FOURIER TRANSFORMS IN ARBITRARY DIMENSION

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Abstract

Fourier Transforms are an important element of undergraduate training in various engineering and scientific fields. This article presents a general derivation of the Fourier Transform for arbitrary dimension. It is shown that Fourier Transforms in even dimensions entail Bessel functions. Then data sets from Monte Carlo simulations for two and four dimensional systems are used to numerically perform the appropriate Fourier Transforms. Such activities expose students to both special functions and numerical methods of integration.

Introduction

In a previous article [1] in this journal we have presented derivations and applications of the Fourier Transform in one and three dimensions. In the present paper we extend this work to arbitrary dimension. It is found that Bessel functions [2, 3] are involved when taking the Fourier Transform in even dimensions. Bessel functions occur in many two dimensional engineering and physics applications such as heat conduction and electromagnetic wave propagation in waveguides of circular cross-section.

The general form of the Fourier transform [4, 5, 6] in any spatial dimension, D, of a function, F(|**R**|), which is symmetric in angular coordinates is given by

$$\tilde{F}(|\mathbf{K}|) = \int e^{i\,\mathbf{K}\cdot\mathbf{R}}\, F(|\mathbf{R}|)\, \mathbf{dR} \qquad (1)$$

where **K** is the wave-vector, $\mathbf{K}\cdot\mathbf{R}$ is the vector dot product between **K** and **R** , **dR** is the appropriate volume element in D dimensional space and | | denotes the magnitude of a vector. In order to simplify the equations we will use bold on a variable to indicate a vector and ordinary text to indicate a vector magnitude.

In two dimensions the volume element in Eq. 1 in Cartesian coordinates is dxdy. If integration is performed employing Cartesian coordinates, two separate one dimensional integrals must be calculated. However, if the problem under investigation has angular symmetry (as is usually the case in many problems), polar coordinates can be employed to reduce the integral over two components, x and y, to a single integral. Then we are left with a one dimensional integral which will be simpler to handle both analytically and numerically than two different component integrals in x and y.

The volume element in polar coordinates is **dR** = RdRdθ. Then the Fourier Transform is given by

$$\tilde{F}(K) = \int_0^{\infty} \int_0^{2\pi} e^{iKR\cos\theta}\, F(R)\, d\theta\, R dR \qquad (2)$$

But the zero-th order Bessel function, $J_0(KR)$, is defined [2, 3] as

$$J_0(KR) = (1 / 2\pi) \int_0^{2\pi} e^{iKR\cos\theta}\, d\theta \qquad (3)$$

Hence,

$$\tilde{F}(K) = 2\pi \int_0^{\infty} J_0(KR)\, F(R)\, R\, dR \qquad (4)$$

This relationship is often called the Hankel Transform in the literature.

To reduce the general D dimensional case, which involves D component integrals, to a single integral over the magnitude of **R** one needs to relate the Cartesian coordinates of **R** to its D dimensional spherical coordinates expressed by |**R**| and D -1 angles $\theta_1\ \theta_2 \ldots \theta_{D-1}$. The resulting infinitesimal solid angle, **de**, is given by [7]

$$\mathbf{de} = \prod_{k=1}^{D-1} \sin^{k-1}\theta_k \, d\theta_k \qquad (5)$$

Then the surface area of a D dimensional sphere would be

$$\Omega_D = \int R^{D-1}\, \mathbf{de} \qquad (6a)$$

$$= R^{D-1} \int_0^{2\pi} d\theta_1 \int_0^{\pi} \sin\theta_2\, d\theta_2 \int_0^{\pi} \sin^2\theta_3\, d\theta_3 \ldots$$

$$\int_0^{\pi} \sin^{D-2}\theta_{D-1}\, d\theta_{D-1} \qquad (6b)$$

or

$$\Omega_D = 2\,\pi^{D/2} R^{D-1} / \Gamma(D/2) \qquad (7)$$

Here, Γ is the Gamma function [3]

$$\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t}\, dt \qquad (8)$$

Eq. 7 follows from the trigonometric integral [7]

$$\int_0^{\pi} \sin^N\theta\, d\theta = \Gamma((N+1)/2)\,\Gamma(1/2) / \Gamma(N/2+1) \qquad (9)$$

Then Eq. 1 becomes

$$\tilde{F}(|\mathbf{K}|) = [\,2\,\pi^{(D-1)/2} / \Gamma((D-1)/2)\,]$$

$$\int_0^{\infty} R^{D-1} F(R)\, dR \int_0^{\pi} e^{iKR\cos\theta} \sin^{D-2}\theta\, d\theta \qquad (10)$$

Here we have integrated over one less angle because of the cosine term in the exponential from the dot product. The angular integration can be expressed [6] in terms of the (D / 2 - 1) -th order Bessel function, $J_{D/2-1}(KR)$:

$$\int_0^{\pi} e^{iKR\cos\theta} \sin^{D-2}\theta\, d\theta = [2^{D/2-1}\Gamma(1/2)\Gamma((D-1)/2)]\; J_{D/2-1}(KR) / (KR)^{D/2-1} \qquad (11)$$

Using Eq. 11 in Eq. 10 one obtains

$$\tilde{F}(|\mathbf{K}|) = [\,(2\pi)^{D/2} / K^{(D-2)/2}\,] \int_0^{\infty} R^{D/2} F(R)\, J_{D/2-1}(KR)\, dR \qquad (12)$$

Eq. 12 is the generalized D dimensional Fourier transform.

When D = 2, Eq. 12 reduces to Eq. 4 and when D = 4, Eq. 12 will involve the first order Bessel function, $J_1(KR)$. The one dimensional integrals required for the Fourier Transform can be handled with either the integration facilities of software packages such as Maple or Mathematica or by numerical integration with Simpson's Rule and the computer routines for the zero and first order Bessel functions provided by Press et al [8].

Application

We have developed an independent studies project using Eq.12 in two and four dimensions, by providing a tabulated function of R as input for students. This function is the total correlation function, H(R), which is defined as,

$$H(R) = G(R) - 1 \qquad (13)$$

The pair correlation function, G(R), measures the order of a fluid at a particular number density, ρ. The Fourier Transform of H(R) is called the structure function, S(K). In this journal Harnett and Bishop [9], Lasky and Bishop [10] and Tiglias and Bishop [1] have described the behavior of G(R) for one, two and three dimensional systems respectively. Bishop, Whitlock and Klein [11] have computed G(R) for hard particle systems for a variety of dimensions and densities by Monte Carlo simulation methods. The Fourier Transform of H(R) has been evaluated by using Eq. 12 and employing Simpson's integration formula with a mesh size of $\Delta R = 0.01$ and a cutoff upper bound of R = 4.0. The numerical integration routines have been written in C and can perform the Fourier Transform of any tabulated data set. For this case the upper bound value in the integral in Eq. 12, only needs to be large enough so that G(R) has essentially become one and therefore, H(R) is zero.

Figure 1 presents the original G(R) Monte Carlo simulation data in two and four dimensions at $\rho = 0.70$. G(R) is zero when $R \leq 1.0$ since particles cannot penetrate each other. When G(R) attains a value of 1.0 the fluid is uniform in its structure. The appearance of the second and even small third peak in two dimensions indicates the onset of ordering at this density but in four dimensions there is essentially only a single peak. In four dimensions particles can easily avoid each other and therefore have a larger free space in which to move. Hence, higher densities are needed before particles start to become localized.

Figure 2 presents the Fourier Transform of the curves in figure 1. The behavior of the S(K) graphs at low values of K reflects the behavior of the pair correlation function at large R values. One needs to be in an R regime in which the pair correlation has decayed smoothly to a value of one and does not display oscillations. Otherwise, one obtains low K values of S(K) which are artifacts of the Fourier Transform

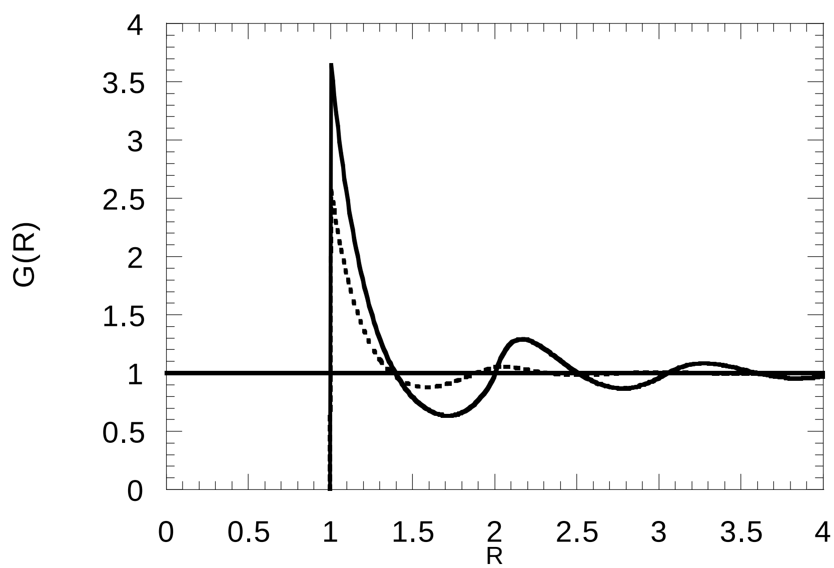

Figure 1: The pair correlation function for D=2 (solid line) and D=4 (dotted line) when $\rho = 0.7$.

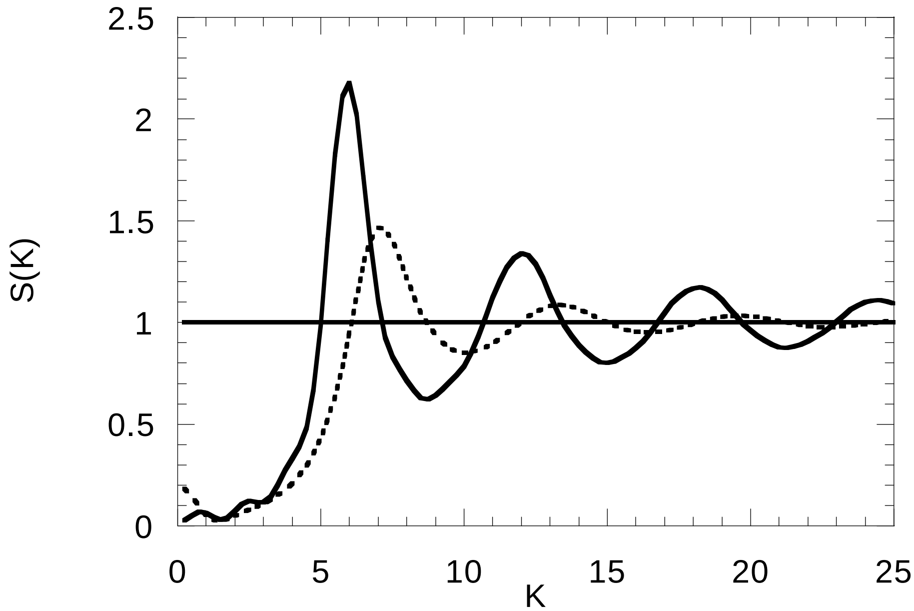

Figure 2: S(K) for D=2 (solid line) and D=4 (dotted line) when ρ = 0.7.

process. In Figure 2 the structure of G(R) is mirrored in S(K). The strong multiple peaks in S(K) for the two dimensional system confirms that it is much more ordered than the four dimensional one.

Conclusions

We have presented a general derivation and an interesting application of Fourier Transforms in arbitrary dimension by studying S(K) of hard particle systems in two and four dimensions. Having students numerically compute the Fourier Transform of tabulated data exposes them to important tools of analysis which will be of great use in their future careers.

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