from the normalization); and $P_B/P_S = \tau^2$ (from the ratio of squares of the pentagons). The above leads to three different values for the intensities of the envelope functions at the origin, *i.e.*

$$I_0(0) = |F(0)|^2 = 1 \quad (\text{for } a = 0)$$
$$I_1(0) = 1/4 \quad (\text{for } a = 1)$$
$$I_2(0) = 0 \quad (\text{for } a = 2).$$

Three different classes of envelopes are obtained, as is shown in Fig. 3(*a*). The intensity of the third class is almost negligible.

## 3. Diffraction pattern along the *y* direction

For the *y* direction, it can easily be shown (Wolny & Kozakowski, 2001; Wolny *et al.*, 2002) that the sums of the corresponding 5D coordinates of scattering vectors modulo 5 ($r_1$ and $r_2$) are equal to zero. This also means that $a = nr_1 + mr_2 \bmod 5$ is equal to zero, where $n$ is an index of the main reflection and $m$ is for the satellite. So along the *y* direction the diffraction pattern looks much simpler (Fig. 3*b*) than the one along the *x* direction. There is only a single type of envelope going through the peak's maximum. The obtained

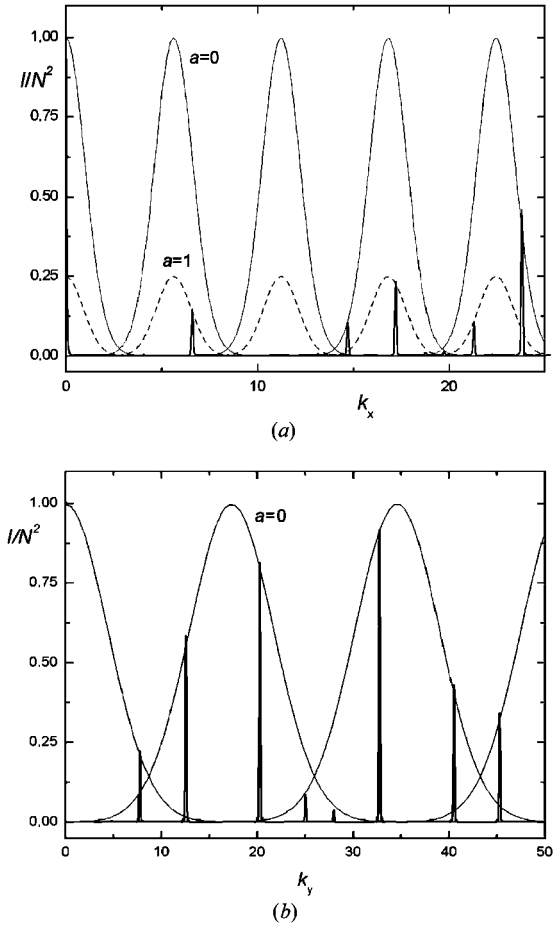


**Figure 3**
(*a*) Diffraction pattern of Penrose tiling calculated along the *x* direction splits into three classes of peaks described by the parameter $a$ = 0, 1, 2 [equation (18)]. The intensity of the third class is almost negligible. Envelope functions have been calculated in the Gaussian approximation [equation (18)] for $a$ = 0 (solid thin line) and $a$ = 1 (dashed line). These lines fit quite well to the calculated diffraction pattern (solid thick line). Small differences between the envelope functions and the intensities of the diffraction peaks completely disappear for proper statistical distribution in the average unit cell. (*b*) All diffraction peaks along the *y* direction are described by a single envelope function with $a$ = 0 [equation (19)].

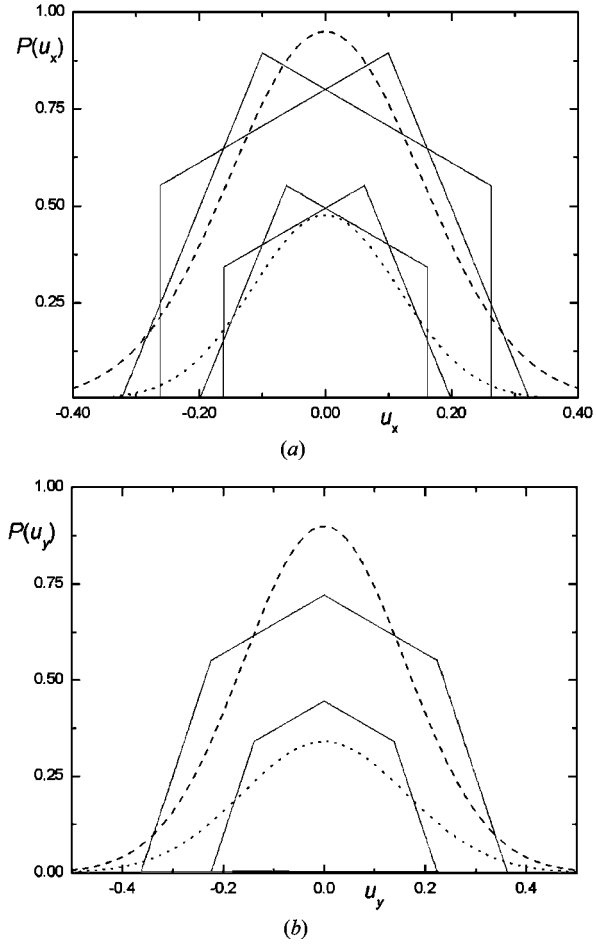


**Figure 4**
(*a*) Probability distributions along the *x* direction for small and big pentagons (solid lines) of the projected atomic surface. These distributions have been approximated by the appropriate Gaussians (broken lines), which lead to the envelope functions shown in Fig. 3(*a*). (*b*) Probability distributions along the *y* direction for small and big pentagons (solid lines) of the projected atomic surface. These distributions have been approximated by the appropriate Gaussians (broken lines), which lead to the envelope functions shown in Fig. 3(*b*).

formula for the structure factor is the same type as (9) [for more details see also formula (37) of Wolny & Kozakowski (2001)] with vanishing second term including $r_1$ and $r_2$, as both of them are equal to zero. The final result is

$$F(0, k_y) = \sum_{j=0}^{5} \int P_j(u_y)\{i[(k_y - 2k_{1y}m5^{1/2})u_y]\}\, \mathrm{d}u_y, \qquad (15)$$

where

$$k_y = 2(nk_{1y} + mq_{1y}) = 2k_{1y}(n + m/\tau). \qquad (16)$$

This single envelope function describes all the main reflections and, when shifted by $k_{\rm shift} = 2k_{1y}m5^{1/2} \approx 17.3m$, also the group of $m$-order satellites.

## 4. Gaussian approximation

The components of the probability distributions along the $x$ and $y$ directions for different pentagons are shown in Figs. 4($a$) and 4($b$). The distributions resemble four pentagons when projected onto $x$ and $y$ axes. However, such distributions are obtained only for perfect and infinite Penrose tiling. For any imperfection, the real distributions are smeared out. The simplest approximation for the new shapes is the use of Gaussian-type distributions for each pentagon (broken lines in Figs. 4$a$ and 4$b$), even if such an approximation is far from the best one. Assuming Gaussian distributions, for small and big pentagons along $x$ and $y$ directions, as

$$P_k(u_i) = A_{ki} \exp(-u_i^2/2\sigma_{ki}^2) \qquad (17)$$

with $k \in \{S, B\}$; $i \in \{x, y\}$, from (13) and (15), one obtains the analytical expressions for the envelope functions:

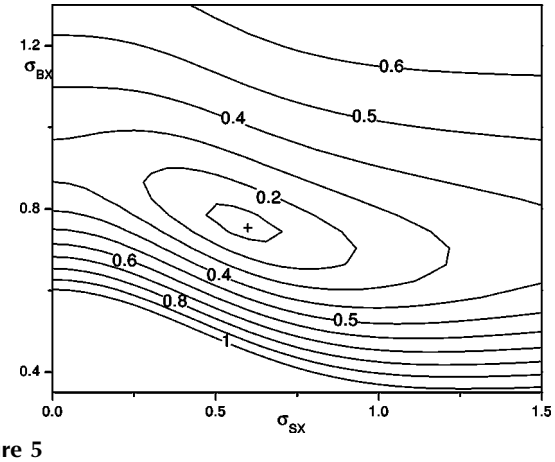


**Figure 5**
Contours of the least-squares fit [equation (21)] to the diffraction pattern in an average unit cell approximated by the Gaussian distributions. A well defined minimum for the $\sigma$ parameter of Gaussian distributions along the $x$ direction is observed. A similar distribution is also observed for the $y$ direction.

$$F(k_{xr}, 0) = \frac{1}{1+\tau^2}\left[\cos\left(\frac{2\pi a}{5}\right)\exp\left(-\tfrac{1}{2}k_{xr}^2\sigma_{Sx}^2\right) + \tau^2\cos\left(\frac{4\pi a}{5}\right)\exp\left(-\tfrac{1}{2}k_{xr}^2\sigma_{Bx}^2\right)\right] \qquad (18)$$

$$F(0, k_{yr}) = \frac{1}{1+\tau^2}\left[\exp\left(-\tfrac{1}{2}k_{yr}^2\sigma_{Sy}^2\right) + \tau^2\exp\left(-\tfrac{1}{2}k_{yr}^2\sigma_{By}^2\right)\right]. \qquad (19)$$

The above equations are very useful and can be used for analysis of diffraction patterns not only along $x$ and $y$ directions but also along other symmetry-related directions. They describe in a very simple way the envelope function (*i.e.* the line that can be fitted directly to the experimental diffraction pattern) using only a few parameters, namely the four widths of the Gaussian distributions. For other diffraction peaks, *e.g.* located on other directions than along $x$ and $y$, one can use more general expressions:

$$P_k(u_x, u_y) = A_k \exp\left(-\frac{u_x^2}{2\sigma_{kx}^2} - \frac{u_y^2}{2\sigma_{ky}^2}\right), \quad k \in \{S, B\} \qquad (20)$$

with the following normalization:

$$A_S\sigma_{Sx}\sigma_{Sy} = \frac{1}{4\pi(1+\tau^2)}$$
$$A_B\sigma_{Bx}\sigma_{By} = \frac{1}{4\pi(1+\tau^2)}.$$

To test the Gaussian approximation, a set of twelve diffraction peaks, six along the $x$ and six along the $y$ axis, were used for the least-squares fit using the formula

$$f = \left\{\frac{1}{n-1}\left[\sum_{j=1}^{n}\left(\frac{I_{0j} - I_j}{I_{0j}}\right)^2\right]\right\}^{1/2}, \qquad (21)$$

where $I_{0j}$ and $I_j$ are the $j$th peak intensities obtained from Fourier transform or Gaussian approximation, respectively, $n$ is the number of diffraction peaks. The results of the calculations are shown in Figs. 3($a$) and 3($b$) for the best fits obtained ($\sigma_{Sx} = 0.578$, $\sigma_{Bx} = 0.758$, $f = 0.061$; $\sigma_{Sy} = 0.162$, $\sigma_{By} = 0.161$, $f = 0.052$). The test function $f$ is shown in Fig. 5 *versus* the fitted parameters ($\sigma_{Sx}$ and $\sigma_{Bx}$ for the $x$ direction). The obtained minimum is rather broad especially for $\sigma_S$, which is quite obvious owing to the $\tau^2$ smaller contribution to the diffraction pattern coming from the small pentagon compared to the big one.

## 5. Conclusions

One can conclude that diffraction analysis of Penrose tiling (and also other quasicrystals) can be successfully performed in physical space using the average unit-cell approach. Such an average unit cell was constructed for some scattering vectors. The Fourier transform of the probability densities of the average unit cell leads to the envelope functions, which fully describe the diffraction intensities of the main reflections and their satellites. For ideal Penrose tiling, this approach is equivalent to the higher-dimensional analysis. The probability distribution in the average unit cell coincides with the pen-

tagons obtained during the oblique projection of the atomic surface into physical space. This leads to another interpretation of the atomic surface in perpendicular space: it can be regarded as the average unit cell expanded up to higher dimensions. However, all the calculations can be done in physical space only and any modifications for defect structures are straightforward and can be easily accomplished. To reduce the number of parameters describing the probability distributions, simple Gaussian distributions were used. As was shown, this approximation quite well describes the diffraction pattern of Penrose tiling. The Gaussian approximation is very useful for defect or random tilings; however, for perfect Penrose tiling much better results can be obtained with flat distributions of elliptical shape (Wolny *et al.*, 2002). The greatest advantages of the presented approximation are formulae (18) and (19), which in a very simple analytical way describe the structure factor for defect Penrose tiling in physical space. Only a few parameters, namely the widths of the Gaussian distributions (two pairs of widths, $\sigma_{Sx}$, $\sigma_{Bx}$ and $\sigma_{Sy}$, $\sigma_{By}$ for $x$ and $y$ directions, respectively) have to be fitted in order to obtain the average unit cell directly from the diffraction pattern. Assuming additionally the ratio of widths for big and small pentagons, one can even reduce the number of fitting parameters to only two. Such an analysis can be successfully used for perfect and imperfect 2D quasicrystals and its extension to 3D is straightforward.

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