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On the calculation of the partial moments of a distribution function from its Fourier transform

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Abstract. A general formula has been obtained for calculating the partial spatial moments of a distribution function directly from its Fourier transform. Examples to illustrate the technique are given based upon neutron diffusion and transport theory. The extensions to other areas of physics and engineering are indicated.

1. Introduction

Many practical situations arise where it is necessary to calculate a particular moment or a set of moments of a distribution function. Such moments are, for example, related to the mean value and variance as well as to skewness and kurtosis, etc. Often we find that the distribution function $F(x)$ is given in terms of a Fourier integral whose subsequent inversion is not always a simple or direct problem. However, even if this can be done, it is necessary to integrate over the result to obtain the desired moments. In this paper we investigate methods for calculating such moments without the intermediate step of inverting the transform.

Applications can be found in the fields of neutron transport theory and radiation damage as well as in statistics and related areas (Davison 1957, Williams 1979a).

2. Theory

2.1. Full-range moments

If the Fourier transform $\bar{F}(k)$ of a function $F(x)$ is defined by

$$\bar{F}(k)=\int_{-\infty}^{\infty} dx\ e^{-ikx}F(x), \tag{1}$$

then clearly

$$\frac{\partial^n \bar{F}(k)}{\partial k^n}=(-i)^n\int_{-\infty}^{\infty} dx\ x^n\ e^{-ikx}F(x). \tag{2}$$

Setting $k=0$ leads to the identity

$$F_n=i^n\frac{\partial^n \bar{F}(k)}{\partial k^n}\bigg|_{k=0}, \tag{3}$$

where

$$F_n = \int_{-\infty}^{\infty} \mathrm{d}x\, x^n F(x). \tag{4}$$

This result is well known and has been used extensively in neutron transport and radiation damage moment calculations. Thus we can define the mean-square distance of travel as

$$\bar{x}^2 = F_2/F_0 = -\bar{F}''(0)/\bar{F}(0), \tag{5}$$

and this may be evaluated directly from the Fourier transform. An example will be given below.

2.2. *Half-range moments*

It is often useful to calculate moments over the regions $0 \leqslant x \leqslant \infty$ or $-\infty \leqslant x \leqslant 0$, where for example

$$\mathscr{F}_n = \int_0^{\infty} \mathrm{d}x\, x^n F(x). \tag{6}$$

For such cases the formula of equation (3) does not apply. Nevertheless, by an artifice we may express $\mathscr{F}_n$ in terms of $\bar{F}(k)$ directly. Thus we rewrite equation (6) as

$$\mathscr{F}_n = \int_{-\infty}^{\infty} \mathrm{d}x\, \Theta(x) x^n F(x), \tag{7}$$

where $\Theta(x)$ is the Heaviside unit function. A similar expression may be written for the negative range of x. Now we note from equation (1) that

$$F(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}kx}\bar{F}(k), \tag{8}$$

and so inserting this into equation (7) and reversing the order of integration leads to

$$\mathscr{F}_n = \int_{-\infty}^{\infty} \mathrm{d}k\, \bar{F}(k)\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}x\, x^n \Theta(x)\, \mathrm{e}^{\mathrm{i}kx}. \tag{9}$$

But it is easily seen that (Roos 1969)

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}x\, \Theta(x)\, \mathrm{e}^{\mathrm{i}kx} = \frac{\delta(k)}{2} + \mathrm{P}.\frac{\mathrm{i}}{2\pi k}, \tag{10}$$

where $\delta(k)$ is the Dirac delta function and P. implies that principal-value integrals are to be taken. Clearly by differentiation, we see that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}x\, x^n \Theta(x)\, \mathrm{e}^{\mathrm{i}kx} = (-\mathrm{i})^n\left(\frac{\delta^{(n)}(k)}{2} - \frac{(-)^n n!}{2\pi \mathrm{i}}\mathrm{P}.\frac{1}{k^{n+1}}\right). \tag{11}$$

For moments over the range $-\infty \leqslant x \leqslant 0$, we find

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}x\, (-x)^n \Theta(-x)\, \mathrm{e}^{\mathrm{i}kx} = \mathrm{i}^n\left(\frac{\delta^{(n)}(k)}{2} + \frac{(-)^n n!}{2\pi \mathrm{i}}\mathrm{P}.\frac{1}{k^{n+1}}\right).$$

Thus the expression for $\mathscr{F}_n$ can be written

$$\mathscr{F}_n = \frac{\mathrm{i}^n}{2}\bar{F}^{(n)}(0) - \frac{\mathrm{i}^n n!}{2\pi \mathrm{i}} \mathrm{P}. \int_{-\infty}^{\infty} \mathrm{d}k \frac{\bar{F}(k)}{k^{n+1}}. \tag{12}$$

The integral appearing in equation (12) is reminiscent of that occurring in dispersion relations; it is an improper integral and must be interpreted accordingly. Roos (1969) shows that the divergent part must be subtracted so that the function is regularised. This leads to

$$\mathrm{P}. \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{k^{n+1}} \bar{F}(k) \equiv \lim_{\varepsilon \to 0} \int_{|k| \geq \varepsilon} \frac{\mathrm{d}k}{k^{n+1}} \left(\bar{F}(k) - \bar{F}(0) - \ldots \frac{k^{n-1}\bar{F}^{(n-1)}(0)}{(n-1)!} \right). \tag{13}$$

This integral is always bounded, and therefore we have a prescription for calculating the $\mathscr{F}_n$.

2.3. Partial moments

A partial moment may be defined as

$$F_n(\alpha, \beta) = \int_{\alpha}^{\beta} \mathrm{d}x\, x^n F(x) \tag{14}$$

which we may rewrite over the full range of x as

$$F_n(\alpha, \beta) = \int_{-\infty}^{\infty} \mathrm{d}x\, x^n F(x) [\Theta(x-\alpha) - \Theta(x-\beta)]. \tag{15}$$

Using the Fourier integral for $F(x)$ and reversing orders of integration we find

$$F_n(\alpha, \beta) = \int_{-\infty}^{\infty} \mathrm{d}k\, \bar{F}(k) \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x\, x^n\, \mathrm{e}^{\mathrm{i}kx} [\Theta(x-\alpha) - \Theta(x-\beta)]. \tag{16}$$

A change of variables leads to

$$F_n(\alpha, \beta) = \int_{-\infty}^{\infty} \mathrm{d}k\, \bar{F}(k) \frac{1}{2\pi} \left(\mathrm{e}^{\mathrm{i}k\alpha} \int_{-\infty}^{\infty} \mathrm{d}z\, (\alpha + z)^n \Theta(z)\, \mathrm{e}^{\mathrm{i}kz} \right.$$

$$\left. - \mathrm{e}^{\mathrm{i}k\beta} \int_{-\infty}^{\infty} \mathrm{d}z\, (\beta + z)^n \Theta(z)\, \mathrm{e}^{\mathrm{i}kz} \right). \tag{17}$$

Using

$$(\alpha + z)^n = \sum_{\nu=0}^{n} \binom{n}{\nu} \alpha^{n-\nu} z^{\nu} \tag{18}$$

we find that equation (17) becomes

$$F_n(\alpha, \beta) = \int_{-\infty}^{\infty} \mathrm{d}k\, \bar{F}(k) \sum_{\nu=0}^{n} \binom{n}{\nu} (\alpha^{n-\nu}\, \mathrm{e}^{\mathrm{i}k\alpha} - \beta^{n-\nu}\, \mathrm{e}^{\mathrm{i}k\beta}) \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}z\, z^{\nu}\, \mathrm{e}^{\mathrm{i}kz} \Theta(z). \tag{19}$$

But from equation (11) we have an expression for the integral over z and hence an expression for $F_n(\alpha, \beta)$ in terms of $\bar{F}(k)$.

2.4. Two-dimensional moments

If we are given a two-dimensional function $\Phi(x, y)$ defined by

$$\Phi(x, y) = \left(\frac{1}{2\pi}\right)^2 \int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2\, e^{ik_1x+ik_2y}\bar{\Phi}(k_1, k_2), \tag{20}$$

then it is clearly a trivial matter to calculate the full-range moments

$$F_{n,m} = \int_{-\infty}^{\infty} dx\, x^n \int_{-\infty}^{\infty} dy\, y^m \Phi(x, y) \tag{21}$$

from

$$F_{n,m} = i^{n+m} \frac{\partial^{n+m}}{\partial k_1^n\, \partial k_2^m} \bar{\Phi}(k_1, k_2)\bigg|_{k_1=k_2=0} \tag{22}$$

The extension to any number of independent variables is clear. A more challenging problem is the calculation of the partial moments

$$\mathscr{F}_{n,m} = \int_0^{\infty} dx\, x^n \int_0^{\infty} dy\, y^m \Phi(x, y) \tag{23}$$

or possibly even

$$\tilde{\mathscr{F}}_{n,m} = \int_0^{\infty} dx\, x^n \int_{-\infty}^{0} dy\, (-y)^m \Phi(x, y). \tag{24}$$

Considering $\mathscr{F}_{n,m}$ we find using the Heaviside function technique that

$$\mathscr{F}_{n,m} = \int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2\, \bar{\Phi}(k_1, k_2) \frac{1}{2\pi} \int_{-\infty}^{\infty} dx\, x^n \Theta(x)\, e^{ik_1x} \frac{1}{2\pi} \int_{-\infty}^{\infty} dy\, y^m \Theta(y)\, e^{ik_2y}. \tag{25}$$

Thus using equation (11) for the integrals over x and y we find after some manipulation that

$$\begin{aligned}
\mathscr{F}_{n,m} = {} & \frac{i^{n+m}}{4} \frac{\partial^{n+m}}{\partial k_1^n\, \partial k_2^m} \bar{\Phi}(k_1, k_2)\bigg|_{k_1=k_2=0} \\
& - \frac{i^{n+m} n!}{4\pi i} \mathrm{P.} \int_{-\infty}^{\infty} dk_1 \frac{1}{k_1^{n+1}} \frac{\partial^m}{\partial k_2^m} \bar{\Phi}(k_1, k_2)\bigg|_{k_2=0} \\
& - \frac{i^{n+m} m!}{4\pi i} \mathrm{P.} \int_{-\infty}^{\infty} dk_2 \frac{1}{k_2^{m+1}} \frac{\partial^n}{\partial k_1^n} \bar{\Phi}(k_1, k_2)\bigg|_{k_1=0} \\
& + \frac{i^{n+m} n!\, m!}{(2\pi i)^2} \mathrm{P.} \int_{-\infty}^{\infty} dk_1\, \mathrm{P.} \int_{-\infty}^{\infty} dk_2 \frac{1}{k_1^{n+1}} \frac{1}{k_2^{m+1}} \bar{\Phi}(k_1, k_2).
\end{aligned} \tag{26}$$

Each of the principal-value integrals must be interpreted according to equation (13). It is also possible to have mixtures of full-range and half-range moments.

3. Examples of applications

We shall consider two examples: one to illustrate diffusion-like behaviour and the other transport-like behaviour.

An equation which arises in diffusion theory and which simulates a first-collision source effect can be written

$$F''(x) - b^2 F(x) + a\,\mathrm{e}^{-ax}\Theta(x) = 0. \tag{27}$$

In this equation, b^{-1} is the diffusion length and a is the total cross section or possibly a removal cross section.

Taking Fourier transforms leads to

$$\bar{F}(k) = a/(k^2 + b^2)(a + \mathrm{i}k). \tag{28}$$

It is of course not difficult to invert this transform by the normal method of residues to find

$$\begin{aligned} F(x) &= \frac{a\,\mathrm{e}^{-bx}}{2b(a-b)} - \frac{a}{a^2 - b^2}\mathrm{e}^{-ax}, \qquad x > 0 \\ &= \frac{a\,\mathrm{e}^{bx}}{2b(a+b)}, \qquad x < 0. \end{aligned} \tag{29}$$

From these expressions all of the desired moments may be obtained. However, it may sometimes be more convenient to use equations (12) and (13). Thus

$$\begin{aligned} \mathscr{F}_0 &= \frac{\bar{F}(0)}{2} - \frac{1}{2\pi\mathrm{i}}\mathrm{P.}\int_{-\infty}^{\infty} \mathrm{d}k\,\frac{\bar{F}(k)}{k} \\ &= \frac{1}{2b^2} - \frac{1}{2\pi\mathrm{i}}\mathrm{P.}\int_{-\infty}^{\infty} \frac{\mathrm{d}k}{k}\,\frac{a}{(k^2+b^2)(a+\mathrm{i}k)} \\ &= \frac{1}{2b^2} + \frac{a}{\pi}\int_0^{\infty} \frac{\mathrm{d}k}{(k^2+b^2)(k^2+a^2)} \\ &= \frac{a+2b}{2b^2(a+b)}. \end{aligned} \tag{30}$$

Similarly

$$\begin{aligned} \mathscr{F}_1 &= \frac{\mathrm{i}}{2}\frac{\mathrm{d}}{\mathrm{d}k}\frac{a}{(k^2+b^2)(a+\mathrm{i}k)}\bigg|_{k=0} - \frac{\mathrm{i}}{2\pi\mathrm{i}}\mathrm{P.}\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{k^2}\left(\frac{a}{(k^2+b^2)(a+\mathrm{i}k)} - \frac{1}{b^2}\right) \\ &= \frac{a^2 + 2ab + 2b^2}{2ab^3(a+b)}. \end{aligned} \tag{31}$$

This simple form of $\bar{F}(k)$ clearly does not show the power of the method since Fourier inversion is quite easy. However, many cases exist in transport theory where direct inversion involves complicated integrations around branch points, and it is with such problems that the present technique becomes very powerful. For example, if we consider the case of an infinite medium with a plane anisotropic source we can write for the neutron flux equation (Davison 1957)

$$\left(\mu\frac{\partial}{\partial z} + 1\right)\phi(z, \mu) = \frac{c}{2}\phi_0(z) + \delta(\mu - \mu_0)\delta(z). \tag{32}$$

After Fourier transformation we have

$$\bar{\phi}_0(k) = \frac{1}{(1 + \mathrm{i}k\mu_0)[1 - (c/k)\tan^{-1}k]}. \tag{33}$$

Now this expression may be inverted and the result is

$$\phi_0(z)=\frac{\nu(1-\nu^2)\,e^{-\nu z}}{(1-\nu\mu_0)(c-1+\nu^2)}+\frac{c}{2}\mathrm{P.}\int_0^1 \frac{d\mu}{\mu-\mu_0}\,e^{-z/\mu}g(c,\mu)$$
$$+\left[1-\frac{c\mu_0}{2}\log\left(\frac{1+\mu_0}{1-\mu_0}\right)\right]g(c,\mu_0)\frac{1}{\mu_0}\,e^{-z/\mu_0},\qquad z>0, \tag{34}$$

$$\phi_0(z)=\frac{\nu(1-\nu^2)\,e^{\nu z}}{(1+\nu\mu_0)(c-1+\nu^2)}-\frac{c}{2}\int_0^1 \frac{d\mu}{\mu+\mu_0}\,e^{z/\mu}g(c,\mu),\qquad z<0, \tag{35}$$

where ν and $g(c,\mu)$ are defined in Williams (1971) and in Case *et al* (1953). These expressions are not only tedious to obtain, but also, when averaged over z to evaluate the moments, lead to principal-value integrals involving complicated transcendental functions. For this reason the methods discussed earlier are much more efficient. As an example, consider the zeroth partial moment of $\phi_0(z)$, which is related to the number of neutrons captured in the medium $z>0$:

$$F_0^+=\frac{1}{2(1-c)}-\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{dk}{k}\,\frac{1}{(1+ik\mu_0)[1-(c/k)\tan^{-1}k]}$$
$$=\frac{1}{2(1-c)}+\frac{\mu_0}{\pi}\int_0^{\infty}\frac{dk}{[1-(c/k)\tan^{-1}k](1+k^2\mu_0^2)} \tag{36}$$

where $F_0^+=\int_0^\infty dz\,\phi_0(z)$.

For captures in the region $z<0$ we note equation (11) and find

$$F_0^-=\frac{1}{2(1-c)}+\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{dk}{k}\,\frac{1}{(1+ik\mu_0)[1-(c/k)\tan^{-1}k]}$$
$$=\frac{1}{2(1-c)}-\frac{\mu_0}{\pi}\int_0^{\infty}\frac{dk}{[1-(c/k)\tan^{-1}k](1+k^2\mu_0^2)}. \tag{37}$$

$F_0^+ + F_0^- = 1/(1-c)$, which is the result obtained from a full-range moment. Clearly, equations (36) and (37) are much easier to evaluate than the corresponding integrals over equations (34) and (35).

As a further example we evaluate the first spatial moments F_1^+ and F_1^-:

$$F_1^+=\frac{i}{2}\frac{d}{dk}\bar{\phi}_0(k)\bigg|_{k=0}-\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{k^2}\left(\frac{1}{(1+ik\mu_0)[1-(c/k)\tan^{-1}k]}-\frac{1}{1-c}\right), \tag{38}$$

which simplifies to

$$F_1^+=\frac{\mu_0}{2(1-c)}-\frac{1}{\pi}\int_0^{\infty}\frac{dk}{k^2}\left(\frac{1}{[1-(c/k)\tan^{-1}k](1+k^2\mu_0^2)}-\frac{1}{1-c}\right), \tag{39}$$

and similarly

$$F_1^-=-\frac{\mu_0}{2(1-c)}-\frac{1}{\pi}\int_0^{\infty}\frac{dk}{k^2}\left(\frac{1}{[1-(c/k)\tan^{-1}k](1+k^2\mu_0^2)}-\frac{1}{1-c}\right). \tag{40}$$

The full-range moment

$$F_1=F_1^+-F_1^-=\mu_0/(1-c). \tag{41}$$

Again, we note the ease with which equations (39) and (40) may be evaluated.

4. Summary and conclusions

A formula has been obtained for calculating the partial moments of a distribution function directly from its Fourier transform. Examples based on the one-speed transport equation show its value in reducing numerical difficulties and generally improving the efficiency of the calculation. The method is of value in other fields of physics and engineering where moments are required rather than the complete solution. Some numerical examples of the use of this technique may be found in Williams (1979b).

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