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Fourier, Gauss, Fraunhofer, Porod and the shape from moments problem

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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 in 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, Porod's law, the shape from moments problem, and Davis's extension of the Motzkin-Schoenberg formula to polygons in the complex plane. [doi:10.1063/1.3676310]

I. 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 Porod's 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 co-workers[4,5] and is related to the overall problem of pattern recognition.

We will not discuss the details here, but the Fourier transform of an area bounded by a smooth curve or a polygon in the plane can also be related to Hopf's Umlaufsatz,[6] Stokes law,[7] the isoperimetric inequality,[8] and Didos' problem.[9] Hopf's Umlaufsatz states that the tangent vector to a smooth or piecewise smooth closed orientable simply connected curve in the plane rotates by $\pm 2\pi$ 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] The isoperimetric inequality is the statement that the shape which maximizes the area enclosed by a curve of a fixed length is the circle.[8] The problem faced by Dido, Queen of Carthage, 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]

As an aside, the Fourier transform is just one of the many techniques that are used for shape discrimination.[10] This problem is both mathematically interesting, and, given the ubiquity of digital databases, 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

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generally different from, the issues concerned with using Fourier transforms explicitly for shape discrimination in digital databases and we will not discuss this aspect further.

The paper is organized as follows. In Sec. II, 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. In Sec. II, we show how this surface integral yields the standard form for the area enclosed inside a smooth curve. We evaluate this integral exactly for polygons in two dimensions which then provides an explicit relation between the vertices of a polygon and its moments. We also 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[4,11] and how the surface integral can be used to compute Fraunhofer diffraction patterns of arbitrary shaped apertures. Section III briefly discusses how the solution for two-dimensional polygons appears when Fourier transforming three-dimensional polyhedrons and how the surface integral form of the Fourier transform can be used to compute volumes and 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 *et al.*[12] The derivation presented here is somewhat more direct.

II. FOURIER AND GAUSS

For generality, we begin in D dimensions but will rapidly particularize to two and three 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 $i = 1, 2, \ldots, D$ to be Cartesian coordinates. The (normalized) moments $\langle x_1^{p_1} \cdots x_D^{p_m} \rangle$ of the shape are then given by

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

where $\int_V = \int \theta_V$ indicates integration over the shape, $v = \int d^D x \theta_V(\vec{x})$ is the finite volume of the shape, and $p_i = 0, 1, 2, 3, \ldots$ 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 $\bar{\phi}\left(\vec{\beta}\right)$ is then given by the Fourier transform of $\theta_V(\vec{x})/v$, i.e.,

$$\bar{\phi}\left(\vec{\beta}\right) = \frac{1}{v} \int_V d^D x \theta_V(\vec{x})\; e^{i\vec{\beta}\cdot\vec{x}}, \tag{2}$$

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 ϕ 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 un-normalized function $\phi\left(\vec{\beta}\right)$.

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

$$\begin{aligned}\bar{\phi}\left(\vec{\beta}\right) &= \frac{1}{v} \int_V d^D x \sum_{n=0}^{\infty} \frac{(i\beta_i x_i)^n}{n!} \\ &= \sum_{n=0}^{\infty} \frac{i^n}{n!} \sum_{p_1+p_2+\cdots+p_D=n} \frac{n!}{p_1!p_2!\cdots p_D!} \beta_1^{p_1} \cdots \beta_D^{p_D} \langle x_1^{p_1} \cdots x_D^{p_D} \rangle.\end{aligned} \tag{3}$$

This result indicates the simple but direct relation that exists between the Fourier transform of a shape and its moments $\langle x_1^{p_1} \cdots x_D^{p_D} \rangle$. We have assumed that we can interchange orders of integration and summation. This is certainly true for all shapes which can be completely enclosed inside a sphere of finite radius.

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

$$e^{i\vec{\beta}\cdot\vec{x}} = \vec{\partial} \cdot \left(\frac{\vec{\beta}}{i\beta^2} e^{i\vec{\beta}\cdot\vec{x}} \right), \tag{4}$$

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

$$\begin{aligned} \int_V d^D x e^{i\vec{\beta}\cdot\vec{x}} &= \int_V d^D x \ \vec{\partial} \cdot \left(\frac{\vec{\beta}}{i\beta^2} e^{i\vec{\beta}\cdot\vec{x}} \right) \\ &= \frac{\vec{\beta}}{i\beta^2} \cdot \int_{\partial V} d^{D-1}s \ \sqrt{g\left(\vec{s}\right)} \hat{n}\left(\vec{s}\right) e^{i\vec{\beta}\cdot\vec{R}(\vec{s})}. \end{aligned} \tag{5}$$

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

$$g\left(\vec{s}\right) = \left| \det\left[g_{ij}\left(\vec{s}\right) \right] \right| = \left| \det\left[\partial_{s_i} \vec{R}\left(\vec{s}\right) \cdot \partial_{s_j} \vec{R}\left(\vec{s}\right) \right] \right|, \tag{6}$$

where $g_{ij}\left(\vec{s}\right)$ is the induced metric on ∂V, $\hat{n}\left(\vec{s}\right)$ is the local outward normal to the surface ∂V, and $|\ldots|$ indicates the absolute value.[14] Below, we show why the square root appears (see (32) and (54)).

Combining (3) and (5) yields

$$\begin{aligned} &\frac{1}{v} \frac{\vec{\beta}}{i\beta^2} \cdot \int_{\partial V} d^{D-1}s \ \sqrt{g\left(\vec{s}\right)} \hat{n}\left(\vec{s}\right) \cdot e^{i\vec{\beta}\cdot\vec{R}(s)} \\ &= \sum_{n=0}^{\infty} \frac{i^n}{n!} \sum_{p_1+p_2+\cdots+p_m=n} \frac{n!}{p_1! p_2! \cdots p_D!} \beta_1^{p_1} \cdots \beta_D^{p_D} \langle x_1^{p_1} \cdots x_D^{p_D} \rangle. \end{aligned} \tag{7}$$

It will be convenient below to work with the un-normalized form of the characteristic function,

$$\phi\left(\vec{\beta}\right) = v\bar{\phi}\left(\vec{\beta}\right), \tag{8}$$

and write the un-normalized moments as

$$M_{p_1,\cdots,p_D} = v\langle x_1^{p_1} \cdots x_D^{p_D} \rangle = \int d^D x \theta_V\left(\vec{x}\right) x_1^{p_1} \cdots x_D^{p_D}. \tag{9}$$

Before particularizing to two and three dimensions, note that expanding the left-hand side of (7) in powers of $\beta = \left|\vec{\beta}\right|$ yields to lowest order a term proportional to $1/i\beta$. This term must vanish, since there is no corresponding power of β on the right and we get the result that

$$\int_{\partial V} d^{D-1}s \ \sqrt{g\left(\vec{s}\right)} \hat{n}\left(\vec{s}\right) = 0, \tag{10}$$

because $\hat{\beta}$ is arbitrary. This can be interpreted as the statement that "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 next order term yields

$$\hat{\beta} \cdot \int_{\partial V} d^{D-1}s \ \sqrt{g\left(\vec{s}\right)} \hat{n}\left(\vec{s}\right) \left(\hat{\beta} \cdot \vec{R}\left(\vec{s}\right) \right), \tag{11}$$

where $\hat{\beta} = \vec{\beta}/\left|\vec{\beta}\right|$. This is the D-dimensional volume v of V. Although this formula looks straightforward, it is actually exceedingly complex to calculate the volume of arbitrary shapes in a large number of dimensions.[16]

The remainder of the paper considers particular cases in two or three dimensions where $\phi\left(\vec{\beta}\right)$ can be computed from the surface integral, either exactly or approximately, and we relate these results to various "classical" problems in physics and mathematics.

III. RESULTS IN TWO DIMENSIONS

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

A. Smooth plane curves

For smooth curves in two dimensions, (5) reduces to

$$\int_V d^2x e^{i\vec{\beta}\cdot\vec{x}} = \frac{\vec{\beta}}{i\beta^2}\cdot\int_{\partial V} ds\hat{n}\left(s\right)e^{i\vec{\beta}\cdot\vec{R}(s)}, \tag{12}$$

where V is the region enclosed by the curve ∂V given by $\vec{R}\left(s\right)$ with the parameter s being the length along the curve. With ds defined as the length of an infinitesimal element of 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

$$\hat{t}\left(s\right) = \partial_s\vec{R}\left(s\right), \tag{13}$$

which is automatically normalized since $ds = \sqrt{d\vec{R}^2}$, i.e., $\left|\partial_s\vec{R}\left(s\right)\right| = 1$. (Generally we will use a hat "^" 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

$$\hat{n}\left(s\right) = \varepsilon\cdot\hat{t}\left(s\right) = \varepsilon\cdot\partial_s\vec{R}\left(s\right), \tag{14}$$

where

$$\varepsilon = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{15}$$

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

$$n_i\left(s\right) = \varepsilon_{ij}n_j\left(s\right), \tag{16}$$

with repeated indices summed over 1,2. Note that ε is the $D = 2$ version of the totally antisymmetric tensor, often called the Levi-Civita tensor,[17] defined as $+1$ for even permutations, of $i, j = 1, 2$, -1 for odd permutations, and 0 if $i = j$.

Substituting (14) into (12) and integrating by parts yields

$$\begin{aligned}\int_V d^2xe^{i\vec{\beta}\cdot\vec{x}} &= -\frac{1}{i\beta^2}\int_{\partial V} ds\ \left(\vec{\beta}\cdot\varepsilon\cdot\vec{R}\left(s\right)\right)\left(i\vec{\beta}\cdot\partial_s\vec{R}\left(s\right)\right)e^{i\vec{\beta}\cdot\vec{R}(s)} \\ &= -\int_{\partial V} ds\ \left(\hat{\beta}\cdot\varepsilon\cdot\vec{R}\left(s\right)\right)\left(\hat{\beta}\cdot\partial_s\vec{R}\left(s\right)\right)e^{i\vec{\beta}\cdot\vec{R}(s)}.\end{aligned} \tag{17}$$

The nominal $1/\beta$ pole in (12) has been cancelled and we can set β to zero for arbitrary nonzero $\hat{\beta} = \vec{\beta}/\left|\vec{\beta}\right|$ which gives

$$v = \int_V d^2x = -\int_{\partial V} ds\ \left(\hat{\beta}\cdot\varepsilon\cdot\vec{R}\left(s\right)\right)\left(\hat{\beta}\cdot\partial_s\vec{R}\left(s\right)\right). \tag{18}$$

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

$$v = -\int_{\partial V} ds\ R_2(s)\,\partial_s R_1(s) = \int_{\partial V} ds\ R_1(s)\,\partial_s R_2(s). \tag{19}$$

Averaging the two forms gives

$$\begin{aligned} v &= \frac{1}{2}\int_{\partial V} ds\ \left(R_1(s)\,\partial_s R_2(s) - R_2(s)\,\partial_s R_1(s)\right) \\ &= \frac{1}{2}\int_{\partial V} ds\ R_i(s)\,\varepsilon_{ij}\partial_s R_j(s). \end{aligned} \tag{20}$$

Both (19) and (20) are standard formulas for the area enclosed by the curve $\vec{R}(s)$.[18]

B. 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 $\vec{v}_i = (x_{1i}, x_{2i})$. For computational convenience, it is useful to let $\vec{v}_{N+1} = \vec{v}_1$. We consider only orientable, i.e., none of the edges cross over or intersect one another, and simply connected polygons. The integral over ∂V in (7) can be evaluated explicitly in this case with the result

$$\begin{aligned} \phi\left(\vec{\beta}\right) &= \frac{\vec{\beta}}{i\beta^2}\cdot\int_{\partial V} d^{D-1}s\ \hat{n}(\vec{s})\cdot e^{i\vec{\beta}\cdot\vec{R}(s)} \\ &= -\frac{1}{\beta^2}\sum_{n=1}^{N}\frac{\vec{\beta}_\perp\cdot(\vec{v}_{n+1}-\vec{v}_n)}{\vec{\beta}\cdot(\vec{v}_{n+1}-\vec{v}_n)}\left(\exp\left(i\vec{\beta}\cdot\vec{v}_{n+1}\right)-\exp\left(i\vec{\beta}\cdot\vec{v}_n\right)\right), \end{aligned} \tag{21}$$

where

$$\vec{\beta}_\perp \equiv \vec{\beta}\cdot\varepsilon = (\beta_1, \beta_2)\cdot\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} = (\beta_2, -\beta_1). \tag{22}$$

The "$\cdot$" stands for standard matrix vector multiplication. Note that (21) makes sense, even if $\vec{\beta}\cdot(\vec{v}_{n+1}-\vec{v}_n)$ vanishes for any given n.

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

$$\begin{aligned} &\sum_{n=0}^{\infty}\frac{i^n}{n!}\sum_{p=0}^{n}\frac{n!}{p!\,(n-p)!}\beta_1^p\beta_2^{(n-p)}M_{p,n-p} \\ &= -\frac{1}{\beta^2}\sum_{n=1}^{N}\frac{\vec{\beta}_\perp\cdot(\vec{v}_{n+1}-\vec{v}_n)}{\vec{\beta}\cdot(\vec{v}_{n+1}-\vec{v}_n)}\left(\exp\left(i\vec{\beta}\cdot\vec{v}_{n+1}\right)-\exp\left(i\vec{\beta}\cdot\vec{v}_n\right)\right). \end{aligned} \tag{23}$$

Now expand the right-hand side in powers of β_i,

$$\begin{aligned} &\frac{1}{\beta^2}\sum_{n=1}^{N}\frac{\vec{\beta}_\perp\cdot(\vec{v}_{n+1}-\vec{v}_n)}{\vec{\beta}\cdot(\vec{v}_{n+1}-\vec{v}_n)}\left(\exp\left(i\vec{\beta}\cdot\vec{v}_{n+1}\right)-\exp\left(i\vec{\beta}\cdot\vec{v}_n\right)\right) \\ &= \frac{1}{\beta^2}\sum_{n=1}^{N}\frac{\vec{\beta}_\perp\cdot(\vec{v}_{n+1}-\vec{v}_n)}{\vec{\beta}\cdot(\vec{v}_{n+1}-\vec{v}_n)}\left(\sum_{m=1}^{\infty}\frac{\left(i\vec{\beta}\cdot\vec{v}_{n+1}\right)^m-\left(i\vec{\beta}\cdot\vec{v}_n\right)^m}{m!}\right) \\ &= \frac{1}{\beta^2}\sum_{m=1}^{\infty}\sum_{n=1}^{N}\frac{i}{m!}\vec{\beta}_\perp\cdot(\vec{v}_{n+1}-\vec{v}_n)\sum_{p=0}^{m-1}\left(i\vec{\beta}\cdot\vec{v}_{n+1}\right)^{m-1-p}\left(i\vec{\beta}\cdot\vec{v}_n\right)^p, \end{aligned} \tag{24}$$

where $\beta^2 = \vec{\beta}^2 = \beta_i \beta_i = \beta_1^2 + \beta_2^2$. In the second step, we have used the identity

$$a^n - b^n = (a-b)\sum_{m=0}^{n-1} a^{n-1-m} b^m. \tag{25}$$

Substituting (24) into (23) gives

$$\sum_{n=0}^{\infty} \frac{i^n}{n!} \sum_{p=0}^{n} \frac{n!}{p!\,(n-p)!} \beta_1^p \beta_2^{n-p} M_{p,n-p}$$
$$= -\frac{1}{\beta^2} \sum_{m=1}^{\infty} \sum_{n=1}^{N} \frac{i}{m!} \vec{\beta}_\perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \sum_{p=0}^{m-1} \left(i\vec{\beta} \cdot \vec{v}_{n+1} \right)^{m-1-p} \left(i\vec{\beta} \cdot \vec{v}_n \right)^p. \tag{26}$$

Letting $\vec{\beta} = \beta \hat{\beta}$ and $\vec{\beta}_\perp = \beta \hat{\beta}_\perp$, we see that the nth term on the left-hand side is proportional to β^n, whereas the mth term on the right is proportional to $\beta^{m\,-\,2}$. Hence, considering each side as a power series in β, 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 $M_{a,\,b}$ and powers of the vertices. Here, we begin by considering the first few terms individually.

1. m = 1 term

The $m = 1$ term on the right of (26) has no corresponding term on the left, and so, we must have

$$0 = \frac{i}{\beta^2} \vec{\beta}_\perp \cdot \sum_{n=1}^{N} (\vec{v}_{n+1} - \vec{v}_n). \tag{27}$$

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 ∂V is everywhere smooth, the form of the dominant term as $\beta \to 0$ is given by

$$\lim_{\beta \to 0} \frac{\vec{\beta}}{i\beta^2} \cdot \int_{\partial V} ds\ \hat{n}(s)\, e^{i\vec{\beta}\cdot\vec{R}(s)} \to \frac{\hat{\beta}}{i\beta} \cdot \int_{\partial V} ds\ \hat{n}(s) \Rightarrow \int_{\partial V} ds\ \hat{n}(s) = 0. \tag{28}$$

The last equality follows from the fact that this term must vanish for any (non-zero) $\vec{\beta}$. The results in (27) and (28) can be seen as a simple version of the more formal statement that the boundary of a boundary is zero,[15] i.e., the curve which bounds an area in two dimensions has no end points. They can also be related to Hopf's Umlaufsatz.[6]

2. m = 2 term

The $m = 2$ term on the right of (26) equals the $n = 0$ term on the left, and so, we have

$$M_{00} = -\frac{i}{2}\frac{1}{\beta^2} \sum_{n=1}^{N} \vec{\beta}_\perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \sum_{p=0}^{1} \left(i\vec{\beta} \cdot \vec{v}_{n+,1} \right)^{1-p} \left(i\vec{\beta} \cdot \vec{v}_n \right)^p$$
$$= -\frac{i}{2}\frac{1}{\beta^2} \sum_{n=1}^{N} \left(\vec{\beta}_\perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \right) \left(i\vec{\beta} \cdot \vec{v}_{n+1} + i\vec{\beta} \cdot \vec{v}_n \right)$$
$$= \frac{1}{2} \sum_{n=1}^{N} \left(\hat{\beta}_\perp \cdot (\vec{v}_{n+1} - \vec{v}_n) \right) \left(\hat{\beta} \cdot (\vec{v}_{n+1} + \vec{v}_n) \right). \tag{29}$$

But, by definition $M_{0,\,0}$ 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

$$M_{0,0} = Area = \sum_{n=1}^{N} \left(\hat{\beta}_\perp \cdot \vec{l}_n\right)\left(\hat{\beta} \cdot \vec{c}_n\right). \tag{30}$$

Taking $\hat{\beta} = (0, 1)$ gives $\hat{\beta}_\perp = (-1, 0)$, and so,

$$Area = -\sum_{n=1}^{N} l_{n,1} c_{n,2}. \tag{31}$$

The geometric interpretation of this is straightforward. Each of the $l_{n,\,1}c_{n,\,2}$ terms corresponds to the area of a four-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, $v_{n,\,i} \geq 0$ for $i = 1, 2$, then all the $c_{n,\,2}$ are non-negative 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 four-sided polygons along the bottom of the net polygon subtracted from the area of the four-sided polygons along the top of the net polygon.

Taking 1/2 the sum of (30) with $\hat{\beta} = (0, 1)$ and with $\hat{\beta} = (1, 0)$, we find that the area can also be written as $\frac{1}{2}\sum_{n=1}^{N} \det[Q_n]$ where the elements of the 2×2 matrices Q_n are given by $Q_{n,\,ij} = v_{n,\,i} v_{n\,+\,1,\,j}$, which is the standard result.[19]

Finally, (30) also shows that the area of a parallelogram formed by two vectors $\vec{a}_i$ with $i = 1, 2$ which therefore has vertices $\vec{v}_1 = \vec{v}_5 = 0$, $\vec{v}_2 = \vec{a}_1$, $\vec{v}_3 = \vec{a}_1 + \vec{a}_2$, and $\vec{v}_4 = \vec{a}_2$ can be written in the coordinate independent form as

$$Area = \sqrt{\left|\det\begin{bmatrix} \vec{a}_1 \cdot \vec{a}_1 & \vec{a}_1 \cdot \vec{a}_2 \\ \vec{a}_1 \cdot \vec{a}_2 & \vec{a}_2 \cdot \vec{a}_2 \end{bmatrix}\right|} = a_{1,1}a_{2,2} - a_{1,2}a_{2,1} = \det\left[a_{i,j}\right]. \tag{32}$$

This follows since for the parallelogram, (30) reduces to

$$\begin{aligned} Area &= \left(\hat{\beta}_\perp \cdot \vec{a}_2\right)\left(\hat{\beta} \cdot \vec{a}_1\right) - \left(\hat{\beta}_\perp \cdot \vec{a}_1\right)\left(\hat{\beta} \cdot \vec{a}_2\right) \\ &= \vec{a}_1 \cdot \varepsilon \cdot \vec{a}_2 \\ &= a_{1,1}a_{2,2} - a_{1,2}a_{2,1}, \end{aligned} \tag{33}$$

where in the second step we have taken $\hat{\beta} = \hat{a}_1$. Note that this is the same as $|\vec{a}_1 \times \vec{a}_2|$ with " $\times$ " the standard cross product.

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

$$\hat{\beta}_1 M_{1,0} + \hat{\beta}_2 M_{0,1} = \frac{1}{3!}\sum_{n=1}^{N} \hat{\beta}_\perp \cdot (\vec{v}_{n+1} - \vec{v}_n)\left(\left(\hat{\beta} \cdot \vec{v}_{n+1}\right)^2 + \left(\hat{\beta} \cdot \vec{v}_{n+1}\right)\left(\hat{\beta} \cdot \vec{v}_n\right) + \left(\hat{\beta} \cdot \vec{v}_n\right)^2\right). \tag{34}$$

It follows from the definition of $M_{a,\,b}$ that

$$M_{1,0} = Area \times X_1 \text{ and } M_{0,1} = Area \times X_2, \tag{35}$$

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

$$M_{1,0} = \frac{1}{3!}\sum_{n=1}^{N} \left(v_{n+1,2} - v_{n,2}\right)\left(v_{n+1,1}^2 + v_{n,1}^2 + v_{n+1,1}v_{n,1}\right), \tag{36}$$

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

$$M_{0,1} = -\frac{1}{3!}\sum_{n=1}^{N}\left(v_{n+1,1} - v_{n,1}\right)\left(v_{n+1,2}^2 + v_{n,2}^2 + v_{n+1,2}v_{n,2}\right). \tag{37}$$

Explicit evaluation of

$$\int_V dx_1 dx_2 x_i, \tag{38}$$

with $i = 1$ or 2 by substituting $x_i = \vec{\partial}\cdot\left(x_i^2\hat{x}_i/2\right)$, with no sum on i, yields the same result as (36) and (37), respectively.

C. 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,

$$\int_V dxdy\partial_z^2 h(z) = \frac{i}{2}\sum_{n=1}^{N}\left(\frac{z_{n-1}^* - z_n^*}{z_{n-1} - z_n} - \frac{z_n^* - z_{n+1}^*}{z_n - z_{n+1}}\right)h(z_n). \tag{39}$$

Here, V is a simply connected orientable polygon with vertices $z_n = x_n + iy_n$ $\left(z_n^* = z_n - iy_n\right)$, $n = 1, \ldots, N$, 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,

$$h(z) = \sum_{n=0}^{\infty} a_n z^n. \tag{40}$$

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

$$a_n = \int_{-\infty}^{+\infty} d\beta\tilde{h}(\beta)\frac{(i\beta)^n}{n!}. \tag{41}$$

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

$$\tilde{h}(\beta) = \sum_{n=0}^{\infty} A_n P_n(\beta), \tag{42}$$

where $P_n(\beta)$ are Legendre polynomials. With this representation, the complex coefficients A_n can be chosen to satisfy (41).

Substituting (41) into (40), interchanging orders of integration and summation, we get

$$h(z) = \int_{-1}^{+1} d\beta\tilde{h}(\beta)\sum_{n=0}^{\infty}\frac{(i\beta z)^n}{n!} = \int_{-1}^{+1} d\beta\tilde{h}(\beta)e^{i\beta z}, \tag{43}$$

which is the analytic continuation of $h(x) = \sum_{n=0}^{\infty} a_n x^n$.

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

$$
\begin{aligned}
\int_V dxdy\partial_z^2 h(z) &= -\int_{-1}^{+1} d\beta \tilde{h}(\beta) \int_V dxdy \beta^2 e^{i\beta z} \\
&= \frac{i}{2}\int_{-1}^{+1} d\beta \tilde{h}(\beta) \int_V dxdy \left(\partial_x, \partial_y\right) \cdot \beta(1, -i) \exp\left[i\beta(1, i)\cdot(x, y)\right] \\
&= \frac{1}{2}\int_{-1}^{+1} d\beta \tilde{h}(\beta) \sum_{n=1}^{N} \frac{\beta(1, -i)\cdot \varepsilon \cdot \left((x, y)_{n+1} - (x, y)_n\right)}{\beta(1, i)\cdot\left((x, y)_{n+1} - (x, y)_n\right)} \\
&\qquad \times \left(\exp\left(i\beta(1, i)\cdot(x, y)_{n+1}\right) - \exp\left(i\beta(1, i)\cdot(x, y)_n\right)\right) \\
&= \frac{i}{2}\int_{-1}^{+1} d\beta \tilde{h}(\beta) \sum_{n=1}^{N} \left(\frac{z_n^* - z_{n-1}^*}{z_n - z_{n-1}} - \frac{z_{n+1}^* - z_n^*}{z_{n+1} - z_n}\right) \exp\left(i\beta z_n\right) \\
&= \frac{i}{2}\sum_{n=1}^{N} \left(\frac{z_{n-1}^* - z_n^*}{z_{n-1} - z_n} - \frac{z_n^* - z_{n+1}^*}{z_n - z_{n+1}}\right) h\left(z_j\right). \qquad (44)
\end{aligned}
$$

In the third line, ε is the matrix defined in (15). In the second step, we have used (5), and in the last step, we have used the definition of $h(z)$ in terms of its Fourier transform. The β'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 $\partial_z^2 h(z)$ 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 co-workers[4,5] 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 $M_{a,b}$ 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) by $\beta^2 = \beta_1^2 + \beta_2^2$ 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 are negative and equal 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 β_1 and β_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 $\vec{v}_n = \left(x_{1,n}, x_{2,n}\right)$,

$$
\begin{aligned}
&\theta(a-2)\frac{M_{a-2,b}}{(a-2)!b!} + \theta(b-2)\frac{M_{a,b-2}}{a!(b-2)!} \\
&= \theta(b-1, a+b-2)\sum_{q=0}^{a}\sum_{p=0}^{a+b-1-q}\left(\begin{array}{c}\theta(p+q-a)\frac{1}{(a+b)!}\frac{(a+b-1-p)!}{q!(a+b-1-p-q)!}\frac{p!}{(a-q)!(p+q-a)!} \\ \times\sum_{n=1}^{N}\left(x_{1,n+1} - x_{1,n}\right)x_{1,n+1}^{q}x_{2,n+1}^{a+b-1-p-q}x_{1,n}^{a-q}x_{2,n}^{p+q-a}\end{array}\right) \\
&- \theta(a-1, a+b-2)\sum_{q=0}^{a-1}\sum_{p=0}^{a+b-1-q}\left(\begin{array}{c}\theta(p+q+1-a)\frac{1}{(a+b)!}\frac{(a+b-1-p)!}{q!(a+b-1-p-q)!}\frac{p!}{(a-q-1)!(p+q+1-a)!} \\ \times\sum_{n=1}^{N}\left(x_{2,n+1} - x_{2,n}\right)x_{2,n+1}^{q}x_{2,n+1}^{a+b-1-p-q}x_{1,n}^{a-q-1}x_{2,n}^{p+q+1-a}\end{array}\right). \qquad (45)
\end{aligned}
$$

The derivation is straightforward but tedious.

D. 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 the aperture itself.[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 λ 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

$$A(\vec{x}) = \int d^2x'\theta_V(\vec{x}')\exp\left[i\frac{k}{L}x_ix_i'\right] = \int\limits_V d^2x'\exp\left[i\frac{k}{L}x_ix_i'\right]. \tag{46}$$

Here, $\theta_V(x_i) = 1$ 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

$$\beta_i = \frac{kx_i}{L} \tag{47}$$

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 (21).

For a circular aperture of radius R centered at $x_i = 0$, it follows from (5) that

$$A(\vec{x}) = \frac{\vec{\beta}R}{i\beta^2}\cdot\int\limits_0^{2\pi} d\varphi\hat{r}(\varphi)\exp\left[i\vec{\beta}\cdot R\hat{r}(\varphi)\right], \tag{48}$$

with $\hat{r}(\varphi) = \vec{x}'/\left|\vec{x}'\right|$. Writing $\vec{\beta}\cdot\hat{r}(\varphi) = \beta\cos\left(\varphi - \varphi_\beta\right)$, where φ_β is the angle $\vec{\beta}$ makes with respect to the x_1-axis and $\beta = \left|\vec{\beta}\right| = k\sqrt{x^2+y^2}/L$, (48) becomes

$$\begin{aligned} A(\vec{x}) &= \frac{R}{i\beta}\int\limits_0^{2\pi} d\varphi\cos\left(\varphi-\varphi_\beta\right)\exp\left[i\beta R\cos\left(\varphi-\varphi_\beta\right)\right] \\ &= \frac{R}{i\beta}\frac{-i}{\beta}\partial_R\int\limits_0^{2\pi} d\varphi\exp\left[i\beta R\cos(\varphi)\right] \\ &= -\frac{R}{\beta^2}2\pi\,\partial_R J_0(\beta R) \\ &= \pi R^2\left(\frac{2J_1(\beta R)}{\beta R}\right). \end{aligned} \tag{49}$$

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 $2a_i$ in the x_i direction, centered at $x_i = 0$, 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 (21) to obtain

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

$$= \frac{1}{\beta^2}\left(\begin{array}{l} \frac{\beta_2}{\beta_1}\left(\exp\left(-ia_1\beta_1+ia_2\beta_2\right)-\exp\left(i\beta_1a_1+i\beta_2a_2\right)\right) \\ -\frac{\beta_1}{\beta_2}\left(\exp\left(-ia_1\beta_1-ia_2\beta_2\right)-\exp\left(-i\beta_1a_1+i\beta_2a_2\right)\right) \\ +\frac{\beta_2}{\beta_1}\left(\exp\left(ia_1\beta_1-ia_2\beta_2\right)-\exp\left(-i\beta_1a_1-i\beta_2a_2\right)\right) \\ -\frac{\beta_1}{\beta_2}\left(\exp\left(ia_1\beta_1+ia_2\beta_2\right)-\exp\left(+i\beta_1a_1-i\beta_2a_2\right)\right) \end{array}\right)$$

$$= (2a_1)(2a_2)\frac{\sin(\beta_1a_1)}{\beta_1a_1}\frac{\sin(\beta_2a_2)}{\beta_2a_2}, \tag{50}$$

which again is the standard result.[2]

Fraunhofer diffraction patterns for arbitrary (orientable) polygons can be calculated simply by substituting the vertex values into (21). It is interesting to compare the patterns generated for a given set of vertices as the vertices are reordered to make the polygon nonorientable.

IV. 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 polygons, 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 book-keeping required to keep proper track of the vertices.

As an example, consider the parallelepiped formed by three vectors $\vec{a}_i, i = 1, 2, 3$. It has six parallelogram faces with positions on the faces $\vec{R}_f(\vec{s})$ given by

$$\begin{array}{lll} \vec{R}_1(\vec{s}) = s_1\hat{a}_1 + s_2\hat{a}_2 & \vec{R}_2(\vec{s}) = s_1\hat{a}_2 + s_2\hat{a}_3 & \vec{R}_3(\vec{s}) = s_1\hat{a}_3 + s_2\hat{a}_1 \\ \vec{R}_4(\vec{s}) = \vec{a}_3 + \vec{R}_1(\vec{s}) & \vec{R}_5(\vec{s}) = \vec{a}_1 + \vec{R}_2(\vec{s}) & \vec{R}_6(\vec{s}) = \vec{a}_2 + \vec{R}_3(\vec{s}). \end{array} \tag{51}$$

The values of s_i in each case range from 0 to the length of the associated vector, e.g., for $f = 3$, $s_1 = 0$ to $|\vec{a}_3| = a_3$ and $s_2 = 0$ to $|\vec{a}_1| = a_1$. We assume the vectors are ordered so that $\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) > 0$. Expanding the exponent in (5) to first order in β, we find that the volume of V is given by

$$v = \hat{\beta}\cdot\int_{\partial V} d^2s\sqrt{g(\vec{s})}\hat{n}(\vec{s})\left(\hat{\beta}\cdot\vec{R}(\vec{s})\right). \tag{52}$$

For the parallelepiped, g_f and $\hat{n}_f$ are constant on each face. Using the fact that the normals point in opposite directions on opposite faces and choosing $\hat{\beta} = \hat{a}_1$ so that $\hat{a}_1\cdot\hat{n}_4(\vec{s}) = \vec{a}_1\cdot\hat{n}_6(\vec{s}) = 0$, we get

$$v = \left(\hat{a}_1\cdot\sqrt{g_5}\hat{n}_5\right)a_1a_2a_3. \tag{53}$$

But $\int d^2s\sqrt{g_5} = \sqrt{g_5}a_2a_3$ is the area of face 5 which is a parallelogram formed by $\vec{a}_2$ and $\vec{a}_3$. As shown above, it has an area given by $|\vec{a}_2\times\vec{a}_3| = |\hat{a}_2\times\hat{a}_3|\,a_2a_3$ and since $\hat{n}_5 = (\hat{a}_2\times\hat{a}_3)/|\hat{a}_2\times\hat{a}_3|$, we have $\sqrt{g_5}\hat{n}_5 = \hat{a}_2\times\hat{a}_3$ and, so, for the parallelepiped

$$v = \vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = \det\left[a_{i,j}\right] = \sqrt{\det\left[\vec{a}_i\cdot\vec{a}_j\right]}. \tag{54}$$

A. Porod's law

Finally, we rederive the anisotropic version of Porod's law as given in the work of Ciccariello *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 $I\left(\vec{k}\right) = I\left(k\hat{k}\right)$ of light of wavelength $\lambda = 2\pi/\left|\vec{k}\right| = 2\pi/k$ scattered off a particle defined by the shape function $\theta_V\left(\vec{x}\right)$ in the direction $\hat{k} = \hat{k}_{out} - \hat{k}_{in}$, where $\hat{k}_{in}\left(\hat{k}_{out}\right)$ is the direction of propagation of incident(scattered) light, is

$$I\left(\vec{k}\right) \sim \left|\int d^D x \exp\left[i\vec{k}\cdot\vec{x}\right]\theta_V\left(\vec{x}\right)\right|^2. \tag{55}$$

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 wave vector k is large, i.e., λ 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 ∂V in the limit of large k by using the method of steepest descents which assumes that the dominant contribution to the integral comes from the regions around the stationary phase points of the exponential, i.e., from positions $\vec{s} = \vec{\sigma}$, such that

$$\vec{\partial}_s\left(\vec{k}\cdot\vec{R}\left(\vec{s}\right)\right)\Big|_{\vec{s}=\vec{\sigma}} = k\vec{\partial}_s\left(\hat{k}\cdot\vec{R}\left(\vec{s}\right)\right)\Big|_{\vec{s}=\vec{\sigma}} = 0, \tag{56}$$

and that the other factors in the integrand, $\sqrt{g\left(\vec{s}\right)}\hat{n}\left(\vec{s}\right)$ in this case, are slowly varying.[20] Here, $\vec{\partial}_s = \left(\partial_{s_1}, \partial_{s_2}, \cdots\right)$ is the gradient with respect to the surface coordinates s_i. For an arbitrary shape, there will generally be multiple points where the phase is stationary. For simplicity, consider a single solution $\vec{\sigma}$. The argument of the exponential in the integrand can be approximated by

$$i\vec{k}\cdot\vec{R}\left(\vec{s}\right) = ik\left(\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right) + \frac{1}{2}\left(\partial_{\sigma_i}\partial_{\sigma_j}\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right)\left(s_i - \sigma_i\right)\left(s_j - \sigma_j\right)\right) \tag{57}$$

to second order in $\vec{s} - \vec{\sigma}$. Substituting into (5) then gives

$$\begin{aligned}
&\int_V d^D x \exp\left[i\vec{k}\cdot\vec{x}\right] \\
&\simeq \exp\left[ik\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right]\frac{\hat{k}}{ik}\cdot\int d^{D-1}s\,\sqrt{g\left(\vec{s}\right)}\hat{n}\left(\vec{s}\right)\exp\left[\frac{ik}{2}\left(\partial_{\sigma_i}\partial_{\sigma_j}\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right)\left(s_i - \sigma_i\right)\left(s_j - \sigma_j\right)\right] \\
&\simeq \exp\left[ik\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right]\left(\frac{\hat{k}}{ik}\cdot\hat{n}\left(\vec{\sigma}\right)\right)\frac{\sqrt{g\left(\vec{\sigma}\right)}\pi^{(D-1)/2}}{\sqrt{\det\left[-\frac{ik}{2}\partial_{\sigma_i}\partial_{\sigma_j}\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right]}}.
\end{aligned} \tag{58}$$

Under the assumption that $\sqrt{g\left(\vec{s}\right)}\hat{n}\left(\vec{s}\right)$ is slowly varying compared to the exponential $\sqrt{g\left(\vec{s}\right)}\hat{n}\left(\vec{s}\right)$ can be replaced with $\sqrt{g\left(\vec{\sigma}\right)}\hat{n}\left(\vec{\sigma}\right)$ and moved outside the integral. Under the assumption that the dominant contribution comes from the region around $\vec{s} = \vec{\sigma}$, the integration range can be extended to $\pm\infty$, thus yielding a standard Gaussian integral which reduces to the result shown above. The determinant in the denominator is taken over the i, j indices.

Using the fact that $\det\left[-\frac{ik}{2}\partial_{\sigma_i}\partial_{\sigma_j}\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right] = k^{D-1}\det\left[-\frac{i}{2}\partial_{\sigma_i}\partial_{\sigma_j}\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right]$, we get

$$\int_V d^D x \exp\left[i\vec{k}\cdot\vec{x}\right] \sim \frac{1}{k}\frac{1}{k^{(D-1)/2}} = \frac{1}{k^{(D+1)/2}}, \tag{59}$$

and so,

$$I\left(\vec{k}\right) \sim \frac{1}{k^{D+1}}. \tag{60}$$

Thus in three dimensions, $I(\vec{k})$ scales as $1/k^4$ for large k. This is the standard isotropic statement of Porod's law.[3] But, as pointed out by Ciccariello, $\det\left[\partial_{\sigma_i}\partial_{\sigma_j}\hat{k}\cdot\vec{R}\left(\vec{\sigma}\right)\right]$ is proportional to the Gaussian curvature (in three dimensions) of the surface ∂V and is the appropriate prefactor. In general, for an arbitrary shaped particle, there will be multiple stationary phase points, i.e., $\vec{\sigma}_1, \vec{\sigma}_2, \ldots$ which must be summed over to get the complete amplitude. There are also issues with positive and negative curvatures which must be carefully considered as well as how to handle cases where the curvature vanishes.[12] The $1/k^3$ dependence predicted for two dimensions, with the relevant prefactor, has recently been reported.[21]

V. 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.

[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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