

FOURIER TRANSFORMS IN ONE AND THREE DIMENSIONS

John L. Tiglias and Marvin Bishop
 Department of Mathematics/Computer Science
 Manhattan College
 Manhattan College Parkway
 Riverdale, New York 10471

Abstract

Fourier transforms are an important element of undergraduate training in engineering and science. This article presents a derivation of the Fourier transform for one and three dimensions. An application from the theory of liquids is presented in which the Fourier transform is performed both numerically and analytically. It is found that there is good agreement between the two approaches.

Introduction

It is well recognized that engineering and science students need to be exposed to Fourier transforms. For example, a variety of digital media continuous signals are sampled at discrete time intervals. Fourier analysis decomposes the sampled signal into its periodic frequency components --- sines and cosines for further analysis. In this article we first present a derivation of the Fourier transform in one and three dimensions. Then we apply Fourier transforms to the study of a model fluid in one and three dimensions.

The general form of the Fourier transform [1,2,3] in any spatial dimension, D , of a function, $F(|\mathbf{R}|)$, which is symmetric in angular coordinates is given by

$$\tilde{F}(|\mathbf{K}|) = \int d\mathbf{R} e^{i\mathbf{K} \cdot \mathbf{R}} F(|\mathbf{R}|) \quad (1)$$

where \mathbf{K} is the wave-vector, $\mathbf{K} \cdot \mathbf{R}$ is the vector dot product between \mathbf{K} and \mathbf{R} , $d\mathbf{R}$ 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 one dimension the volume element $d\mathbf{R}$ is $2dX$ and $e^{i\mathbf{K} \cdot \mathbf{R}}$ reduces to $\cos(KX)$ for any real function, $F(X)$, so that the Fourier Transform is

$$\tilde{F}(K) = 2 \int_0^{\infty} dX \cos(KX) F(X) \quad (2)$$

which is a straightforward integral to evaluate.

However, in three dimensions, the volume element in Cartesian coordinates is $dx dy dz$. If integration is performed employing Cartesian coordinates three one dimensional integrals must be done. If the problem under investigation has spherical symmetry (as is usually the case in most physical problems) spherical coordinates can be used to integrate out the angular dependence. Then we are left with a one dimensional integral which will be simpler to handle both analytically and numerically than three different component integrals in x , y and z .

In spherical coordinates the volume element is $d\mathbf{R} = R^2 dR \sin\theta d\theta d\phi$ and $e^{i\mathbf{K} \cdot \mathbf{R}}$ becomes $e^{iKR\cos\theta}$. Thus,

$$\tilde{F}(K) = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} e^{iKR\cos\theta} F(R) d\phi \sin\theta d\theta R^2 dR \quad (3)$$

After performing the integrals over θ and ϕ we find that

$$\tilde{F}(K) = 4\pi \int_0^{\infty} F(R) \left[\frac{\sin(KR)}{KR} \right] R^2 dR \quad (4)$$

There are many applications of the Fourier transform in engineering and science. An interesting area of study is the structure of

model fluids in one and three dimensions. A fluid model is specified by the pair potential, $U(R)$, of particle interaction when the particles are separated by the distance R . One very important model of fluids consists of hard particles of diameter, σ , for which $U(R)$ is given in any dimension by

$$U(R) = \begin{cases} \infty & R < \sigma \\ 0 & R \geq \sigma \end{cases} \quad (5)$$

This rather simple model goes a long way toward explaining the properties of real fluids.

Various probes have been developed in order to examine the nature of the onset of molecular ordering in such model fluids and the manner in which the structure of the fluid is altered as the density is increased. One such important function is the pair correlation function[4], $G(R)$. The change in the shape of the pair correlation function directly mirrors the underlying particle rearrangements. Indeed, the appearance of peaks in $G(R)$ is an indication of the increased molecular ordering. On the other hand in the ideal state, $G(R)$ has a constant value of one reflecting the non-interaction of particles. Recently, in this journal, Harnett and Bishop[5] have published their Monte Carlo (MC) simulation of the pair correlation of one dimensional hard particles. Also, Bishop, Whitlock and Klein[6] have presented their MC simulations for hard particles in three dimensions. Figure 1 and Figure 2 illustrate the variation of the pair correlation function for a variety of densities, $\rho = 0.30, 0.50$ and 0.70 , in one and three dimensions, respectively. These studies demonstrate very clearly the onset of ordering as the density is increased.

A different measure of structural order is the structure function[7], $S(K)$, where K is the momentum transfer. This function is related to the Fourier transform of the pair correlation function as will be shown below. $S(K)$ probes spatial correlations at both large and small

scales so that at low values of K one is examining large R behavior and vice versa. Moreover, at least in three dimensions, $S(K)$ can be experimentally determined[7]. The structure factor is linked to the pair correlation function through the total correlation function, $H(R)$. This is defined as

$$H(R) = G(R) - 1 \quad (6)$$

so that $H(R)$ measures the deviation from ideal behavior. Many years ago, Ornstein and Zernike[7] proposed an equation which related the $S(K)$ to the Fourier transform of $H(R)$:

$$S(K) = 1 + \rho \tilde{H}(K), \quad (7)$$

Moreover, they were also able to obtain another equation which related $S(K)$ to the Fourier transform of $C(R)$ (the direct correlation function);

$$S(K) = 1 / (1 - \rho \tilde{C}(K)) \quad (8)$$

Hence, $S(K)$ can be obtained either by the Fourier transform of $C(R)$ or $H(R)$.

Method

The analytical solution for $S(K)$ from Eq. 8 for hard particle systems in one and three dimensions follows from other workers who were able to exactly solve for $\tilde{C}(K)$.

The exact solution for $C(X)$ in one dimension has been known for a long time[8]. In a system of units in which $\sigma = 1$, the direct correlation function is:

$$C(X) = - (1 - \eta X) / (1 - \eta)^2 \quad 0 \leq X \leq 1 \quad \text{and } 0 \text{ otherwise} \quad (9)$$

where the packing fraction, η , is $\eta = \rho$. Then using the one dimensional Fourier transform of Eq. 2 one finds that

$$S(K) = 1 / (1 + 2(n/K)^2 [1 - \cos K + (K/n) \sin K]) \quad (10)$$

where

$$n = \rho / (1 - \rho) \quad (11)$$

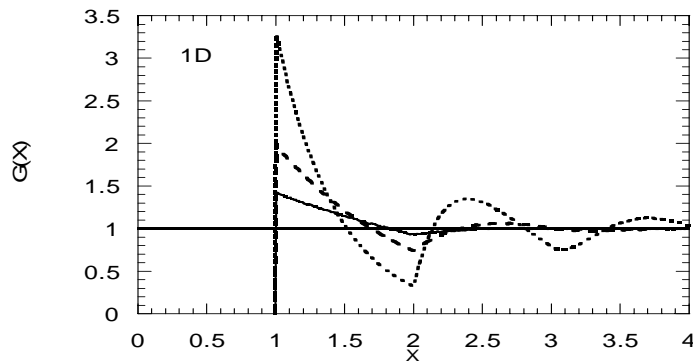


Figure 1: The one dimensional pair correlation function. Solid line: $\rho = 0.30$, dashed line: $\rho = 0.50$ and dotted line: $\rho = 0.70$. At the highest density, distinct peaks indicate the increased ordering of the particles.

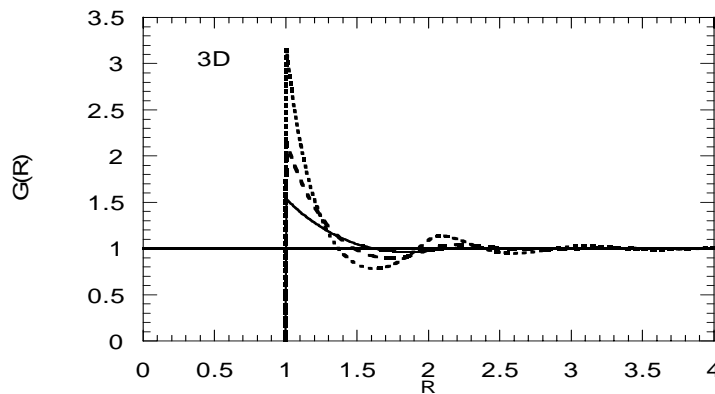


Figure 2: The three dimensional pair correlation function. Solid line: $\rho = 0.30$, dashed line: $\rho = 0.50$ and dotted line: $\rho = 0.70$. In this case, at the highest density, less ordering has occurred than in one dimension.

The $C(R)$ has also been determined exactly in three dimensions[9,10]

$$C(R) = - [\alpha + \beta R + \gamma R^3] \quad (12)$$

where

$$\alpha = (1 + 2\eta)^2 / (1 - \eta)^4 \quad (13a)$$

$$\beta = -6\eta(1 + \eta/2)^2 / (1 - \eta)^4 \quad (13b)$$

$$\gamma = \eta(1 + 2\eta)^2 / 2(1 - \eta)^4 \quad (13c)$$

and now the packing fraction is given by

$$\eta = \pi\rho / 6 \quad (14)$$

Employing the three dimensional Fourier transform of Eq. 4 yields the closed form

$$S(K) = 1 / (1 + 4\pi\rho [I_1 + I_3 + I_3] / K) \quad (15)$$

where

$$I_1 = \alpha [\sin K - K \cos K] / K^2 \quad (16a)$$

$$I_2 = \beta [(2 - K^2) \cos K + 2K \sin(K) - 2] / K^3 \quad (16b)$$

$$I_3 = \gamma [4K(K^2 - 6) \sin K - (24 - 12K^2 + K^4) \cos K + 24] / K^5 \quad (16c)$$

Results

The $C(R)$ results discussed above provide an analytic form of $S(K)$ for hard particle systems at any density. Alternatively, we have performed MC simulations[5,6] to obtain $G(R)$ numerically. Then $S(K)$ has been determined from the MC $G(R)$ values by performing the appropriate integrals, Eq. 2 in one dimension and Eq. 4 in three dimensions, using Simpson's integration formula with a mesh size of $\Delta R = 0.01$ and a cutoff upper bound of $R = 4.0$. The upper bound value needs to be large enough so that $G(R)$ has essentially become one. Alternatively, a symbolic software package such as Maple or Mathematica could be used.

A comparison between the theoretically predicted $S(K)$ from the exact equation, Eq. 10, and the MC simulation results at a variety of densities is presented in Figure 3 for one dimensional systems. The agreement is excellent.

Figure 4 presents a similar comparison, using the exact Eq. 15 and the MC results, for three dimensions. Here there is fine agreement for $K > 2$ but there is some discrepancy at the lowest K values. That regime corresponds to large R values and it is difficult to accurately determine $G(R)$ there which in turn affects the accuracy of the $S(K)$ calculation.

Conclusions

We have presented the derivation and an interesting application of Fourier transforms in one and three dimensions by studying the structure factor of hard particle systems. The values obtained by numerically Fourier transforming the Monte Carlo simulations agree well with theoretical predictions.

Projects

1) Given an exponential function in one dimension, $F(X) = e^{-a|X|}$, use Eq. 2 to find $\tilde{F}(K)$

analytically. [Hint: This is easier if the cosine is rewritten as a complex exponential.]

2) Given a Gaussian function in one dimension, $F(X) = e^{-bX^2}$, show analytically that the Fourier transform is another Gaussian function. [Hint: Rewrite the cosine function as a complex exponential and complete the square.]

3) Alternatively, redo questions 1 and 2 by computing $\tilde{F}(K)$ numerically employing some software package such as Maple or Mathematica. Also compute the Fourier transform by using Simpson's rule (see any calculus book) to perform the integral numerically. In this case the error in your solution is dependent upon the mesh size you choose.

4) Find $S(K)$ analytically using Eq. 4 if $G(R)$ in three dimensions is the Heaviside function:

$$G(R) = \begin{matrix} 0 & R < 1 \\ 1 & R \geq 1 \end{matrix}$$

[Hint: Divide the region of integration into two parts, $R = [0,1]$ and $R = [1, \infty]$.]

Acknowledgements

This research has been supported by the Manhattan College computer center. We wish to thank Professor Paula A. Whitlock for many helpful discussions about Monte Carlo computer simulations.

References

1. A. Papoulis, "The Fourier Integral and Its Application", (McGraw Hill, New York, 1962).
2. R.N. Bracewell, "The Fourier Transform and its Applications", (McGraw Hill, New York, 2000).
3. I. N. Sneddon, "Fourier Transforms", (Dover, New York, 1995).
4. M. Bishop and C. Bruin, "The Pair Correlation Function: A Probe of Molecular Order", Am. J. Phys., 52, 1106 (1984).

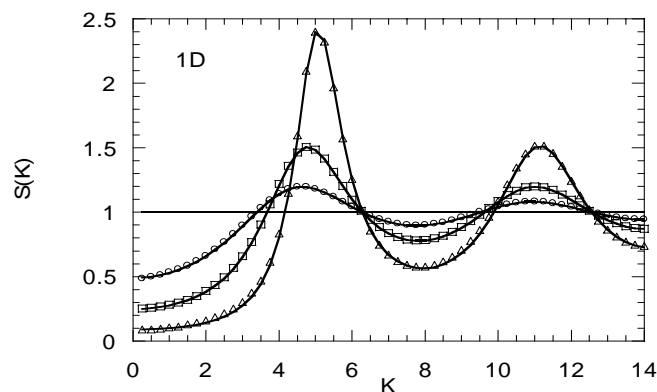


Figure 3: $S(K)$ vs. K in one dimension. Lines: exact equations, circles: MC $\rho = 0.30$, squares: MC $\rho=0.50$, triangles: MC $\rho=0.70$.

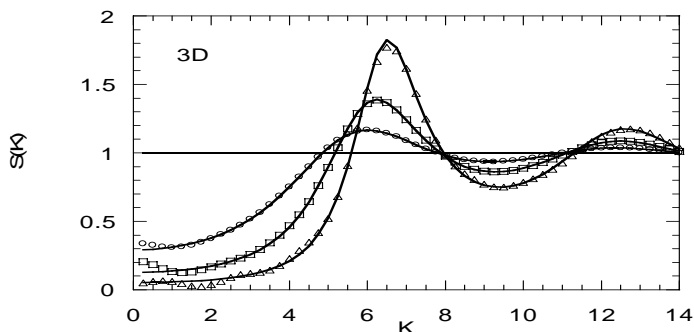


Figure 4: $S(K)$ vs. K in three dimensions. Lines: exact equations, circles: MC $\rho = 0.30$, squares: MC $\rho=0.50$, triangles: MC $\rho=0.70$.

5. J. Harnett and M. Bishop, "Monte Carlo Simulation of One Dimensional Hard Particle Systems", Computers in Education Journal, in press.
6. M. Bishop, P.A. Whitlock and D. Klein, "The structure of Hyperspherical Fluids in Various Dimensions", J. Chem. Phys., 122, 074508-1 (2005).
7. D.A. McQuarrie, "Statistical Mechanics", (Harper and Row, New York, 1976).
8. M. Chen, "On the Equivalence of the Ornstein-Zernike relation and Baxter's relations for a one-dimensional simple fluid", J. Math. Phys., 16, 1150 (1975).
9. E. Thiel, "Equation of State for Hard Spheres", J. Chem. Phys., 39, 474 (1963).
10. M. S. Wertheim, "Exact Solution of the Percus-Yevick Integral Equation for Hard Spheres", Phys. Rev. Lett., 10, 321 (1963).

Biographical Information

John L. Tiglias completed a B.S. in computer science at Manhattan College and is currently a graduate student in computer science at Stevens Institute of Technology.

Marvin Bishop is a Professor in the Department of Mathematics and Computer Science at Manhattan College. He received his Ph.D. from Columbia University, his M.S. from New York University and his B.S. from City College of New York. His research interests include simulation and modeling and parallel processing.