6 Central symmetry of the squared modulus of the Fourier transform and the Friedel law

The diffraction patterns of the Fraunhofer type — both in optics and in structure analysis — frequently attract one’s attention by their beauty (Figure 1). Their grace may issue from their symmetry. Very often the patterns have central symmetry, even in the case when the object which originated the diffraction does not boast central symmetry (Figure 2). This fact is remarkable not only from an aesthetic point of view but it has also considerable practical consequences. In structure analysis it even bears a special name — the Friedel law. It will be proved in this chapter that the diffraction patterns display the central symmetry whenever the function \( f(\vec{x}) \) characterizing the specimen is real.

![Figure 1: The Fraunhofer diffraction pattern from the system of eight circular openings in an opaque foil regularly distributed along the circle whose radius is 20 times as large as the radius of the openings.](image)

6.1 Central symmetry of the Fourier transform

The necessary and sufficient condition for the central symmetry of the Fourier transform (i.e. not only of the modulus of the Fourier transform) is expressed by the following theorem:

**Theorem:** Let the Fourier integral of the function \( f(\vec{x}) \) exist. The function \( f(\vec{x}) \) has the central symmetry (antisymmetry) if and only if its Fourier transform \( F(\vec{X}) \) has the central symmetry (antisymmetry). Expressed by formula

\[
f(\vec{x}) = \pm f(-\vec{x}) \iff F(\vec{X}) = \pm F(-\vec{X}).
\]

(1)
Figure 2: The Fresnel portrait adorning the front-page of his collected papers (*Œuvres complètes d’Augustin Fresnel, tome 1*. Imprimerie impériale, Paris 1866) and the Fraunhofer diffraction pattern from the negative of the portrait pen–and–ink drawing.

**Proof:** Let us suppose that the function $f(\vec{x})$ has central symmetry, i.e. $f(\vec{x}) = f(-\vec{x})$. We take advantage of that property in the definition integral of the Fourier transform $F(\vec{X})$:

$$
F(\vec{X}) = A^N \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(\vec{x}) \exp(-ik \vec{x} \cdot \vec{X}) d^N \vec{x} = 
$$

$$
= A^N \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(-\vec{x}) \exp(-ik \vec{x} \cdot \vec{X}) d^N \vec{x}.
$$

The substitution $\vec{x}' = -\vec{x}$ leads to

$$
F(\vec{X}) = A^N \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(\vec{x}') \exp(-ik \vec{x}' \cdot (-\vec{X})) d^N \vec{x}' = 
$$

$$
= F(-\vec{X})
$$

and the statement of the theorem is proved in one direction. To prove the statement in the opposite direction we proceed in the similar way. And in the similar way we prove the theorem also in the case of antisymmetry, i.e. $f(\vec{x}) = -f(-\vec{x})$.

The proved theorem does not explain why the diffraction patterns have the central symmetry even if the objects from which the diffraction comes from does not possess the central symmetry. To advance in this direction it is convenient to become aware of two facts:

(i) For the central symmetry of the diffraction pattern it is not necessary to require the central symmetry (or antisymmetry) of the Fourier transform $F(\vec{X})$. The central symmetry of its modulus $|F(\vec{X})|$ is sufficient.
The functions \( f(\vec{x}) \) characterizing the diffraction specimen are often real. As examples may serve empty openings in an opaque screen in optical diffraction, electron density in X-ray diffraction, etc. Therefore, it is rewarding to pursue the Fourier transform of real functions.

6.2 The Fourier transform of real functions

**Theorem:** Let the Fourier integral of the function \( f(\vec{x}) \) exist. The function \( f(\vec{x}) \) is real if and only if its Fourier transform \( F(\vec{X}) \) is hermitian. Expressed by symbols

\[
f(\vec{x}) = f^*(\vec{x}) \quad \iff \quad F(\vec{X}) = F^*(-\vec{X}).
\]  

**Proof:**

(i) We suppose that the function \( f(\vec{x}) \) is real, i.e. \( f(\vec{x}) = f^*(\vec{x}) \) and employ this property in the definition integral of the Fourier transform:

\[
F(\vec{X}) = A \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(\vec{x}) \exp(-ik\vec{x} \cdot \vec{X}) d^n\vec{x} =
\]

\[
= A \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f^*(\vec{x}) \exp(i k \vec{x} \cdot (-\vec{X})) d^n\vec{x} = F^*(-\vec{X}).
\]

In this way the theorem is proved in one direction.

(ii) Now we suppose that the Fourier transform \( F(\vec{X}) \) is hermitian, i.e. \( F(\vec{X}) = F^*(-\vec{X}) \) and employ it in the definition integral of the inverse Fourier transform:

\[
f(\vec{x}) = B \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} F(\vec{X}) \exp(ik\vec{x} \cdot \vec{X}) d^n\vec{X} =
\]

\[
= B \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} F^*(-\vec{X}) \exp(i k \vec{x} \cdot \vec{X}) d^n\vec{X}.
\]

If we substitute \( \vec{X}' = -\vec{X} \) in the last integral the theorem is proved in the opposite direction:

\[
f(\vec{x}) = B \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} F^*(\vec{X}') \exp(-ik\vec{x} \cdot \vec{X}') d^n\vec{X}' = f^*(\vec{x}).
\]

6.2.1 The Friedel law

Theorem 6.2(1) evidently has the following consequence:

If the function \( f(\vec{x}) \) is real the squared modulus of its Fourier transform exhibits the central symmetry. Expressed by formula

\[
f(\vec{x}) = f^*(\vec{x}) \quad \implies \quad F(\vec{X}) F^*(\vec{X}) = F^*(-\vec{X}) F(-\vec{X}).
\]  

The statement (2) — restricted to a special case of periodic functions — bears the name Friedel law (see e.g. [1], [2], p. 33, [3], pp. 40, 47, [4], p. 278) in crystallography. We will make a remark about it at the end of chapter 6.

Now we will keep a formal aspect of the statement and emphasize that the statement (2) provides only sufficient condition for the central symmetry of the squared modulus of the Fourier transform but not the necessary one. Another sufficient condition is e.g. the central symmetry or antisymmetry of the function \( f(\vec{x}) \). It is difficult (see [5]), if possible at all, to find the necessary and sufficient condition for the central symmetry of the modulus of the Fourier transform.
6.2.2 The Fourier transform of real functions with central symmetry or antisymmetry

Further useful consequences of theorems 6.1(1) and 6.2(1) are statements:

The function \( f(\vec{x}) \) is real and centrosymmetric if and only if its Fourier transform \( F(\vec{X}) \) is real and centrosymmetric. Written as a formula:

\[
\begin{align*}
  f(\vec{x}) &= f^*(\vec{x}) = f(-\vec{x}) \iff F(\vec{X}) = F^*(\vec{X}) = F(-\vec{X}).
\end{align*}
\]

(3)

The function \( f(\vec{x}) \) is real and antisymmetric if and only if its Fourier transform is purely imaginary and antisymmetric. Written as a formula:

\[
\begin{align*}
  f(\vec{x}) &= f^*(\vec{x}) = -f(-\vec{x}) \iff F(\vec{X}) = -F(-\vec{X}) = -F^*(\vec{X}).
\end{align*}
\]

(4)

Proofs of these statements follow immediately from theorems 6.1(1) and 6.2(1) and we dismiss them. Rather we point out that the statements (3) and (4) may serve as useful tests of calculations. We have found in examples of the previous chapters that the Fourier transforms of real and even functions are real and even (e.g., the Gaussian function, \( \text{rect}(x) \), \( \text{tri}(x) \), \( \cos ax \), and integer positive powers of \( \cos ax \), even and positive powers of \( \sin ax \), and so on). Also we have seen that the Fourier transform of odd and real functions are odd and purely imaginary functions (e.g., \( \text{sgn}(x) \), \( \sin ax \), and odd positive powers of \( \sin ax \)).

6.2.3 Loci of zero intensity in the Fraunhofer diffraction patterns

The Fraunhofer diffraction patterns from diffraction filters with a real transmission function \( f(x_1, x_2) \) are then always centrosymmetric irrespective of whether the transmission function itself is centrosymmetric. Hence, a question arises whether there are indications which allow us to distinguish between diffraction patterns from centrosymmetric filters and those from filters without central symmetry. Some hints in these decisions provide loci of zero intensity in the Fraunhofer diffraction patterns.

(i) If the transmission function \( f(x_1, x_2) \) is real and centrosymmetric, then according to (3), also its Fourier transform \( F(X_1, X_2) \) is real (and centrosymmetric). The intensity

\[
\begin{align*}
  I(X_1, X_2) = F(X_1, X_2)F^*(X_1, X_2) = F^2(X_1, X_2).
\end{align*}
\]

is then given by the squared Fourier transform and the loci of zero intensity are determined by the single condition

\[
\begin{align*}
  F(X_1, X_2) = 0.
\end{align*}
\]

(5)

This condition usually specifies a system of lines in the plane \( X_1, X_2 \). Hence, we may expect that the Fraunhofer diffraction patterns from centrosymmetric filters with a real transmission function have lines of zero intensity.

(ii) If, however, the real transmission function \( f(x_1, x_2) \) does not possess central symmetry, we may apply theorem (2) only, so that the intensity is

\[
\begin{align*}
  I(X_1, X_2) = F(X_1, X_2)F^*(X_1, X_2) = (\text{Re} F(X_1, X_2))^2 + (\text{Im} F(X_1, X_2))^2.
\end{align*}
\]

The loci of zero intensity are now determined by two conditions

\[
\begin{align*}
  \text{Re} F(X_1, X_2) = 0, \quad \text{Im} F(X_1, X_2) = 0.
\end{align*}
\]

(6)

Each of these conditions specifies a system of lines in the plane \( X_1, X_2 \). The two systems are independent and have possibly common points of intersection. Hence, we may expect that loci of zero intensity in the Fraunhofer diffraction patterns from filters with real transmission function
but without central symmetry are mostly points. (The uncertainty in formulation is here intentional. There are exceptions, namely when the filter consists from identical centrosymmetric objects arranged in such a way that they have mutually the same orientation, but the arrangement as a whole does not have central symmetry. (As an example it may serve a system of odd number of circular openings in an opaque screen situated at the vertices of regular polygon.) The intensity distribution is then characterized by the product of two functions \( I_1, I_2 \); one of them, \( I_1 \), characterizes one of the identical objects, and the other, \( I_2 \), is specified just by mutual positions of the objects (cf. Section 9.2 below). Such a diffraction pattern has both points of zero intensity originated in the function \( I_2 \) (cf. (6)) and lines of zero intensity corresponding to the function \( I_1 \) (cf. (5)). These lines of zero intensity are usually distinct, as they are "broad" in comparison with the more sharply painted details of the diffraction pattern.)

Hence, the Fraunhofer diffraction patterns from filters with a real centrosymmetric transmission function have lines of zero intensity and exhibit therefore "higher contrast" than diffraction patterns from filters without the center of symmetry which have usually just points of zero intensity. Figures 3 to 5 illustrate this fact.

Figure 3: The Fraunhofer diffraction from windmill with three–fold and six–fold symmetry.

6.2.4 Imperfect centrosymmetry of the Fraunhofer diffraction patterns

To get the Fraunhofer diffraction patterns with perfect central symmetry from filters which do not possess centrosymmetry it is necessary to make sure that the transmission function is real. The best is to work
Figure 4: The Fraunhofer diffraction from triagonal and hexagonal aperture.

Figure 5: The Fraunhofer diffraction from forty eight and forty nine circular apertures regularly distributed along the circle with the twenty times larger diameter.

with empty opening in an opaque screen (in a metal foil, for example). The filters consisting from from photographic emulsion usually do not have a real transmission function. The places with different density have also different thickness of the gelatine. This causes differences in phase shifts of the transmitted light, so that the transmission function is then complex. This happens also with fine photographic materials (holographic plates) and with filters which should have only two levels of photographic density. The diffraction patterns then are not centrosymmetric (see Figure 6). It is rather demanding to ensure the
central symmetry of the diffraction patterns from filters with photographic emulsion. (For example, it is possible to immerse such a filter in oil between two plan–parallel plates.)

The diffraction patterns without central symmetry arise also in X–ray diffraction patterns from crystals. It is related with different phase shifts by planes \((h k l)\) and \((\bar{h} \bar{k} \bar{l})\) in polar structures (see e.g. [2], p. 33).

References


6 CENTRAL SYMMETRY OF THE SQUARED MODULUS