Fourier, Gauss, Fraunhofer, Porod and the Shape from Moments Problem

Gregg M. Gallatin
National Institute of Standards and Technology
Center for Nanoscale Science and Technology
Gaithersburg, MD
gregg.gallatin@nist.gov

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Abstract

We show how the Fourier transform of a shape in any number of dimensions can be simplified using Gauss’s law and evaluated explicitly for polygons in two dimensions, polyhedra three dimensions, etc. We also show how this combination of Fourier and Gauss can be related to numerous classical problems in physics and mathematics. Examples include Fraunhofer diffraction patterns, Porods law, Hopfs Umlaufsatz, the isoperimetric inequality and Didos problem. We also use this approach to provide an alternative derivation of Davis’s extension of the Motzkin-Schoenberg formula to polygons in the complex plane.

1 Introduction

A shape can be defined mathematically in many ways. Here we consider defining it by a function that has the value unity inside the shape and zero outside the shape. Only simply connected orientable [1] shapes will be considered. The Fourier transform of a shape defined in this way has interesting applications and connections to many areas of physics and mathematics. For example, in physical optics the Fourier transform of the shape of an aperture or opening in an opaque screen yields the Fraunhofer or far field diffraction pattern that is generated when light passes through the aperture [2]. In X-ray scattering, the Fourier transform of a volumetric shape in three dimensions reduces in the appropriate limit to Porods law [3]. From a probabilistic point of view the Fourier transform of a shape properly normalized can be considered as the characteristic function or moment generating function of the shape. Hence the Fourier transform of the shape is intimately related to the moments of the shape and hence to the ”shape from moments problem”, which has been studied recently for polygons by Golub, Milanfar and others [4] [5] and is related to the overall problem of pattern recognition. The Fourier transform of an area bounded by a smooth curve or a polygon in the plane can be shown to imply Hopf’s Umlaufsatz [6], which states that the tangent vector (or the normal vector or any linear combination thereof) to a smooth or piecewise smooth closed orientable simply connected curve in the plane rotates by ±2π as it goes completely around the curve. The +/− signs correspond to counterclockwise/clockwise rotation. This seemingly obvious geometrical fact is rather subtle to prove [6] We also use this formula to derive the planar version
Stokes law [7] and to show that a circle maximizes the area for a given perimeter length which is known as the isoperimetric inequality [6] [8]. Finally there is the famous problem faced by Dido, Queen of Carthage, which was to determine what shape open curve of a given length encloses the maximum area when its endpoints are connected by a straight line with an arbitrary length [9]. Here I show how combining the Fourier transform with Gauss’s Law provides a central platform for relating and solving all these problems.

As an aside, the Fourier transform is just one of many techniques that are used for shape discrimination [10]. This problem is both mathematically interesting, and, given the ubiquity of digital data bases, technologically important. Here our specific interest is in the relation of the Fourier transform of a shape to its moments and to the problems mentioned above. This is related to, but generally different from, the issues concerned with using Fourier transforms explicitly for shape discrimination in digital data bases and we will not discuss this aspect further.

The paper is organized as follows. In the Section 2, Gauss’s Law is used to rewrite the Fourier transform of a $D$ dimensional volume as the surface integral over the $D-1$ surface of that volume. This surface integral can then be evaluated exactly for polygons in two dimensions, polyhedra in three dimensions, etc. In particular in two dimensions this then provides an explicit relation between the vertices of a polygon and its moments. This section also discusses how this result is related to the isoperimetric inequality, Dido’s problem and Hopf’s Umlaufsatz. Finally we show how the combination of Fourier and Gauss provides an alternative derivation of a famous result of Davis concerning the integral of an analytic function over a polygon in the complex plane [11] [4]. Section 3 briefly discusses how the solution for two dimensional polyhedra appears when Fourier transforming three dimensional polyhedrons before showing how the surface integral form of the three dimensional Fourier transform can be used to derive not only the standard Porod’s law [3] for X-ray scattering from spherical particles but also the extension of this law to anisotropic particles. This extension has been discussed recently in a series of papers by Ciccariello and colleagues [12]. The derivation presented here is somewhat more direct than that used by Ciccariello and colleagues.

2 Fourier and Gauss

For generality we begin in $D$ dimensions but will rapidly particularize to 2 and 3 dimensions. Define a shape, in $D$ dimensions, by the function $\theta_V(\vec{x})$ where $\theta_V(\vec{x}) = 1$ for $\vec{x} = (x_1, x_2, \cdots, x_D)$ inside $V$ and 0 for $\vec{x}$ outside. This is known in certain circles as an indicator function [13]. Here we take $x_i$ for $i = 1, 2, \cdots, D$ to be Cartesian coordinates. The (normalized) moments $\langle x_1^{p_1} \cdots x_D^{p_D} \rangle$ of the shape are then given by

$$\langle x_1^{p_1} \cdots x_D^{p_D} \rangle = \frac{1}{v} \int d^Dx \theta_V(\vec{x}) x_1^{p_1} \cdots x_D^{p_D} \equiv \frac{1}{v} \int_V d^Dx x_1^{p_1} \cdots x_D^{p_D}$$

where $\int_V = \int \theta_V$ indicates integration over the shape, $v = \int d^Dx \theta_V(\vec{x})$ is the finite volume of the shape and $p_i = 0, 1, 2, 3, \cdots$ for each $i$. The symbols $V$ and $v$ are used to distinguish between the shape itself and its volume as a numerical value. Also the terms ”volume” and ”surface” are used generically and should be understood to refer to a $D$ dimensional submanifold in $D$ dimensions and to its $D-1$ dimensional boundary, respectively.

Note that $\frac{1}{v} \theta_V(\vec{x})$ can be thought of as a probability density for $\vec{x}$ to be inside the shape. The characteristic function or moment generating function $\bar{\phi}(\vec{\beta})$ is then given by the Fourier transform
\[ \theta_V(\vec{x})/v, \text{ i.e.,} \]

\[ \bar{\phi}(\vec{\beta}) = \frac{1}{v} \int_V d^Dx \theta_V(\vec{x}) e^{i\vec{\beta} \cdot \vec{x}} \]  

(2)

with \( \vec{\beta} \cdot \vec{x} = \sum_{i=1}^D \beta_i x_i \equiv \beta_i x_i \). (Unless noted otherwise the Einstein summation convention, wherein repeated indices are summed over their appropriate range, will be used throughout the paper.) The bar on \( \phi \) is meant to indicate that this is the normalized characteristic function, i.e., \( \bar{\phi}(0) = 1 \). Below we will find it convenient to work with the unnormalized function \( \phi(\vec{\beta}) \).

Using the power series representation of \( \exp \left[ i\vec{\beta} \cdot \vec{x} \right] \) and the multinomial theorem it follows that

\[ \bar{\phi}(\vec{\beta}) = \frac{1}{v} \int_V d^Dx \sum_{n=0}^{\infty} \frac{(i\beta_i x_i)^n}{n!} \]

\[ = \sum_{n=0}^{\infty} \frac{i^n}{n!} \sum_{p_1+p_2+\cdots+p_D = n} \frac{n!}{p_1!p_2!\cdots p_D!} \beta_1^{p_1} \cdots \beta_D^{p_D} \langle x_1^{p_1} \cdots x_D^{p_D} \rangle \]  

(3)

This result indicates the simple but direct relation that exists between the Fourier transform of a shape and its moments \( \langle x_1^{p_1} \cdots x_D^{p_D} \rangle \). Note that we have assumed that since \( v \) is finite we can interchange orders of integration and summation. For all practical cases this is certainly true.

We see from this result that if we can compute \( \bar{\phi}(\vec{\beta}) \) explicitly then the moments \( \langle x_1^{p_1} \cdots x_D^{p_D} \rangle \) follow directly from a Taylor expansion of \( \bar{\phi}(\vec{\beta}) \) about \( \vec{\beta} = 0 \). An explicit form for \( \bar{\phi}(\vec{\beta}) \) can be found by applying Gauss law to the Fourier integral. Noting that

\[ e^{i\vec{\beta} \cdot \vec{x}} = \vec{\partial} \cdot \left( \frac{\vec{\beta}}{i\beta^2} e^{i\vec{\beta} \cdot \vec{x}} \right) \]  

(4)

with \( \vec{\partial} = (\partial/\partial x_1, \partial/\partial x_2, \cdots, \partial/\partial x_D) \equiv (\partial_1, \partial_2, \cdots, \partial_D) \) we get

\[ \int_V d^Dx e^{i\vec{\beta} \cdot \vec{x}} = \int_V d^Dx \vec{\partial} \cdot \left( \frac{\vec{\beta}}{i\beta^2} e^{i\vec{\beta} \cdot \vec{x}} \right) \]

\[ = \frac{\vec{\beta}}{i\beta^2} \cdot \int_{\partial V} d^{D-1}s \sqrt{|\det g(\vec{s})|} n(\vec{s}) e^{i\vec{\beta} \cdot \vec{R}(\vec{s})} \]  

(5)

Here \( \partial V \) indicates the surface of \( V \) with \( \vec{s} = (s_1, s_2, \cdots, s_{D-1}) \) being coordinates on the surface \( \partial V \). \( \vec{R}(\vec{s}) \) gives the position in \( D \) dimensions of the point on the surface labeled by \( \vec{s} \) and

\[ g(\vec{s}) = |\det [g_{ij}(\vec{s})]| = |\det [\partial_\sigma \vec{R}(\vec{s}) \cdot \partial_{\sigma_i} \vec{R}(\vec{s})]| \]  

(6)

where \( g_{ij}(\vec{s}) \) is the induced metric on \( \partial V \), \( n(\vec{s}) \) is the local outward normal to the surface \( \partial V \) and \( |\cdots| \) indicates the absolute value [14]. Below we use (5) to prove that \( \sqrt{|\det [\partial_\sigma \vec{R}(\vec{s}) \cdot \partial_{\sigma_i} \vec{R}(\vec{s})]|} d^2s \) is the area element of a parallelogram in 2 dimensions with sides defined by the vectors \( d\vec{R}_i = \)
The boundary of a boundary is zero. This boundary of a boundary principle has been considered to have interesting implications with respect to the origin of physical laws. [15]

The remainder of the paper considers particular cases in 2 or 3 dimensions where \( \phi (\vec{\beta}) \) can be computed from the surface integral either exactly or approximately. We now relate these results to various "classical" problems in physics and mathematics.

### 3 Results in Two Dimensions

In this section we show how (5) and (7) can be used to derive various two dimensional classical results in physics and mathematics.

#### 3.1 Smooth Curves

For smooth curves in two dimensions (5) reduces to

\[
\int_V d^2 x e^{i\vec{\beta} \cdot \vec{x}} = \frac{\vec{\beta}}{|i\vec{\beta}|^2} \cdot \int_{\partial V} ds \, \hat{n} (s) e^{i\vec{\beta} \cdot \vec{R}(s)}
\]
where \( V \) is the region enclosed by the curve \( \partial V \) given by \( \vec{R}(s) \) with the parameter \( s \) being the length along the curve. With \( ds \) defined as the unit of length on the curve, i.e., \( ds^2 = d\vec{R}^2 \), it follows that \( g(s) = 1 \). The unit tangent vector to the curve at \( s \) is given by

\[
\hat{t}(s) = \partial_s \vec{R}(s)
\]

(12)

which is automatically normalized since \( ds = \sqrt{d\vec{R}^2} \), i.e., \( \left| \partial_s \vec{R}(s) \right| = 1 \). (Generally we will use a hat "\( \hat{\cdot} \)" to indicate the vector has been normalized to have unit length. Also we will switch back and forth between vector and component notation, e.g., between writing \( \hat{u}_1 \) and \((1, 0)\).)

We take increasing \( s \) to correspond to counterclockwise circulation of the curve so that

\[
\hat{n}(s) = \varepsilon \cdot \hat{t}(s) = \varepsilon \cdot \partial_s \vec{R}(s)
\]

(13)

where

\[
\varepsilon = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}
\]

(14)

and the "\( \cdot \)" indicates matrix multiplication, i.e.,

\[
n_i(s) = \varepsilon_{ij} n_j(s)
\]

(15)

with repeated indices summed over 1, 2. Note that \( \varepsilon \) is the \( D = 2 \) version of the totally antisymmetric tensor, often called the Levi-Civita tensor \([16]\), defined as +1 for even permutations of \( i, j = 1, 2 \), −1 for odd permutations and 0 if \( i = j \).

Substituting (13) into (11) and integrating by parts yields

\[
\int_V d^2x e^{i\hat{\beta} \cdot \vec{x}} = -\frac{1}{i\beta} \int_{\partial V} ds \left( \hat{\beta} \cdot \varepsilon \cdot \vec{R}(s) \right) \left( \hat{\beta} \cdot \partial_s \vec{R}(s) \right) e^{i\hat{\beta} \cdot \vec{R}(s)}
\]

\[
= -\int_{\partial V} ds \left( \hat{\beta} \cdot \varepsilon \cdot \vec{R}(s) \right) \left( \hat{\beta} \cdot \partial_s \vec{R}(s) \right) e^{i\hat{\beta} \cdot \vec{R}(s)}
\]

(16)

The nominal \( 1/\beta \) pole in (11) has been cancelled and we can set \( \beta \) to zero for arbitrary nonzero \( \hat{\beta} = \frac{\beta}{|\beta|} \) which gives

\[
v = \int_V d^2x = \int_{\partial V} ds \left( \hat{\beta} \cdot \varepsilon \cdot \vec{R}(s) \right) \left( \hat{\beta} \cdot \partial_s \vec{R}(s) \right)
\]

(17)

Letting \( \hat{\beta} \) be \((1, 0)\) or \((0, 1)\) with \( \vec{R}(s) = (R_1(s), R_2(s)) \) yields

\[
v = -\int_{\partial V} ds \ R_2(s) \partial_s R_1(s) = \int_{\partial V} ds \ R_1(s) \partial_s R_2(s)
\]

(18)

Averaging the two forms gives

\[
v = \frac{1}{2} \int_{\partial V} ds \ \left( R_1(s) \partial_s R_2(s) - R_2(s) \partial_s R_1(s) \right)
\]

\[
= \frac{1}{2} \int_{\partial V} ds \ R_i(s) \varepsilon_{ij} \partial_s R_j(s)
\]

(19)

Both (18) and (19) are standard formulae for the area \( v \) enclosed by the curve \( \vec{R}(s) \) \([17]\).
**Isoperimetric Inequality** There are numerous proofs of this inequality [6] [8]. One rather cute and straightforward proof uses Fourier Series. Since $\partial V$ is a closed curve (the boundary of a boundary is zero) the functions $R_i(s)$ are periodic in the length

$$L = \int_{\partial V} ds$$

and so can be written as $R_i(s) = \sum_{n=-\infty}^{+\infty} \hat{R}_{i,n} \exp [i 2\pi s/L]$ with $\hat{R}_{i,n} = \hat{R}_{i,-n}^*$ so that $X_i(s)$ is real (" *" indicates complex conjugation). Substituting into (5) and using some very simple inequalities yields one proof of the isoperimetric inequality (see for example, Lut hy in [8]).

The approach we will use is to extremize $v$ with the constraint that $(\partial_s \vec{R}(s))^2 = 1$ imposed using a Lagrange multiplier $\lambda$. Minimizing

$$v = \frac{1}{2} \int_{\partial V} ds \; R_i(s) \varepsilon_{ij} \partial_s R_j(s) + \lambda \left( \int_0^L ds \; (\partial_s R_i(s))^2 - L \right)$$

with respect to $R_i(s)$, and $\lambda$ yields

$$0 = \frac{\delta v}{\delta R_1(s)} = \partial_s R_2(s) - 2\lambda \partial_s^2 R_1(s)$$
$$0 = \frac{\delta v}{\delta R_2(s)} = -\partial_s R_1(s) - 2\lambda \partial_s^2 R_2(s)$$
$$0 = \frac{\partial v}{\partial \lambda} = \int_0^L ds \; (\partial_s R_i(s))^2 - L$$

Here $\delta/\delta R_i(s)$ indicates functional differentiation [18]. Combining the first and second equations in (22) gives

$$(\partial_s R_i) + 2\lambda \partial_s^2 (\partial_s R_i) = 0 \text{ for } i = 1, 2$$

Taking $\partial_s R_1(s = 0) = 0$ so that $\partial_s R_2(s = 0) = 1$, the solutions are

$$\partial_s R_1(s) = -\sin (s/2\lambda)$$
$$\partial_s R_2(s) = \cos (s/2\lambda)$$

where the minus sign was chosen for convenience. Integrating both sides yields

$$R_1(s) = 2\lambda \cos (s/2\lambda) + R_{0,1}$$
$$R_2(s) = 2\lambda \sin (s/2\lambda) + R_{0,2}$$

which is a circle of radius $2\lambda$ centered at the arbitrary position $\vec{R}_0 = (R_{0,1}, R_{0,2})$. Note that the radius $2\lambda$ is indeterminate since substituting these solutions into the third equation above yields an identity. This is as it should be since the circle does not have to be a particular size to maximize an unspecified value of $v$. It just has to be a circle. Of course once a particular value of $v$ is given then $\lambda$ can be determined. Note that the above calculation shows only that the circle is one shape which
extremizes the area. In other words, we have only shown that the circle is a local extremum, to formally complete the proof requires showing that it is the global extremum.

We will not show it here but isoperimetric inequality is generalizable to arbitrary dimensions with the result that the shape that maximizes the "volume" for a given surface "area" is always a "ball" [6] [8], i.e., circle for $D = 2$, sphere for $D = 3$, etc.

The isoperimetric inequality can be used to solve Dido’s problem which is to find the open curve of fixed length $L$ which encloses the maximum area when the end points are connected by a straight line of arbitrary length [9]. Combining this closed curve with its reflection relative to the straight line yields a closed curve of length $2L$. Via the isoperimetric inequality the circle with circumference $2L$ encloses the maximum area and hence the original open curve which maximizes the area is a semicircle.

**Stokes Law** We now use (5) to derive the planar version of Stokes law as used in classical electrodynamics [7]. It should come as no surprise that we can relate Gauss’s law to Stokes law and indeed to Green’s theorem as well since they are all different aspects of the general version of Stokes theorem represented compactly using differential forms [16]. Consider the integral over an area $V$ in the $x_1x_2$ plane of the curl of a smooth 3 dimensional vector field $\vec{F}(\vec{x})$. Let indices from the beginning of the alphabet $a, b, c, \cdots$ range over 1,2,3 and indices from the middle of the alphabet $i, j, k, \cdots$ range over 1,2. This way $\vec{F}(\vec{x}) = F_a(\vec{x}) \hat{u}_a$ and $\vec{x} = x_a \hat{u}_a$ with $\hat{u}_a$ the unit vectors with respect to $x_a$. Represent $\vec{F}(\vec{x})$ as a Fourier transform

$$F_i(\vec{x}) = \int d^3 \beta \hat{F}_i\left(\vec{\beta}\right) e^{i \vec{\beta} \cdot \vec{x}}$$

with $\vec{\beta} = \beta_a \hat{u}_a$. Again we assume that orders of integration can be freely exchanged. Using index notation the $a^{th}$ component of the curl can be written

$$\left(\vec{\partial} \times \vec{F}(\vec{x})\right)_a = \varepsilon_{abc} \partial_b F_c(\vec{x})$$

Here $\varepsilon_{abc}$ is the $D = 3$ totally antisymmetric Levi-Civita tensor defined as $+1$ for even permutations of $a, b, c = 1,2,3$, $-1$ for odd permutations and 0 if any two of the indices have the same value. Repeated $a, b, c, \cdots$ indices are summed over the range 1,2,3. The normal to $V$, which lies in the $x_1x_2$ plane, is $\hat{u}_3$ and so

$$\int_V d^2 x \ \hat{u}_3 \cdot \left(\vec{\partial} \times \vec{F}(\vec{x}_V)\right) = \int_V d^2 x \varepsilon_{3bc} \partial_b F_c(\vec{x}_V)$$

where $\vec{x}_V = x_i \hat{u}_i$. But $\varepsilon_{3bc}$vanishes unless $b$ and $c$ are restricted to the range 1,2 and so $\varepsilon_{3bc} \partial_b F_c(\vec{x}) = \varepsilon_{ij} \partial_i F_j(\vec{x})$ where $\varepsilon_{jk}$ are the elements of the $2 \times 2$ Levi-Civita matrix $\varepsilon$ defined above. Putting this
together and using (5) and (26) gives

\[
\int_V d^2 x \, \hat{u}_3 \cdot \left( \hat{\partial} \times \vec{F}(\vec{x}_V) \right) = \int_V d^2 x \, \varepsilon_{ij} \partial_i \vec{F}_j(\vec{x}_V)
\]

\[
= \int_V d^2 \beta_i \bar{\varepsilon}_{ij} \hat{F}_j\left(\vec{\beta}\right) \int d^2 x \, e^{i \bar{\beta} \cdot \vec{x}_V}
\]

\[
= \int d^2 \beta_i \varepsilon_{ij} \hat{F}_j\left(\vec{\beta}\right) \frac{\beta_k \varepsilon_{kl}}{\beta^2} \int d s \, t_1(s) \, e^{i \bar{\beta} \cdot \vec{R}(s)}
\]

\[
= \int d s \, t_1(s) \int d^2 \beta e^{i \bar{\beta} \cdot \vec{R}(s)} \hat{F}_1\left(\vec{\beta}\right)
\]

\[
= \int d s \, \hat{\gamma}(s) \cdot \vec{F}(\vec{R}(s))
\]

(29)

which is the planar form of Stokes law. To get the fourth line we used

\[
\beta_1 \int d s \, t_1(s) \, e^{i \bar{\beta} \cdot \vec{R}(s)} = -\beta_2 \int d s \, t_2(s) \, e^{i \bar{\beta} \cdot \vec{R}(s)}
\]

(30)

which follows from

\[
\int d s \, \hat{\beta} \cdot \hat{\gamma}(s) = \int d s \, \hat{\beta} \cdot \partial_s \vec{R}(s) \, e^{i \bar{\beta} \cdot \vec{R}(s)}
\]

\[
= \int d s \, \partial_s e^{i \bar{\beta} \cdot \vec{R}(s)}
\]

\[
= 0
\]

(31)

### 3.2 Polygons

A polygon with \(N\) sides and \(N\) vertices in two dimensions can be defined by its vertices, arranged in a particular order, \(\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_N\) with \(\vec{v}_1 = (x_1, x_2)\). For computational convenience it is useful to let \(\vec{v}_{N+1} = \vec{v}_1\). We consider only orientable polygons, i.e., none of the edges cross over or intersect one another. The integral over \(\partial V\) in (7) can be evaluated explicitly in this case with the result

\[
\phi\left(\vec{\beta}\right) = \frac{\vec{\beta}}{i \beta^2} \cdot \int_{\partial V} d^{D-1} s \, \hat{n}(s) \cdot e^{i \bar{\beta} \cdot \vec{R}(s)}
\]

\[
= -\frac{1}{\beta^2} \sum_{n=1}^{N} \frac{\vec{\beta} \cdot (\vec{v}_{n+1} - \vec{v}_n)}{\vec{\beta} \cdot (\vec{v}_{n+1} - \vec{v}_n)} \left( \exp\left(i \bar{\beta} \cdot \vec{v}_{n+1}\right) - \exp\left(i \bar{\beta} \cdot \vec{v}_n\right) \right)
\]

(32)

where

\[
\vec{\beta}_\perp \equiv \vec{\beta} \cdot \varepsilon = (\beta_1, \beta_2) \cdot \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} = (\beta_2, -\beta_1)
\]

(33)
The "·" stands for standard matrix vector multiplication.

Equating the surface integral to the series expansion in terms of moments gives

\[
\sum_{n=0}^{\infty} \frac{i^n}{n!} \sum_{p=0}^{n!} \frac{n!}{p!(n-p)!} \beta_1^p \beta_2^{n-p} M \left(x_1^n x_2^{n-p}\right)
\]

\[
= -\frac{1}{\beta^2} \sum_{n=1}^{N} \beta_1 \cdot (\vec{v}_{n+1} - \vec{v}_n) \left( \exp \left( i\beta \cdot \vec{v}_{n+1} \right) - \exp \left( i\beta \cdot \vec{v}_n \right) \right)
\]

Now expand the right hand side in powers of \( \beta_i \)

\[
\frac{1}{\beta^2} \sum_{n=1}^{N} \beta_1 \cdot (\vec{v}_{n+1} - \vec{v}_n) \left( \exp \left( i\beta \cdot \vec{v}_{n+1} \right) - \exp \left( i\beta \cdot \vec{v}_n \right) \right)
\]

\[
= \frac{1}{\beta^2} \sum_{n=1}^{N} \beta_1 \cdot (\vec{v}_{n+1} - \vec{v}_n) \left( \sum_{m=1}^{\infty} \frac{(i\beta \cdot \vec{v}_{n+1})^m - (i\beta \cdot \vec{v}_n)^m}{m!} \right)
\]

\[
= \frac{1}{\beta^2} \sum_{m=1}^{\infty} \sum_{n=1}^{N} \frac{i}{m!} \beta_1 \cdot (\vec{v}_{n+1} - \vec{v}_n) \sum_{p=0}^{m-1} (i\beta \cdot \vec{v}_{n+1})^{m-1-p} (i\beta \cdot \vec{v}_n)^{p}
\]

where \( \beta^2 = \beta_1 \beta_4 = \beta_1^2 + \beta_2^2 \). In the second step we have used the identity

\[
a^n - b^n = (a - b) \sum_{m=0}^{n-1} a^{n-1-m} b^m
\]

Substituting (35) into (34) gives

\[
\sum_{n=0}^{\infty} \frac{i^n}{n!} \sum_{p=0}^{n!} \frac{n!}{p!(n-p)!} \beta_1^p \beta_2^{n-p} M \left(x_1^n x_2^{n-p}\right)
\]

\[
= -\frac{1}{\beta^2} \sum_{m=1}^{\infty} \sum_{n=1}^{N} \frac{i}{m!} \beta_1 \cdot (\vec{v}_{n+1} - \vec{v}_n) \sum_{p=0}^{m-1} (i\beta \cdot \vec{v}_{n+1})^{m-1-p} (i\beta \cdot \vec{v}_n)^{p}
\]

Letting \( \bar{\beta} = \beta \beta_1 \) and \( \bar{\beta}_2 = \beta_2 \) we see that the \( n \)th term on the left hand side is proportional to \( \beta^n \) whereas the \( m \)th on the right is proportional to \( \beta^{m-2} \). Hence considering each side as a power series in \( \beta \) the coefficients of the \( m \) term on the right must equal the coefficient of \( n = m - 2 \) term on the left. Below we write out the general relation between \( M \left(x_1^n x_2^n\right) \) and powers of the vertices. Here we begin by considering the first few terms individually.

### 3.2.1 \( m = 1 \) term

The \( m = 1 \) term on the right has no corresponding term on the left of (34) and so we must have

\[
0 = \frac{i}{\beta^2} \bar{\beta}_2 \sum_{n=1}^{N} (\vec{v}_{n+1} - \vec{v}_n)
\]
The fact that this should vanish follows from the fact that it scales as $1/\beta$ whereas the left hand side remains finite as $\beta \to 0$. Also this term is imaginary and the result must be real. And indeed this term does vanish, trivially, since we have defined $\vec{v}_{N+1} = \vec{v}_1$ and the sum of the directed sides, $\vec{v}_{n+1} - \vec{v}_n$, of a closed polygon must vanish. For the case where the boundary $\partial V$ is everywhere smooth the form of the dominant term as $\beta \to 0$ is given by

$$\lim_{\beta \to 0} \frac{\vec{\beta}}{i\beta^2} \cdot \int_{\partial V} ds \, \hat{n}(s) e^{i\vec{\beta} \cdot \vec{R}(s)} = \frac{\vec{\beta}}{i\beta} \cdot \int_{\partial V} ds \, \hat{n}(s) \Rightarrow \int_{\partial V} ds \, \hat{n}(s) = 0 \quad (39)$$

The last equality follows from the fact that this term must vanish for any (non-zero) $\vec{\beta}$. The results in (38) and (39) can also be related to Hopf’s Umlaufsatz [6] which states that the tangent vector (or the normal vector or a linear combination thereof) to a smooth or piecewise smooth orientable curve in two dimensions rotates by $2\pi$ on making a complete circuit of the curve if the curve is traversed in a counterclockwise direction and by $-2\pi$ if traversed in a clockwise direction. For nonorientable curves, i.e., curves which crossover or intersect themselves it is an integer multiple of $2\pi$ with the integer value counting the net number of signed (+/− for counterclockwise/clockwise) loops. This seems obvious but in fact is rather subtle to prove [6].

**Hopf’s Umlaufsatz** The results in (38) and (39) can also be related to Hopf’s Umlaufsatz [6] which states that the tangent vector (or the normal vector or a linear combination thereof) to a smooth or piecewise smooth orientable curve in two dimensions rotates by $2\pi$ on making a complete circuit of the curve if the curve is traversed in a counterclockwise direction and by $-2\pi$ if traversed in a clockwise direction. For nonorientable curves, i.e., curves which crossover or intersect themselves it is an integer multiple of $2\pi$ with the integer value counting the net number of signed (+/− for counterclockwise/clockwise) loops. This seems obvious but in fact is rather subtle to prove [6].

The following is an argument in favor of the Hopf Umlaufsatz but is not a proof in the strict mathematical sense. Consider first the piecewise smooth, actually piecewise linear, case of a polygon (clockwise/counterclockwise) loops. This seems obvious but in fact is rather subtle to prove [6].

The results in (38) and (39) can also be related to Hopf’s Umlaufsatz [6] which states that the tangent vector (or the normal vector or a linear combination thereof) to a smooth or piecewise smooth orientable curve in two dimensions rotates by $2\pi$ on making a complete circuit of the curve if the curve is traversed in a counterclockwise direction and by $-2\pi$ if traversed in a clockwise direction. For nonorientable curves, i.e., curves which crossover or intersect themselves it is an integer multiple of $2\pi$ with the integer value counting the net number of signed (+/− for counterclockwise/clockwise) loops. This seems obvious but in fact is rather subtle to prove [6].

The same type of argument can be applied to the smooth curve case. Write the tangent vector $\hat{t}$ at distance $s$ along the curve as

$$\hat{t}(s + ds) = R(\partial_s \theta(s) \, ds) \cdot \hat{t}(s) \quad (43)$$
where $\theta(s)$ is the angle between the tangent vector at $s$ and the tangent vector at $s=0$ so that

$$\hat{t}(s) = R(\theta(s)) \cdot \hat{t}(0)$$  \hspace{1cm} (44)$$

Then using the fact that the curve is smooth ($\partial_s \hat{t}(s)$ is everywhere defined) and closed we have, with $L$ the total distance around the curve, that

$$\hat{t}(L) = R(\theta(L)) \cdot \hat{t}(0) = \hat{t}(0)$$  \hspace{1cm} (45)$$

and so $\theta(L)$ must be an integer times $2\pi$. Again this result must be combined with the fact that the curve is orientable to specify the integer value as unity.

### 3.2.2 $m=2$ term

The $m=2$ term on the right equals the $n=0$ term on the left and so we have

$$M(1) = -\frac{i}{2} \frac{1}{\beta^2} \sum_{n=1}^{N} \beta \perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \sum_{p=0}^{1} (i\beta \cdot \vec{v}_{n+1})^{1-p} (i\beta \cdot \vec{v}_n)^p$$

$$= -\frac{i}{2} \frac{1}{\beta^2} \sum_{n=1}^{N} \left( \beta \perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \right) \left( i\beta \cdot \vec{v}_{n+1} + i\beta \cdot \vec{v}_n \right)$$

$$= \frac{1}{2} \sum_{n=1}^{N} \left( \beta \perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \right) \left( \beta \cdot (\vec{v}_{n+1} + \vec{v}_n) \right)$$  \hspace{1cm} (46)$$

But by definition $M(1)$ is the area of the polygon. Defining $\vec{l}_n = \vec{v}_{n+1} - \vec{v}_n = $ the vector from vertex $n$ to vertex $n+1$ and $\vec{c}_n = (\vec{v}_{n+1} + \vec{v}_n)/2 = $ position of the center of side $n$ we have

$$M(1) = \text{Area} = \sum_{n=1}^{N} \left( \beta \perp \cdot \vec{l}_n \right) \left( \beta \cdot \vec{c}_n \right)$$  \hspace{1cm} (47)$$

Taking $\beta = (0,1)$ gives $\beta \perp = (-1,0)$ and so

$$\text{Area} = -\sum_{n=1}^{N} l_{n,1} c_{n,2}$$  \hspace{1cm} (48)$$

The geometric interpretation of this is straightforward. Each of the $l_{n,1} c_{n,2}$ terms correspond to the area of a 4-sided polygon of width $|l_{n,1}|$ in the $x_1$ direction and mean height $|c_{n,2}|$ in the $x_2$ direction. If we take all the vertices to lie in the first quadrant, $v_{n,i} > 0$ for $i = 1, 2$ then all the $c_{n,2}$ are positive but the $l_{n,1}$ change sign depending on whether $\vec{l}_n$ points generally in the $+x_1$ or $-x_1$ direction. If we consider that the $n = 1, \ldots, N$ ordering corresponds to following the vertices in a counterclockwise direction around the polygon then the positive $l_{n,1}$ will generally run along the bottom sides of the net polygon and the negative $l_{n,1}$ will generally run along the top sides of the net polygon, then the area of the net polygon is the total area of all the 4-sided polygons along
the bottom of the net polygon subtracted from the area of the 4-sided polygons along the top of
the net polygon.

Taking 1/2 the sum of (47) with \( \hat{\beta} = (0, 1) \) and with \( \hat{\beta} = (1, 0) \) we find that the area can
also be written as \( \frac{1}{2} \sum_{n=1}^{N} \det [M_n] \) where the elements of the 2×2 matrices \( M_n \) are given by
\( M_{n,ij} = \nu_{n,i} \nu_{n+1,j} \), which is the standard result [19].

**Area Element** We now show that the area element \( dv \) of a 2 dimensional surface \( \partial V \) defined by
\( \tilde{R}(\tilde{s}) \), which is a vector in \( 3 \) dimensional Euclidean space and \( \tilde{s} = (s_1, s_2) \) labels points on \( \partial V \), is
given by

\[
dv = \sqrt{\det \left[ \partial_{s_1} \tilde{R}(\tilde{s}) \cdot \partial_{s_2} \tilde{R}(\tilde{s}) \right]} ds_1 ds_2 = \sqrt{\det \left[ \hat{t}_i(\tilde{s}) \cdot \hat{t}_j(\tilde{s}) \right]} ds_1 ds_2
\]  

(49)

The two vectors \( d\tilde{R}_i = \partial_{s_i} \tilde{R}(\tilde{s}) ds_i = \hat{t}_i(\tilde{s}) ds_i \) for \( i = 1, 2 \) (no sum on \( i \)) form a parallelogram with
area \( dv \) whose vertices are \( \tilde{v}_1 = (0, 0) \), \( \tilde{v}_2 = d\tilde{R}_1 \), \( \tilde{v}_3 = d\tilde{R}_1 + d\tilde{R}_2 \), \( \tilde{v}_4 = d\tilde{R}_2 \) and \( \tilde{v}_5 = \tilde{v}_1 \) all of
which lie on \( \partial V \). (For simplicity we have assumed that \( s_i \) has units of length so that \( \partial_{s_i} \tilde{R}(\tilde{s}) = \hat{t}_i(\tilde{s}) \)
with \( \hat{t}_i(\tilde{s}) \) automatically normalized to unity.) The area of this parallelogram \( dv \) can be computed
directly from (46).

\[
dv = \frac{1}{2} \left[ \left( \hat{\beta} \cdot d\tilde{R}_1 \right) \left( \hat{\beta} \cdot \hat{t}_1 \right) + \left( \hat{\beta} \cdot d\tilde{R}_2 \right) \left( \hat{\beta} \cdot \hat{t}_2 \right) \right] + \left( \hat{\beta} \cdot d\tilde{R}_1 \hat{\beta} \cdot d\tilde{R}_2 \right)
\]

\[
= \left( \hat{\beta} \cdot \hat{t}_2 \right) \left( \hat{\beta} \cdot \hat{t}_1 \right) - \left( \hat{\beta} \cdot \hat{t}_1 \right) \left( \hat{\beta} \cdot \hat{t}_2 \right)
\]

(50)

The vector \( \hat{\beta} \) can be written as an arbitrary linear combination of the unit vectors \( \hat{t}_i(\tilde{s}) \). Letting
\( \hat{\beta} = \hat{t}_1 \) gives

\[
dv = \hat{t}_1 \cdot \hat{t}_2 ds_1 ds_2
\]

\[
= \left( t_{1,1} t_{2,2} - t_{1,2} t_{2,1} \right) ds_1 ds_2
\]

(51)

where \( t_{i,a} \) are the components of \( \hat{t}_i \) in an orthonormal coordinate system indexed by \( a = 1, 2 \) erected
on \( \partial V \) at \( \tilde{s} \). But

\[
\sqrt{\det \left[ \hat{t}_i \cdot \hat{t}_j \right]} ds_1 ds_2 = \sqrt{\det \left[ \hat{t}_1 \cdot \hat{t}_1 \hat{t}_2 \cdot \hat{t}_2 \right]} ds_1 ds_2
\]

\[
= \sqrt{\left( \hat{t}_1 \cdot \hat{t}_1 \right) \left( \hat{t}_2 \cdot \hat{t}_2 \right) - \left( \hat{t}_1 \cdot \hat{t}_2 \right)^2} ds_1 ds_2
\]

\[
= \left( t_{1,1} t_{2,2} - t_{1,2} t_{2,1} \right) ds_1 ds_2
\]

\[
= dv
\]

(52)

For the purposes of the above derivation even though \( \hat{t}_1 \cdot \hat{t}_1 = \hat{t}_2 \cdot \hat{t}_2 = 1 \) it is more convenient leave
them as \( \hat{t}_1 \cdot \hat{t}_1 \) and \( \hat{t}_2 \cdot \hat{t}_2 \). Finally note that from simple geometry we have \( dv = \left| d\tilde{R}_1 \right| \left| d\tilde{R}_2 \right| \sin(\theta) \)
where \( \theta \) is the angle between \( d\tilde{R}_1 \) and \( d\tilde{R}_2 \), and if we do use \( \hat{t}_1 \cdot \hat{t}_1 = \hat{t}_2 \cdot \hat{t}_2 = 1 \) then \( \sqrt{\det \left[ \hat{t}_i \cdot \hat{t}_j \right]} =\)
\[
\sqrt{1 - (\hat{t}_1 \cdot \hat{t}_2)^2} = \sqrt{1 - \cos(\theta)^2} = \sin(\theta)
\]
and we get the same result for \(dv\). In general it is much more convenient to work with \(\sqrt{|\det [\hat{t}_i \cdot \hat{t}_j]|}\) than other forms since the inner product \(\hat{t}_i \cdot \hat{t}_j\) is coordinate independent.

### 3.2.3 \(m = 3\) term

The \(m = 3\) term on the right hand side corresponds to the \(n = 1\) term on the left and so after cancelling \(i\) from both sides we have

\[
\hat{\beta}_1 M(x_1) + \hat{\beta}_2 M(x_2) = \frac{1}{3!} \sum_{n=1}^{N} \hat{\beta}_\perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \left( \frac{\hat{\beta} \cdot \vec{v}_{n+1}}{\hat{\beta} \cdot \vec{v}_n} \right)^2 + \left( \hat{\beta} \cdot \vec{v}_{n+1} \right) \left( \hat{\beta} \cdot \vec{v}_n \right) + \left( \hat{\beta} \cdot \vec{v}_n \right)^2 \tag{53}
\]

It follows from the definition of \(M\) that

\[
M(x_i) = \text{Area} \times X_i \tag{54}
\]

where \(X_i\) is the "center of mass" or centroid of the polygon in the \(i = 1, 2\) directions.

For \(\hat{\beta} = (1, 0), \hat{\beta}_\perp = (0, 1)\) we have

\[
M(x_1) = \frac{1}{3!} \sum_{n=1}^{N} (v_{n+1,2} - v_{n,2}) \left( v_{n+1,1}^2 + v_{n,1}^2 + v_{n+1,1}v_{n,1} \right) \tag{55}
\]

and for \(\hat{\beta} = (0, 1), \hat{\beta}_\perp = (-1, 0)\) we have

\[
M(x_2) = -\frac{1}{3!} \sum_{n=1}^{N} (v_{n+1,1} - v_{n,1}) \left( v_{n+1,2}^2 + v_{n,2}^2 + v_{n+1,2}v_{n,2} \right) \tag{56}
\]

Explicit evaluation of

\[
\int_V dx_1 dx_2 x_i \tag{57}
\]

with \(i = 1\) or 2 by substituting \(x_i = \hat{\partial} \cdot (x_i^2 \hat{x}_i/2)\), with no sum on \(i\), yields the same result as in (55) and (56).

### 3.3 Moments and Shapes of Polygons

We begin this section by using a version of (5) modified to live in the complex plane to provide an alternative derivation of the result of Davis which is a generalization from triangles to polygons of the Motzkin-Schoenberg formula [11]. This result is also related to the so-called "shape from moments" problem which is to find the ordered vertices of a polygon given an appropriate set of the polygon moments [4] [5]. As shown by Milanfar [4], in the complex plane with \(z = x + iy\), the result of Davis can be written

\[
\int_V dx dy \partial_z^2 h(z) = \frac{i}{2} \sum_{n=1}^{N} \left( \frac{z_{n+1}^* - z_n^*}{z_{n+1} - z_n} - \frac{z_n^* - z_{n+1}^*}{z_n - z_{n+1}} \right) h(z_n) \tag{58}
\]
Here $V$ is a simply connected orientable polygon with vertices $z_n = x_n + iy_n$ ($z_n^* = z_n - iy_n$), $n = 1, \ldots, N$, in the complex plane and the function $h(z)$ is analytic (= holomorphic = regular) in the closure of $V$. In the sum we have let $z_0 = z_N$ and $z_1 = z_{N+1}$. For the remainder of this section we follow the standard notation for variables in the complex plane, i.e., we replace $x_1$ with $x$, $x_2$ with $y$, etc.

To write $h(z)$ as a Fourier transform start with the definition of an analytic function, i.e., that it can be written as a power series in non-negative powers of $z$

$$h(z) = \sum_{n=0}^{\infty} a_n z^n \quad (59)$$

Now define the function $\tilde{h}(\beta)$, with $\beta$ real, by

$$a_n = \int d\beta \tilde{h}(\beta) \frac{(i\beta)^n}{n!} \quad (60)$$

This may seem restrictive but if we take $\tilde{h}(\beta)$ to vanish outside $|\beta| \leq 1$ then we can represent $\tilde{h}(\beta)$ as

$$\tilde{h}(\beta) = \sum_{n=0}^{\infty} A_n P_n(\beta) \quad (61)$$

where $P_n(\beta)$ are Legendre polynomials. With this representation the complex coefficients $A_n$ can be chosen to satisfy (35). Again assuming we can interchange sums and integrals at will we can write

$$h(z) = \int d\beta \tilde{h}(\beta) \sum_{n=0}^{\infty} \frac{(i\beta z)^n}{n!} = \int d\beta \tilde{h}(\beta) e^{i\beta z} \quad (62)$$

Using the obvious notation $(a, b) \cdot (x, y) = ax + by$, we now have

$$\int_V \int \int d\beta (\partial_x^2 + \partial_y^2) h(z) = - \int \int d\beta \tilde{h}(\beta) \int_{V'} dx dy \beta^2 e^{i\beta z}$$

$$= \frac{i}{2} \int d\beta \tilde{h}(\beta) \int_V dx dy (\partial_x \partial_y) \cdot \beta (1, -i) \exp [i\beta (1, i) \cdot (x, y)]$$

$$= \frac{1}{2} \int d\beta \tilde{h}(\beta) \sum_{n=1}^{N} \beta (1, -i) \cdot \varepsilon \cdot ((x, y)_{n+1} - (x, y)_n)$$

$$\cdot (\frac{\beta (1, i) \cdot ((x, y)_{n+1} - (x, y)_n)}{\beta (1, i) \cdot ((x, y)_{n+1} - (x, y)_n)} - \exp (i\beta (1, i) \cdot (x, y)_n))$$

$$= \frac{i}{2} \int d\beta \tilde{h}(\beta) \sum_{n=1}^{N} \left( \frac{z_n^* - z_{n-1}^*}{z_n - z_{n-1}} - \frac{z_{n+1}^* - z_n^*}{z_{n+1} - z_n} \right) \exp (i\beta z_n)$$

$$= \frac{i}{2} \sum_{n=1}^{N} \left( \frac{z_{n-1}^* - z_n^*}{z_{n-1} - z_n} - \frac{z_{n+1}^* - z_n^*}{z_{n+1} - z_n} \right) h(z_j) \quad (63)$$

In the third line $\varepsilon$ is the Levi-Civita matrix defined in (14). In the second step we have used (5) and in the last step the definition of $h(z)$ in terms of its Fourier transform. The $\beta$’s cancel in the coefficient of the exponents in line three and hence we reproduce the result of Davis that the
integral over a polygon of $\partial^2 h(z)$ is the sum of $h(z)$ evaluated at the vertices of the polygon times coefficients which depend only on the vertices and not on $h(z)$.

The moments of a polygon obviously contain the polygon shape information. The order of the vertices is important as reordering them nominally leads to a polygon with a different shape and/or can make it nonorientable. For $N$ vertices there are $2N$ independent real numbers corresponding to the $\vec{v}_1, \ldots, \vec{v}_N$ vertices which define the polygon. Thus the infinite set of all possible moments of the polygon must be highly redundant. We will not solve this "shape from moments" problem here. Milanfar and others \cite{4} \cite{5} have shown how to solve for the vertices given a particular set of complex moments which can be easily computed from (63) by letting $h(z) = z^k$. Here we merely present the complete set of relations between all possible moments $M(x^a, y^b)$ and the vertices $(x, y)_n$ of a polygon that follows from (34).

To derive an explicit relation between the moments and the vertices of an arbitrary orientable polygon multiply (32) through by $\beta_1^a \beta_2^b$ and use the fact that the $m = 1$ term on the right hand side vanishes identically. The derivation is facilitated by defining a function $\theta(\cdots)$ which vanishes if any one or more of its arguments is negative and equals 1 otherwise. This function can be used to keep track of the limits on the sums when the summation indices are redefined so that the powers of $\beta_1$ and $\beta_2$ are written as $\beta_1^a \beta_2^b$ on both sides of the equation. Then using the fact that the coefficient of $\beta_1^a \beta_2^b$ on the left must equal the coefficient of $\beta_1^a \beta_2^b$ on the right for the same given non-negative integer values of $a$ and $b$ we find, with $\vec{v}_n = (x_{1,n}, x_{2,n})$

$$\theta(a - 2) \frac{M(x_1^{a-2} x_2^b)}{(a - 2)! b!} + \theta(b - 2) \frac{M(x_1^a y_2^{b-2})}{a! (b - 2)!}$$

$$= \theta(b - 1, a + b - 2) \sum_{q=0}^{a} \sum_{p=0}^{a+b-1-q} \left( \sum_{n=1}^{N} \frac{\theta(p + q - a)}{(a + b)!} \frac{1}{q!} \frac{1}{(a + b - 1 - p - q)!} \frac{1}{(a - q)! (p + q - a)!} \right) \frac{1}{(a + b - 1 - p)!} \frac{1}{q!} \frac{1}{(a + b - 1 - p - q)!} \frac{1}{(a - q - 1)! (p + q + 1 - a)!} \times \left( x_1, x_2, x_{1,1}, x_{1,2}, x_{1,3}, \ldots, x_{1,n}, x_{2,1}, x_{2,2}, x_{2,3}, \ldots, x_{2,n} \right)$$

$$- \theta(a - 1, a + b - 2) \sum_{q=0}^{a} \sum_{p=0}^{a+b-1-q} \left( \sum_{n=1}^{N} \frac{\theta(p + q + 1 - a)}{(a + b)!} \frac{1}{q!} \frac{1}{(a + b - 1 - p - q)!} \frac{1}{(a - q - 1)! (p + q + 1 - a)!} \right) \frac{1}{(a + b - 1 - p)!} \frac{1}{q!} \frac{1}{(a + b - 1 - p - q)!} \frac{1}{(a - q - 1)! (p + q + 1 - a)!} \times \left( x_2, x_2, x_{2,1}, x_{2,2}, x_{2,3}, \ldots, x_{2,n}, x_{1,1}, x_{1,2}, x_{1,3}, \ldots, x_{1,n} \right)$$

The derivation is straightforward but tedious.

3.4 Fraunhofer Diffraction

Fraunhofer diffraction occurs when the light diffracted from an aperture or opening in an opaque screen is observed in a plane far from aperture itself \cite{2}. By "far" we mean that the distance between the opaque screen and the plane of observation, which is by convention taken to be parallel to the screen, is much larger than the maximum dimension of the aperture. For the case where the opaque screen lies in the $x_1x_2$ plane and the illumination is a unit amplitude plane wave of wavelength $\lambda$ incident on the screen from the side opposite the observation plane, the amplitude of the diffracted light at position $x_i$ in the observation plane a distance $L$ away from the screen is given by

$$A(\vec{x}) = \int d^2 x' \theta_V(\vec{x}') \exp \left[ \frac{i}{L} x_i x_i' \right] = \int d^2 x' \exp \left[ \frac{i}{L} x_i x_i' \right]$$
Here $\theta_V(x,y) = 1$ inside the aperture and 0 outside describes the aperture shape and $k = 2\pi/\lambda$. This is essentially the left hand side of (5) but with
\[
\beta = \frac{kx_1}{L} \tag{66}
\]
and without the normalization factor. The intensity of the diffraction pattern is given by $I(\vec{x}) = |A(\vec{x})|^2$.

We consider two cases, a circular aperture whose solution follows almost trivially from (5) and a slit whose solution is already implicit in (32).

For a circular aperture of radius $R$ centered at $x_1 = 0$ it follows from (5) that
\[
A(\vec{x}) = \frac{\vec{\beta}R}{i\beta^2} \int_0^{2\pi} d\varphi \hat{r}(\varphi) \exp \left[ i\vec{\beta} \cdot \vec{R} \hat{r}(\varphi) \right] \tag{67}
\]
with $\hat{r}(\varphi) = \vec{x}'/|\vec{x}'|$. Writing $\vec{\beta} \cdot \hat{r}(\varphi) = \beta \cos(\varphi - \varphi_\beta)$ where $\varphi_\beta$ is the angle $\vec{\beta}$ makes with respect to the $x_1$-axis and $\beta = |\vec{\beta}| = k\sqrt{x^2 + y^2}/L$, (67) becomes
\[
A(\vec{x}) = \frac{R}{i\beta} \int_0^{2\pi} d\varphi \cos(\varphi - \varphi_\beta) \exp \left[ i\beta R \cos(\varphi - \varphi_\beta) \right]
\]
\[
= \frac{R}{i\beta} \int_0^{2\pi} d\varphi \exp \left[ i\beta R \varphi \right] \tag{68}
\]
Here the $J_n(x)$ are the Bessel functions of the first kind. This is the standard result for a circular aperture [2].

For a slit (rectangular) aperture of width $2a_1$ in the $x_1$ direction, centered at $x_1 = 0$, we merely have to substitute $\vec{v}_1 = (a_1, a_1)$, $\vec{v}_2 = (-a_1, a_2)$, $\vec{v}_3 = (-a_1, -a_2)$, $\vec{v}_4 = (a_1, -a_2)$, and $\vec{v}_5 = \vec{v}_1$ into (32) to obtain
\[
A(\vec{x}) = \frac{1}{\beta^2} \sum_{n=1}^{N} \frac{\beta \cdot \hat{e} \cdot (\vec{v}_{n+1} - \vec{v}_n)}{\beta \cdot (\vec{v}_{n+1} - \vec{v}_n)} \left( \exp \left( i\vec{\beta} \cdot \vec{v}_{n+1} \right) - \exp \left( i\vec{\beta} \cdot \vec{v}_n \right) \right)
\]
\[
= \frac{1}{\beta^2} \left( \frac{\beta_1}{\beta_1} \left( \exp (-ia_1\beta_1 + ia_2\beta_2) - \exp (i\beta_1 a_1 + i\beta_2 a_2) \right) 
\right.
\]
\[
- \frac{\beta_1}{\beta_2} \left( \exp (-ia_1\beta_1 - ia_2\beta_2) - \exp (-i\beta_1 a_1 + i\beta_2 a_2) \right) 
\]
\[
+ \frac{\beta_1}{\beta_1} \left( \exp (ia_1\beta_1 + ia_2\beta_2) - \exp (-i\beta_1 a_1 - i\beta_2 a_2) \right) 
\]
\[
- \frac{\beta_1}{\beta_2} \left( \exp (ia_1\beta_1 - ia_2\beta_2) - \exp (i\beta_1 a_1 - i\beta_2 a_2) \right) \right) 
\]
\[
= (2a_1) (2a_2) \frac{\sin(\beta_1 a_1) \sin(\beta_2 a_2)}{\beta_1 a_1 \beta_2 a_2} \tag{69}
\]
which again is the standard result [2].

Fraunhofer diffraction patterns for arbitrary (orientable) polygons can be calculated simply by substituting the vertex values into (32). It is interesting to compare the patterns generated for a given set of vertices as the vertices are reordered to make the polygon nonorientable.

4 Results in Three Dimensions

Before discussing Porod’s law we point out an essentially obvious but useful fact. Since the faces of a polyhedron are themselves polyhedra it follows that applying (5) to a polyhedron reduces the integral over the volume to a sum of integrals over the areas of polygonal faces and then applying (32) to the faces themselves reduces the volume integral to a sum of integrals over the edges. These integrals can of course be evaluated exactly. The only issue is the bookkeeping required to keep proper track of the vertices.

4.1 Volume Element

We use (5) to show that the volume in three dimensions of a parallelepiped formed by three vectors \( \vec{a}_i \) is given by \( \det [a_{ij}] \) where \( a_{ij} \) the 3×3 matrix of the components of the \( \vec{a}_i \), i.e., the first column is \( a_{11} \), the second \( a_{21} \), and the third \( a_{31} \) with of course, \( i = 1, 2, 3 \). If the \( \vec{a}_i \) are infinitesimals given by \( d\vec{R}_i = \partial_x \vec{R} ds_i \) with no sum on \( i \), then \( \det [d\vec{R}_i] \, d^3s \) forms the fundamental volume element \( dv \) for integration. Expanding the right hand side of (5) to first order in \( \beta \) we have that the volume of a shape in three dimension is given by

\[
v = \int_V d^3x = \hat{\beta} \cdot \int_{\partial V} d^2s \sqrt{g(\vec{s})} \hat{n}(\vec{s}) \left( \hat{\beta} \cdot \vec{R}(\vec{s}) \right)
\]

(70)

A parallelepiped, defined by three (non coplanar) vectors \( \vec{a}_i, i = 1, 2, 3 \), in three dimensions has 6 parallelogram faces. The functions \( \vec{R}_f(\vec{s}) \) for positions on the faces with \( f \) labeling the faces, are

\[
\vec{R}_1(\vec{s}) = s_1\hat{a}_1 + s_2\hat{a}_2 \quad \vec{R}_2(\vec{s}) = s_1\hat{a}_2 + s_2\hat{a}_3 \quad \vec{R}_3(\vec{s}) = s_1\hat{a}_3 + s_2\hat{a}_1
\]

\[
\vec{R}_4(\vec{s}) = \hat{a}_3 + s_1\hat{a}_1 + s_2\hat{a}_2 \quad \vec{R}_5(\vec{s}) = \hat{a}_1 + s_1\hat{a}_2 + s_2\hat{a}_3 \quad \vec{R}_6(\vec{s}) = \hat{a}_2 + s_1\hat{a}_3 + s_2\hat{a}_1
\]

(71)

The values of \( s_i \) in each case range from 0 to the corresponding length of the associated vector \( \vec{a}_i \). For example, for \( f = 3 \), \( s_1 \) ranges from 0 to \( |\vec{a}_3| = a_3 \) and \( s_2 \) ranges from 0 to \( |\vec{a}_1| = a_1 \). We assume that the vectors \( \vec{a}_i \) are ordered so that \((\vec{a}_2 × \vec{a}_3)\) points in the general direction of \( \vec{a}_1 \), i.e., \( \vec{a}_1 \cdot (\vec{a}_2 × \vec{a}_3) > 0 \) where “×” is the standard cross product. On each face \( g_f(\vec{s}) \) and \( \hat{n}_f(\vec{s}) \) are constants and so factor out of the integrals. The outward normals \( \hat{n}_f \) on the opposite faces, 1 and 4, 2 and 5, 3 and 6, point in opposite directions. Thus, the integrals over the \( \vec{s} \) dependent parts of \( \vec{R}_f(\vec{s}) \) completely cancel and we are left with

\[
v = \left( \hat{\beta} \cdot \sqrt{g_4} \hat{n}_4 \right) \left( \hat{\beta} \cdot \hat{a}_1 \right) a_1 a_2 + \left( \hat{\beta} \cdot \sqrt{g_5} \hat{n}_5 \right) \left( \hat{\beta} \cdot \hat{a}_1 \right) a_2 a_3 + \left( \hat{\beta} \cdot \sqrt{g_6} \hat{n}_6 \right) \left( \hat{\beta} \cdot \hat{a}_2 \right) a_3 a_1
\]

(72)
But $\hat{\beta}$ is arbitrary. Choose it to be $\hat{a}_1$. Then since $\hat{n}_4 = (\hat{a}_1 \times \hat{a}_2) / |\hat{a}_1 \times \hat{a}_2|$ and $\hat{n}_6 = (\hat{a}_3 \times \hat{a}_1) / |\hat{a}_3 \times \hat{a}_1|$, we have $\hat{a}_1 \cdot \hat{n}_4 = \hat{a}_1 \cdot \hat{n}_6 = 0$ and $v$ reduces to

$$v = (\hat{a}_1 \cdot \sqrt{g_5} \hat{n}_5) a_1 a_2 a_3$$

But, as shown above in the derivation of the area element in two dimensions, $\sqrt{g}$ is the sine of the angle between the two corresponding vectors and so equals the magnitude of the cross product of those vectors, hence $\sqrt{g_5} = |\hat{a}_2 \times \hat{a}_3|$ and thus $\sqrt{g_5} \hat{n}_5 = \hat{a}_2 \times \hat{a}_3$. So finally

$$v = \hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3) a_1 a_2 a_3$$

$$= \hat{a}_1 \cdot \hat{a}_2 \times \hat{a}_3$$

$$= \varepsilon_{ijk} a_1 a_2 a_3 k$$

$$= \det [a_{ij}]$$

$$= \sqrt{ \det [\hat{a}_i \cdot \hat{a}_j] }$$

Again the form in the last line is the most useful since it is coordinate independent.

### 4.2 Porod's Law

Finally, we rederive the anisotropic version of Porod's law as given in the work of Cicciariello, et al. [12]. The anisotropic result of course reduces to the isotropic result for spherical particles. Here we use the notation $\vec{k}$ rather than $\vec{\beta}$ as is more common in this context.

The intensity $I \left( \vec{k} \right) = I \left( \vec{k} \hat{k} \right) = I \left( \frac{2\pi}{\lambda} \vec{k} \right)$ of light of wavelength $\lambda$ scattered off a particle defined by the shape function $\theta_\nu \left( \vec{x} \right)$ in the direction $\vec{k} = \hat{k}_{out} - \hat{k}_{in}$ where $\hat{k}_{in} \left( \vec{k}_{out} \right)$ is the direction of propagation of incident (scattered) light is

$$I \left( \vec{k} \right) \sim \left| \int d^Dx \exp \left[ i\vec{k} \cdot \vec{x} \right] \theta_\nu \left( \vec{x} \right) \right|^2$$

To be general, for now, we start in $D$ dimensions. Porod's law [12] follows from this in the case where the magnitude of the scattering wavevector $k = \mid \vec{k} \mid = 2\pi / \lambda$ is large, i.e., $\lambda$ is small and so Porod's law is often associated with X-ray scattering.

To obtain Porod's law, use (5) and evaluate the integral over $\partial V$ in the limit of large $k$ using the method of stationary phase. The positions $\vec{s}_p$ on the surface $\vec{R} \left( \vec{s} \right)$ where the phase is stationary satisfy

$$\partial_s \left( \vec{k} \cdot \vec{R} \left( \vec{s} \right) \right)_{\vec{s} = \vec{s}_p} = k \partial_s \left( \vec{k} \cdot \vec{R} \left( \vec{s} \right) \right)_{\vec{s} = \vec{s}_p} = 0$$

(76)

Here $\partial_s = (\partial_{s_1}, \partial_{s_2}, \cdots)$ is the gradient with respect to the surface coordinates and the index $p$ runs from 1 up to the number of solutions of (76).

For simplicity consider a single solution $\vec{s}$ to this equation. The argument of the exponential in the integrand can now be approximated by

$$i\vec{k} \cdot \vec{R} \left( \vec{s} \right) = ik \left( \vec{k} \cdot \vec{R} \left( \vec{s} \right) + \frac{1}{2} \partial_{s_i} \partial_{s_j} \vec{k} \cdot \vec{R} \left( \vec{s} \right) (s_i - \sigma_i) (s_j - \sigma_j) \right)$$

(77)
to second order in \( \mathbf{s} - \mathbf{\bar{\sigma}} \). Substituting into (5) gives

\[
\int_V d^D x \exp \left[ i \hat{\mathbf{k}} \cdot \mathbf{x} \right] \\
\simeq \exp \left[ i k \hat{\mathbf{k}} \cdot \hat{\mathbf{R}}(\mathbf{\bar{\sigma}}) \right] \frac{k}{ik} \int d^{D-1} s \sqrt{g(s)} \hat{n}(\mathbf{s}) \exp \left[ i k \left( \partial_{\sigma_i} \partial_{\sigma_j} \hat{\mathbf{k}} \cdot \hat{\mathbf{R}}(\mathbf{\bar{\sigma}}) \right) (s_i - \sigma_i)(s_j - \sigma_j) \right] \\
\simeq \exp \left[ i k \hat{\mathbf{k}} \cdot \hat{\mathbf{R}}(\mathbf{\bar{\sigma}}) \right] \frac{k}{ik} \hat{n}(\mathbf{\bar{\sigma}}) \frac{\sqrt{g(\mathbf{\bar{\sigma}})} \pi^{(D-1)/2}}{\sqrt{\det \left[ -\frac{i k}{2} \partial_{\sigma_i} \partial_{\sigma_j} \hat{\mathbf{k}} \cdot \hat{\mathbf{R}}(\mathbf{\bar{\sigma}}) \right]}} \tag{78}
\]

where the determinant in the denominator is taken over the \( i, j \) indices. Using the fact that

\[
\det \left[ -\frac{i k}{2} \partial_{\sigma_i} \partial_{\sigma_j} \hat{\mathbf{k}} \cdot \hat{\mathbf{R}}(\mathbf{\bar{\sigma}}) \right] = k^{D-1} \det \left[ -\frac{i}{2} \partial_{\sigma_i} \partial_{\sigma_j} \hat{\mathbf{k}} \cdot \hat{\mathbf{R}}(\mathbf{\bar{\sigma}}) \right]
\]

we get

\[
\int_V d^D x \exp \left[ i \hat{\mathbf{k}} \cdot \mathbf{x} \right] \sim \frac{1}{k k^{(D-1)/2}} = \frac{1}{k^{(D+1)/2}} \tag{79}
\]

and so

\[
I(\hat{\mathbf{k}}) \sim \frac{1}{k^{D+1}} \tag{80}
\]

Thus in 3 dimensions \( I(\hat{\mathbf{k}}) \) scales as \( 1/k^4 \) for large \( k \). This is the standard isotropic statement of Porod’s law [3]. But as pointed out by Cicciariello, \( \det \left[ -\frac{i k}{2} \partial_{\sigma_i} \partial_{\sigma_j} \hat{\mathbf{k}} \cdot \hat{\mathbf{R}}(\mathbf{\bar{\sigma}}) \right] \) is proportional to the Gaussian curvature (in 3 dimensions) of the surface \( \partial V \). In general for an arbitrary shaped particle there will be multiple stationary phase points, i.e., \( \mathbf{\bar{\sigma}}_1, \mathbf{\bar{\sigma}}_2, \ldots \) which must be summed to get the complete amplitude. There are also issues with positive and negative curvature which must be carefully considered as well along with how the handle the case when the curvature vanishes [12].

## 5 Conclusion

We have shown how a simple idea, that of combining Gauss’s law with the Fourier transform provides alternative solutions and/or derivations of many different classical results in physics and mathematics. No doubt there are many other problems and proofs to which this idea can be applied.

## References

[1] Simply connected here means that the shape is a single connected area in two dimensions, a single connected volume in three dimensions and not multiple disconnected shapes. By orientable here we mean simply that the boundary manifold of the shape (the curve enclosing an area in two dimensions, the surface enclosing a volume in three dimensions, etc.) does not intersect itself.

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