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The concept of resolution in the domain of rotations

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The metric of the $SO(3)$ group of rotations can be used to define the angular resolution of a function of rotations. The resolution is related to the degree of the highest representation present in the expansion of the function in terms of Wigner functions. The peculiar non-Euclidean metric of the rotation domain, however, implies that the terms which effectively contribute to the expansion vary through two-dimensional sections of the rotation domain and are within limiting resolution circles in two-dimensional reciprocal sections. This reconciles an economic sampling of the expansion with the acceleration provided by fast Fourier transform (FFT) techniques.

1. Introduction

The group of rotations $SO(3)$ is frequently the domain of definition of functions. Since rotations can be parametrized using triples of real numbers, the abstract $SO(3)$ domain is often represented as a subset of $\mathbb{R}^3$. Though the metric of $SO(3)$ is not equivalent to the standard Euclidean metric of $\mathbb{R}^3$ (Chevalley, 1946), an adequate parametrization of the rotations permits the $SO(3)$ domain to be partitioned into two-dimensional sections, in each one of which the rotation metric reduces to a Euclidean one (Burdina, 1971; Lattman, 1972).

The matrix elements of the irreducible representations of $SO(3)$, also known as Wigner functions, constitute a complete set of functions defined on $SO(3)$ (Wigner, 1959); real or complex functions of rotations can therefore be expanded in this basis. Also, by using the Euler parametrization of rotations, the Wigner expansion reduces to a Fourier series allowing faster calculations of the functions [see Trapani & Navaza (2006) and references therein]. In practical cases, the Wigner series includes matrices of representations up to a degree $\ell_{\max}$ related to a certain angular resolution of the expanded function.

In Fourier theory, the concept of resolution of a function defined on a Euclidean space is related to the maximum length of the corresponding reciprocal-space vectors. In this work, we have applied the same idea to functions defined on the Euclidean two-dimensional sections of the $SO(3)$ domain. We will show that $\ell_{\max}$ naturally defines a limiting circle – the angular resolution – in the corresponding two-dimensional reciprocal sections, outside which the Fourier coefficients are practically negligible. As a consequence, the set of Wigner functions up to a given degree $\ell_{\max}$ are not all necessary in order to faithfully represent a function of rotations at the corresponding angular resolution. This implies that any function of rotations may be evaluated on a more economic distortion-free sampling grid that satisfies the fast Fourier transform (FFT) prescriptions. This approach has been applied to the calculation of the self-rotation function of the IBDV VP2 subviral particle.

2. Background

In this section, we briefly recall some notions and results regarding the rotation group, its metric and the complete set of Wigner functions defined on the group.

A rotation $\mathbf{R}$ is an isometric transformation of the three-dimensional Euclidean space characterized by an invariant axis (the rotation axis) and a spin angle around the rotation axis. The set of all rotations having a common invariant point (the intersection of their rotation axes) constitutes an infinite group, $SO(3)$, isomorphic to the group of the 3 by 3 orthogonal matrices.

The notion of distance between rotations can be introduced in the rotation group. It can be demonstrated that the quantity

$$ds^2 = \mathrm{trace}(d\mathbf{R}d\mathbf{R}^+) = \sum_{i,j=1}^{3}(dR_{ij})^2 \qquad (1)$$

defines a metric on $SO(3)$, unique up to a multiplicative constant, which cannot be reduced to a Euclidean metric (Chevalley, 1946). This is a topological property of the group, independent of its parametrization. The length element ds, which corresponds to a rotation spin angle, is interpreted as the distance between the rotations $\mathbf{R}$ and $\mathbf{R} + d\mathbf{R}$.

There exists a countably infinite number of irreducible matrix representations of $SO(3)$. The matrix associated with a rotation $\mathbf{R}$ in the representation of degree ℓ has elements

$$\{D^{\ell}_{m,m'}(\mathbf{R})\}, \quad -\ell \le m,\ m' \le \ell.$$

ℓ takes integer values from 0 to ∞. Altogether, they constitute a complete set of orthogonal complex-valued functions defined on $SO(3)$. Therefore, any well behaved function $\mathcal{R}$,

$$\mathcal{R} : SO(3) \rightarrow \mathbb{C},$$

can be expressed as a series of $D^{\ell}_{m,m'}$,

$$\mathcal{R}(\mathbf{R}) = \sum_{\ell=0}^{\ell_{\max}} \sum_{m,m'=-\ell}^{\ell} C^{\ell}_{m,m'} D^{\ell}_{m,m'}(\mathbf{R}), \qquad (2)$$

where the $C^{\ell}_{m,m'}$ are the expansion coefficients. The summation limit $\ell_{\max}$, which should be ∞ in theory, is set to a convenient finite number in all practical cases. In the following, we will call 'Wigner expansion' the expansion in equation (2).

A rotation can be represented using a triple of real numbers. Several parametrizations can be established, each one of which leads to a different mapping of some subset of $\mathbb{R}^3$ onto the $SO(3)$ group. The Wigner expansion can be conveniently expressed in terms of Euler angles, while the $SO(3)$ metric is more faithfully represented using the Burdina–Lattman parametrization, as described below.

2.1. The Wigner expansion using Euler angles

According to Euler, a rotation $\mathbf{R}$ can be specified by three angles (α, β, γ) associated with an orthonormal frame $\{X, Y, Z\}$. We will follow the convention by which (α, β, γ) denotes a rotation of α about the Z axis, followed by a rotation of β about the rotated Y axis, and finally a rotation of γ about the rotated Z axis. In this way, a mapping from the parallelepiped

$$\{0 \le \alpha < 2\pi\} \times \{0 \le \beta \le \pi\} \times \{0 \le \gamma < 2\pi\} \subset \mathbb{R}^3$$

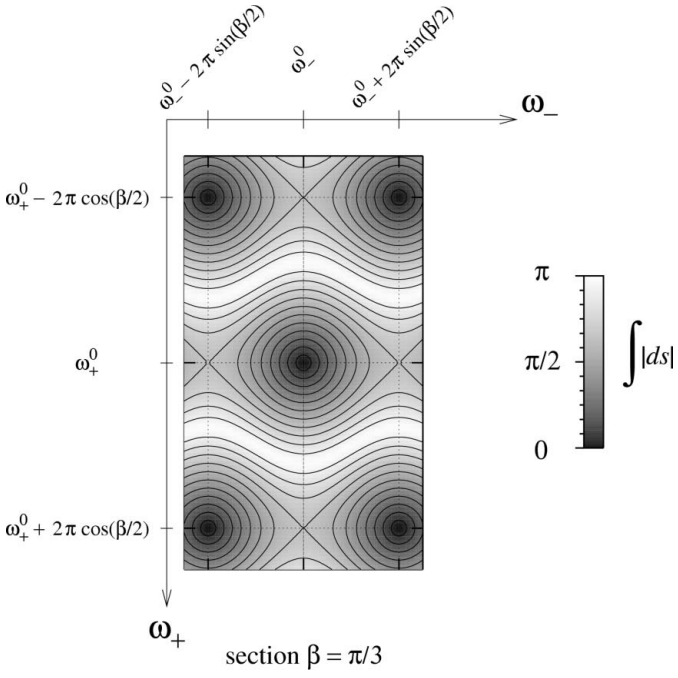

Figure 1
Two-dimensional plot of the angular distance from a reference rotation $(\omega^0_-, \beta, \omega^0_+)$ plotted as a function of the coordinates (ω_-, ω_+) at constant $\beta = \pi/3$. The angular distance values are represented using gray colour levels and equispaced contours. These differ from 'Euclidean' circumferences only at long distances from the reference point (ω^0_-, ω^0_+). Notice the periodic structure corresponding to a centred rectangular lattice with unit-cell lengths $\{4\pi\sin(\beta/2), 4\pi\cos(\beta/2)\}$. The plotted function is independent of the choice of (ω^0_-, ω^0_+). Similar plots, with different unit-cell parameters, are obtained for different β sections.

onto the $SO(3)$ group is established. This correspondence, though complete, is not exactly one-to-one. In fact, different values of α and γ may correspond to the same rotation when $\beta = 0$ or π:

$$\mathbf{R}(\alpha, 0, \gamma) = \mathbf{R}(\alpha + \gamma, 0, 0)$$
$$\mathbf{R}(\alpha, \pi, \gamma) = \mathbf{R}(\alpha - \gamma, \pi, 0).$$

It is sometimes convenient to extend the Euler domain to the entire $\mathbb{R}^3$. In this case, the correspondence between Euler angles and rotations is 2π-periodic in α, β and γ and possesses a diagonal glide plane of symmetry which results from the equivalence

$$\mathbf{R}(\alpha, \beta, \gamma) = \mathbf{R}(\alpha + \pi, -\beta, \gamma + \pi).$$

The rotation length element [equation (1)] in the Euler domain becomes

$$ds^2 = d\alpha^2 + 2\cos(\beta) d\alpha d\gamma + d\gamma^2 + d\beta^2. \qquad (3)$$

The Wigner functions take a simple form in Euler coordinates:

$$D^{\ell}_{m,m'}(\alpha, \beta, \gamma) = d^{\ell}_{m,m'}(\beta) \exp[i(m\alpha + m'\gamma)], \qquad (4)$$

where the $d^{\ell}_{m,m'}(\beta)$, known as the reduced Wigner functions, are real trigonometric polynomials that can be represented by a Fourier summation with maximum oscillation frequency $\ell/2\pi$.

According to equation (4), the Wigner expansion [equation (2)] can be reduced, for each β section, to a simple Fourier expansion in α and γ:

$$\mathcal{R}(\alpha, \beta, \gamma) = \sum_{m,m'=-\ell_{\max}}^{\ell_{\max}} S_{m,m'}(\beta) \exp[i(m\alpha + m'\gamma)], \qquad (5)$$

where the two-dimensional Fourier coefficients $S_{m,m'}(\beta)$ are given by

$$S_{m,m'}(\beta) = \sum_{\ell=\max(|m|,|m'|)}^{\ell_{\max}} C^{\ell}_{m,m'} d^{\ell}_{m,m'}(\beta). \qquad (6)$$

Functions of rotations are frequently evaluated using equation (5) as it allows the rapid sampling of β sections by means of FFT algorithms (Crowther, 1972). When the $d^{\ell}_{m,m'}(\beta)$ are represented by a Fourier summation then the whole three-dimensional angular domain can be assessed by FFT (Kovacs & Wriggers, 2002).

2.2. The $SO(3)$ metric expressed in terms of the Burdina–Lattman parameters

Although the $SO(3)$ metric cannot be reduced to a Euclidean one in three dimensions, it is possible to do so for two-dimensional sections (Burdina, 1971; Lattman, 1972). Indeed, for fixed β, the transformations

$$\begin{bmatrix} \theta_- \\ \theta_+ \end{bmatrix} = 1/2 \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \alpha \\ \gamma \end{bmatrix} \qquad (7)$$

$$\begin{bmatrix} \omega_- \\ \omega_+ \end{bmatrix} = \begin{bmatrix} 2\sin(\beta/2) & 0 \\ 0 & 2\cos(\beta/2) \end{bmatrix} \begin{bmatrix} \theta_- \\ \theta_+ \end{bmatrix} \qquad (8)$$

reduce equation (3) to

$$ds^2 = d\omega_-^2 + d\omega_+^2. \quad (9)$$

Equation (7) orthogonalizes the Euler (α, γ) angles, while the resulting $\theta_\mp$ coordinates are normalized by equation (8). The $\omega_\mp$ parametrization permits a distortion-free graphical representation of $SO(3)$ β sections (see Fig. 1). A set of points regularly spaced in these variables will correspond to regular distances between points. The $\omega_\mp$ parametrization has the periodicity of a two-dimensional centred rectangular lattice with unit-cell parameters $\{4\pi \sin(\beta/2), 4\pi \cos(\beta/2)\}$. Notice that these are β-dependent and that for β equal to 0 or π the sections reduce to lines.

3. The concept of resolution in $SO(3)$

The concept of resolution of a function is related to the maximal frequency present in its Fourier spectrum. In crystallography, the resolution is commonly expressed as the inverse of the maximum reciprocal-vector length. In direct space, this corresponds approximately to the smallest possible distance between two points of oscillation of the function. This relationship results from interpreting the argument of the complex exponential in the Fourier expansion as a scalar product. It is therefore meaningful only if the direct-space metric is Euclidean with respect to the coordinates used in the Fourier expansion.

In the domain of rotations, the notion of 'angular resolution' of a function can be associated with the upper limit $\ell_{\max}$ in its Wigner expansion [equation (2)]. It is related to the maximum Fourier frequency of the expansion, which is $\ell_{\max}/2\pi$ for each one of the three Euler variables [equation (4)]. These Fourier frequencies cannot be directly related, in the way described above, to an angular distance in $SO(3)$. Nevertheless, they can in two-dimensional β sections, where the $SO(3)$ metric is equivalent to a Euclidean one.

In the following, we will apply the concepts of distance and resolution to direct and reciprocal β sections of the $SO(3)$ domain. We will show that standard FFT requirements for a uniform sampling [in terms of the $SO(3)$ distance given by equation (1)] imply that some terms in a Wigner expansion must have vanishingly small contributions.

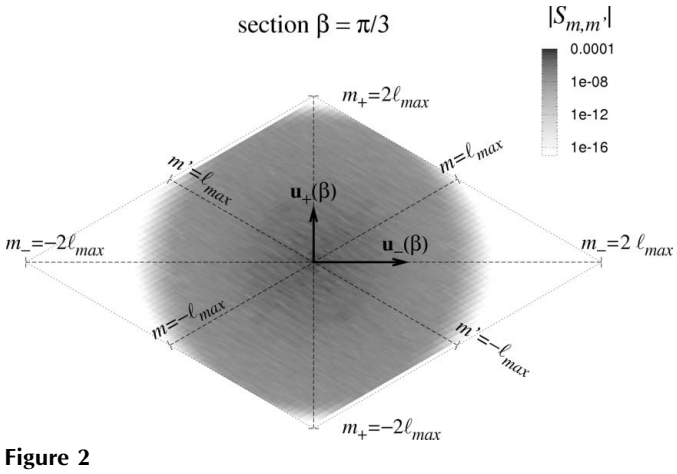

Figure 2
Plot of one β section of the $S_{m,m'}(\beta)$ self-rotation coefficients for the IBDV VP2 subviral particle.

3.1. Direct and reciprocal vectors in β sections

The argument of the exponential in a two-dimensional Wigner expansion [equation (5)] may be interpreted as a scalar product between two vectors. One of them is associated with the rotation of fixed β angle, with components (α, γ) in a non-orthonormal basis [because of equation (3)], the direct basis. The other one has components (m, m') in another non-orthonormal basis, the reciprocal basis. After orthogonalizing by equation (7) and defining

$$m_\mp = m \mp m', \quad (10)$$

we obtain, for the argument of the imaginary exponential,

$$m\alpha + m'\gamma = m_-\theta_- + m_+\theta_+. \quad (11)$$

The rotation now has components (θ_-, θ_+) in an orthogonal basis with parameters $\{2\sin(\beta/2), 2\cos(\beta/2)\}$, and the reciprocal vector has components (m_-, m_+), analogous to Miller indexes, in the associated orthogonal reciprocal basis. As the sum of the $m_\mp$ indexes is always even, the reciprocal vectors correspond to a rectangular centred lattice. This implies that only half of the direct cell is an independent domain. It can be chosen as

$$0 \le \theta_- \le \pi$$
$$0 \le \theta_+ \le 2\pi$$

or the equivalent one obtained by interchanging θ_- and θ_+. The length of the reciprocal vector of coordinates (m_-, m_+) is now given by

$$\left[\left(\frac{m_-}{2\sin(\beta/2)}\right)^2 + \left(\frac{m_+}{2\cos(\beta/2)}\right)^2\right]^{1/2}. \quad (12)$$

Notice that, for m_- (or m_+) $\neq 0$, the reciprocal vector length tends to infinity as $\beta \to 0$ (or π).

3.2. FFT-based *versus* metric based sampling

The sampling of β sections of the Wigner expansion of a function $\mathcal{R}$ is dictated by the standard FFT requirements: the number N of sampling points along a coordinate and the highest index M of the Fourier coefficients that represent $\mathcal{R}$ along the same coordinate must satisfy (see Brillouin, 1956)

$$N \ge 2M + 1. \quad (13)$$

This inequality may be used in two different ways. If the maximum index M of the Fourier series is known then we can determine the minimum number of equidistant sampling points needed to recover $\mathcal{R}$ from the samples. Conversely, if we know that the function can be recovered from N samples, then we know that the maximum index of the Fourier series that represents $\mathcal{R}$ cannot be greater than $(N-1)/2$. According to equation (5), the indices m and m' take values in the interval

$$-\ell_{\max} \le m, m' \le \ell_{\max} \quad (14)$$

independently of β. The number of sampling points in α and γ (N_α and N_γ, respectively) must therefore satisfy

$$\begin{aligned} N_\alpha &\geq 2\ell_{\max} + 1 \\ N_\gamma &\geq 2\ell_{\max} + 1. \end{aligned} \tag{15}$$

On the other hand, in terms of $\theta_\mp$, any β section has period 2π and has Fourier coefficients with indexes $m_\mp$ in the interval

$$-2\ell_{\max} \leq m_\mp \leq 2\ell_{\max} \tag{16}$$

so that the number of sampling points in $\theta_\mp$ must satisfy

$$N_{\theta_\mp} \geq 4\ell_{\max} + 1. \tag{17}$$

Let us now use the metric ds^2 in order to define a set of sampling points for $\mathcal{R}$, which we choose as a Cartesian grid of approximately equally spaced $\omega_\mp$ points. The number of sampling points along $\omega_\mp$ is defined in terms of a distance Δ, in radians, as

$$\begin{aligned} N_-(\beta) &= [\sin(\beta/2)4\pi/\Delta] \\ N_+(\beta) &= [\cos(\beta/2)4\pi/\Delta], \end{aligned} \tag{18}$$

where $[x]$ denotes the smallest positive integer greater than x, from which the actual spacings

$$\begin{aligned} \Delta_-(\beta) &= \sin(\beta/2)4\pi/N_-(\beta) \\ \Delta_+(\beta) &= \cos(\beta/2)4\pi/N_+(\beta) \end{aligned} \tag{19}$$

are determined. The spacings $\Delta_-(\beta)$ and $\Delta_+(\beta)$ usually differ but remain close to the original distance Δ. For the sampling based on the distance between rotations, the left-hand member of equation (13) varies monotonically between $4\pi/\Delta$ and unity [see equation (18)], while the right-hand member is always $4\ell_{\max} + 1$ [see equation (17)] irrespective of the β section. Thus, either $\mathcal{R}$ is not faithfully represented by our samples or the coefficients $S_{m,m'}(\beta)$ go to zero for indices that do not satisfy the sampling criterion. We have investigated this problem numerically.

3.3. The limiting resolution circles

The crystallographic self-rotation function (Crowther, 1972; Navaza, 1993) of the IBDV VP2 subviral particle (Coulibaly *et al.*, 2005) has been calculated using data up to 5 Å resolution and an integration radius of 130 Å, resulting in $\ell_{\max} = 154$.

The amplitudes of the $S_{m,m'}(\beta)$ coefficients for $\beta = \pi/3$ are plotted in Fig. 2. In the plot, the reciprocal β section and both the $\{m, m'\}$ and $\{m_-, m_+\}$ systems of coordinates are drawn in order to faithfully represent distances in reciprocal space. The reciprocal basis vectors

$$\begin{aligned} \mathbf{u}_- &\equiv (m_- = 1, m_+ = 0) \\ \mathbf{u}_+ &\equiv (m_- = 0, m_+ = 1) \end{aligned}$$

are therefore represented as orthogonal arrows with relative lengths $[2\sin(\beta/2)]^{-1}$ and $[2\cos(\beta/2)]^{-1}$, respectively. In Fig. 3, the $S_{m,m'}(\beta)$ amplitudes are plotted *versus* the reciprocal vector length for different β sections.

All the non-null $S_{m,m'}$ coefficients were found inside approximately circular regions – which we will call the limiting resolution circles – that do not fill completely the reciprocal β sections. The radius of these circles represents the maximum allowed reciprocal vector length. As expected, this value is constant throughout the different β sections (see Fig. 3). An estimation of the radius can be made by considering the section $\beta = 0$, where the rotation function is independent of θ_- and, as a consequence, the corresponding Fourier frequencies with index $m_- \neq 0$ must be null [this can also be derived from equation (6) using the identity $d^\ell_{m,m'}(0) = \delta_{m,m'}$]. In that section, only the $(0, m_+)$ reciprocal line can contribute to the rotation function, and the longest vectors on this line have moduli equal to

$$2\ell_{\max}/[2\cos(0)] = \ell_{\max}.$$

The same conclusion can be drawn by considering the section $\beta = \pi$ and the line $(m_-, 0)$. For a general β section, therefore, the $S_{m,m'}(\beta)$ coefficients are expected to effectively contribute to the rotation function only if

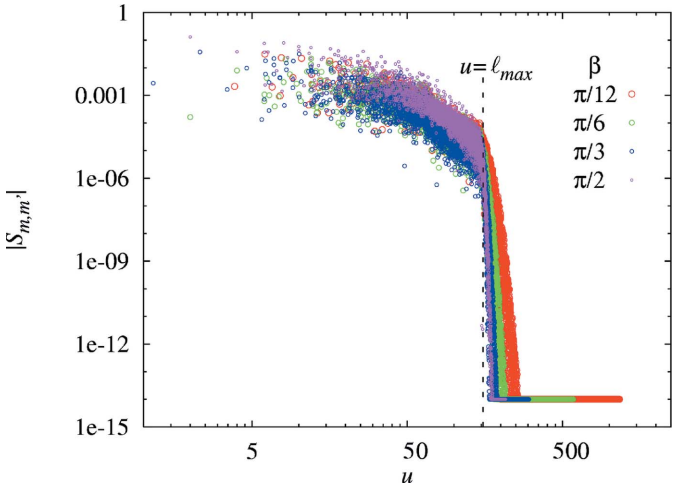

Figure 3
Plot of the IBDV VP2 $S_{m,m'}(\beta)$ amplitudes *versus* the distance from the reciprocal-space origin.

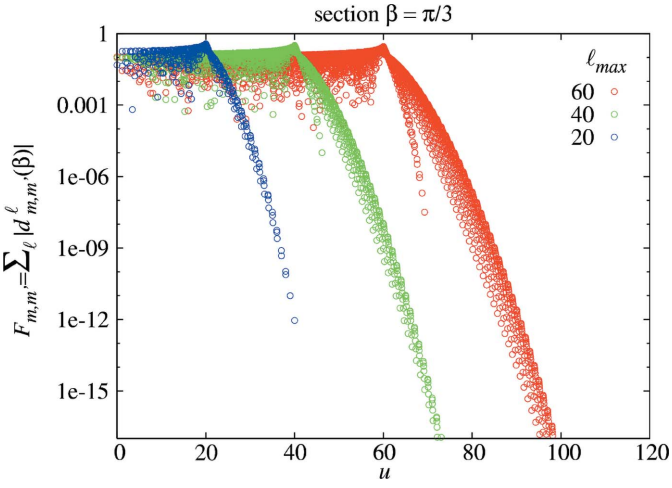

Figure 4
Plot of the $F_{m,m'}$ coefficients *versus* the distance from the reciprocal-space origin.

$$\left(\frac{m_-}{2\sin(\beta/2)}\right)^2 + \left(\frac{m_+}{2\cos(\beta/2)}\right)^2 \leq \ell_{\max}^2. \qquad (20)$$

Notice that, when the indices (m, m') or (m_-, m_+) are plotted on a regular orthogonal grid, the limiting circle becomes an ellipse if $\beta \neq \pi/2$ and tends to a segment as $\beta \rightarrow 0$ or π.

The existence of a limiting resolution circle of radius $\ell_{\max}$ is a built-in feature of the reduced Wigner functions themselves, independently of any experimental data [*i.e.* the $C^{\ell}_{m,m'}$ coefficients in equation (6)]. Indeed, the quantity

$$F_{m,m'} = \sum_{\ell=\max(|m|,|m'|)}^{\ell_{\max}} |d^{\ell}_{m,m'}(\beta)| \qquad (21)$$

decays rapidly to zero beyond the above radius (Fig. 4).

4. Computing Wigner expansions

In crystallography, the maximum Miller index in any direction is obtained by dividing the corresponding cell parameter by the resolution of the Fourier coefficients. In the two-dimensional angular domain, we have seen that the length of the longest reciprocal vector included in the Wigner expansion, *i.e.* the inverse of the resolution, is $\ell_{\max}$, so that the highest indices are

$$\begin{aligned} M_-(\beta) &= 2\sin(\beta/2)\ell_{\max} \\ M_+(\beta) &= 2\cos(\beta/2)\ell_{\max} \end{aligned} \qquad (22)$$

and the minimum numbers of sampling points, $N_{\mp}(\beta)$, are given by equation (13). Taking into account that only half of the rectangular centred cell has to be considered, the number of sampling points per section is

$$N_-(\beta)N_+(\beta)/2 \approx (2\ell_{\max})^2 \sin(\beta). \qquad (23)$$

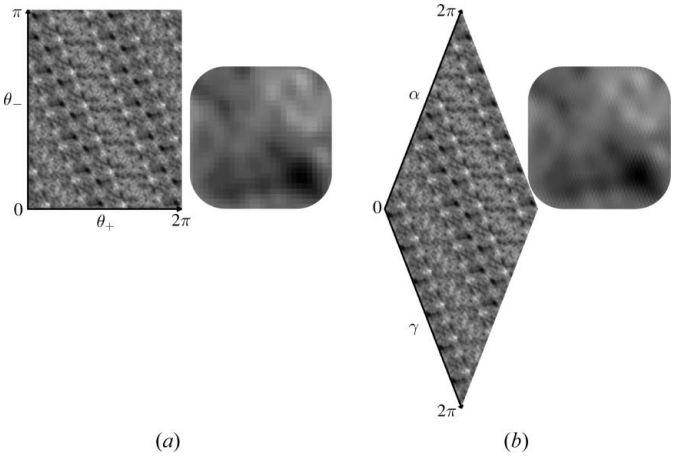

Figure 5
Plot of the $\beta = 137.8^\circ$ section of the self-rotation function corresponding to the IBDV VP2 subviral particle, evaluated by FFT techniques. (*a*) Metric based sampling; (*b*) classical sampling. A detail of the two plots is also shown. The extra periodicity along γ is due to a crystal sixfold axis parallel to the Z axis.

On the other hand, the number of sampling points corresponding to the classical prescription is [see equation (15)]

$$N_\alpha N_\gamma \approx (2\ell_{\max})^2 \qquad (24)$$

for any β section. Thus, there are $\sin(\beta)$ times fewer points with the sampling based on the indices (22).

In summary, the results of the preceding section allow us to sample β sections of any function of rotations at fewer points while computing it by FFT techniques, and recover distortion-free sections, which facilitates peak-searching procedures.

In Fig. 5, we show two plots of the same section ($\beta = 137.8^\circ$) of the IBDV VP2 self-rotation function computed by FFT using, respectively, the classical sampling (96100 points) and the metric based sampling (64736 points). The (α, γ) points are represented on an oblique grid in order to permit a direct comparison with the metric based plot. As expected, the two plots display the same features.

5. Conclusions

The angular resolution of a function $\mathcal{R}$ defined on the group $SO(3)$ of three-dimensional rotations, if correctly expressed in terms of the $SO(3)$ metric as a rotational distance Δ (in radians), corresponds to an upper limit $\ell_{\max} = \pi/\Delta$ of the Wigner expansion of the function $\mathcal{R}$. The peculiar non-Euclidean metric of the rotation domain, however, implies that not all the terms of degree less than $\ell_{\max}$ contribute to the Wigner expansion. Those which effectively contribute vary through two-dimensional sections of the rotation domain and are determined by limiting resolution circles in the two-dimensional reciprocal sections. As a consequence, β sections of any function of rotations may be evaluated by means of FFT techniques on equally spaced distortion-free grids. This reconciles the acceleration of the fast rotation function (Crowther, 1972) with the metric based sampling (Burdina, 1971; Lattman, 1972).

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References

Brillouin, L. (1956). *Science and Information Theory*, pp. 78–79. New York: Academic Press.
Burdina, V. I. (1971). *Sov. Phys. Crystallogr.* **15**, 545–550.
Chevalley, C. (1946). *Theory of Lie Groups.* Princeton University Press.
Coulibaly, F., Chevalier, C., Gutsche, I., Pous, J., Navaza, J., Delmas, B. & Rey, F. A. (2005). *Cell*, **120**, 761–772.
Crowther, R. A. (1972). *The Molecular Replacement Method*, edited by M. G. Rossmann, pp. 173–178. New York: Gordon and Breach.
Kovacs, J. A. & Wriggers, W. (2002). *Acta Cryst.* D**58**, 1282–1286.
Lattman, E. E. (1972). *Acta Cryst.* B**28**, 1065–1068.
Navaza, J. (1993). *Acta Cryst.* D**49**, 588–591.
Trapani, S. & Navaza, J. (2006). *Acta Cryst.* A**62**, 262–269.
Wigner, E. P. (1959). *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra.* New York: Academic Press.