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ALA MOANA HOTEL, HONOLULU, HAWAII

# THE FOURIER TRANSFORM SOLUTION FOR THE GREEN'S FUNCTION OF MONOENERGETIC NEUTRON TRANSPORT THEORY

GANAPOL, BARRY D.

UNIVERSITY OF ARIZONA

DEPARTMENT OF AEROSPACE AND MECHANICAL ENGINEERING

Ganapol, Barry D.  
Department of Aerospace and Mechanical Engineering  
University of Arizona

## **The Fourier Transform Solution for the Green's Function of Monoenergetic Neutron Transport Theory**

Nearly 65 years ago, Ken Case published his seminal paper on the singular eigenfunction solution for the Green's function of the monoenergetic neutron transport equation with isotropic scattering. Previously, the solution had been obtained by Fourier transform. While it is apparent the two had to be equivalent, a convincing equivalence proof for general anisotropic scattering remained a challenge until now.

## **The Fourier Transform Solution for the Green's Function of Monoenergetic Neutron Transport Theory**

### **INTRODUCTION**

It has been nearly 55 years since the derivation of the most meaningful analytical solution of neutron transport theory. Ken Case, in a remarkably insightful paper [1] applied separation of variables to express the Green's function for monoenergetic, isotropically scattering neutrons in terms of singular eigenfunctions. Previously, the solution had been found analytically through Fourier transform inversion [2,3,4]. Here, we will address the question of equivalence between the two approaches. Showing equivalence for other than isotropic scattering is anything but straightforward (as shown by the author in [5]). While equivalence was indeed demonstrated, it lacked intuitive simplicity. In the following, we revisit equivalence in a more unified manner through the Legendre polynomial expansion of the Fourier transformed solution in terms of analytically determined moments.

### **1. The Monoenergetic Green's Function**

Our focus is the Green's function given by the neutron transport equation,

$$\left[ \mu \frac{\partial}{\partial x} + 1 \right] \psi(x, \mu; \mu_0) = \frac{c}{2} \sum_{l=0}^{\infty} \omega_l P_l(\mu) \psi_l(x; \mu_0) + \delta(\mu - \mu_0) \delta(x), \quad (1a)$$

satisfying the condition  $\lim_{|x| \rightarrow \infty} \psi(x, \mu; \mu_0) < \infty$ . By translational invariance, the source, emitting neutrons in direction  $\mu_0$ , is located at  $x = 0$ . The total cross section is unity and  $c$  is the number of scattering secondaries [ $0 \leq c < 1$ ].  $\omega_l$  is the  $l^{\text{th}}$  scattering coefficient for a Legendre polynomial [ $P_l(\mu)$ ] series expansion of the scattering kernel. The Legendre moments,

$$\psi_l(x; \mu_0) \equiv \int_{-1}^1 d\mu P_l(\mu) \psi(x, \mu; \mu_0); \quad l = 0, 1, \dots, \quad (1b)$$

will play a key role in what follows. As usual,  $\mu$  and  $x$  are the neutron direction and position of the angular flux distribution  $\psi(x, \mu; \mu_0)$ .

## 2. The Standard Solution

The angular flux solution derives from the Fourier transform of Eq(1a)

$$\bar{\psi}(k, \mu; \mu_0) \equiv \int_{-\infty}^{\infty} dx e^{-ikx} \psi(x, \mu; \mu_0), \quad (2a)$$

and the Legendre moments

$$\bar{\psi}_l(k; \mu_0) \equiv \int_{-\infty}^{\infty} dk e^{-ikx} \psi_l(x; \mu_0), \quad (2b)$$

to give

$$(1 + ik\mu) \bar{\psi}(k, \mu; \mu_0) = \frac{c}{2} \sum_{l=0}^{\infty} \omega_l P_l(\mu) \bar{\psi}_l(k; \mu_0) + \delta(\mu - \mu_0). \quad (3)$$

Solving for the angular flux and projecting gives the moments as the solution to

$$\sum_{l=0}^L [\delta_{j,l} - c\omega_l L_{j,l}(z)] \bar{\psi}_l(k; \mu_0) = \frac{z}{z + \mu_0} P_j(\mu_0), \quad (4)$$

where the matrix element is explicit

$$L_{j,l}(z) \equiv (-1)^{l+j} z \begin{cases} Q_l(z) P_j(z), & j \leq l \\ Q_j(z) P_l(z), & l < j \end{cases}$$

and  $z \equiv 1/ik$ .  $Q_l$  is the Legendre function of the second kind of order  $l$ . The solution to Eq(4) requires truncation of the scattering kernel, for which we have assumed the scattering coefficient  $\omega_l$  to vanish for  $l \geq L+1$ . In vector notation, Eq(4) becomes

$$[\mathbf{I} - c\mathbf{L}(z)\mathbf{W}] \bar{\psi}(k; \mu_0) = \frac{z}{z + \mu_0} \mathbf{P}(\mu_0), \quad (5)$$

with

$$\begin{aligned} \mathbf{L}(z) &\equiv \{L_{j,l}(z); j, l = 1, 2, \dots, L\} \\ \mathbf{W} &\equiv \text{diag}(\omega_l) \\ \mathbf{P}(\mu_0) &\equiv \{P_j(\mu_0); j = 0, \dots, L\}; \end{aligned}$$

and whose solution by matrix inversion

$$\bar{\psi}(k; \mu_0) = \frac{z}{z + \mu_0} [\mathbf{I} - c\mathbf{L}(z)\mathbf{W}]^{-1} \mathbf{P}(\mu_0), \quad (6)$$

gives the angular moments vector,

$$\bar{\psi}(k; \mu_0) = [\bar{\psi}_1(k; \mu_0) \quad \bar{\psi}_2(k; \mu_0) \quad \dots \quad \bar{\psi}_L(k; \mu_0)]^T.$$

The angular flux transform comes from Eq(3)

$$\bar{\psi}(k, \mu; \mu_0) = \frac{z}{z + \mu_0} \delta(\mu - \mu_0) + \frac{c}{2} \frac{z}{z + \mu} \mathbf{P}^T(\mu) \mathbf{W} \bar{\psi}(k; \mu_0).$$

From the inversion integral

$$\psi(x, \mu; \mu_0) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} \bar{\psi}(k, \mu; \mu_0),$$

therefore

$$\begin{aligned} \psi(x, \mu; \mu_0) &= \frac{e^{-|x/\mu_0|}}{|\mu_0|} \Theta(x/\mu_0) \delta(\mu - \mu_0) + \\ &+ \frac{c}{4\pi} \mathbf{P}^T(\mu) \mathbf{W} \int_{-\infty}^{\infty} dk e^{ikx} \frac{z}{z + \mu} \frac{z}{z + \mu_0} [\mathbf{I} - c\mathbf{L}(z)\mathbf{W}]^{-1} \mathbf{P}(\mu_0), \end{aligned} \quad (7)$$

where  $\Theta(x/\mu_0)$  is the unit step function in the uncollided contribution, which is the first term.

While Eq(7) is a valid solution, an explicit analytical form from the inversion is not forthcoming. One can only say poles come from the zeros of  $\text{Det}\left[\mathbf{I} - c\mathbf{L}(z)\mathbf{W}\right]$  and branch points  $\pm i$  come from the logarithm in the Legendre functions in  $\mathbf{L}$ .

### 3. The Non-Standard Solution

#### 3.1 Moments Solution

We find a more useful moments solution by projection of Eq(3) over Legendre polynomials to give the following three-term recurrence for the transformed Legendre moments:

$$zh_l\bar{\psi}_l(k; \mu_0) + (l+1)\bar{\psi}_{l+1}(k; \mu_0) + l\bar{\psi}_{l-1}(k; \mu_0) = zS_l(\mu_0), \quad (8)$$

with

$$\begin{aligned} h_l &\equiv 2l + 1 - \omega_l \\ S_l(\mu_0) &\equiv (2l + 1)P_l(\mu_0). \end{aligned}$$

From the theory of recurrence [6], the general solution to this recurrence is

$$\bar{\psi}_l(k; \mu_0) = a(z; \mu_0)g_l(z) + b(z; \mu_0)\rho_l(z) + z\sum_{j=0}^l \alpha_{l,j}(z)S_j(\mu_0), \quad (9)$$

where the functions  $g_l(z)$  and  $\rho_l(z)$  are solutions to the homogeneous form of Eq(8), followed by the particular solution. The coefficients,  $a(z; \mu_0)$  and  $b(z; \mu_0)$ , are determined from the starting condition at  $l = 0$

$$\begin{aligned} a(z; \mu_0) &\equiv \bar{\psi}_0(k; \mu_0) \\ b(z; \mu_0) &\equiv -S_0(\mu_0) = -1 \end{aligned}$$

with  $g_0(z) \equiv 1$ ;  $\rho_0(z) \equiv 0$ ;  $\alpha_{0,0}(z) \equiv 0$  giving the recurrences

$$\begin{aligned} zh_l g_l(z) + (l+1)g_{l+1}(z) + lg_{l-1}(z) &\equiv 0 \\ zh_l \rho_l(z) + (l+1)\rho_{l+1}(z) + l\rho_{l-1}(z) &\equiv 0. \end{aligned}$$

Using the properties of the homogeneous solutions, one can show the coefficient in the particular solution is

$$z\alpha_{l,j}(z) = \rho_j(z)g_l(z) - g_j(z)\rho_l(z)$$

to give

$$\begin{aligned}\bar{\psi}_l(k; \mu_0) &= g_l(z) \bar{\psi}_0(k; \mu_0) - \\ &- \sum_{j=0}^l (2j+1) [g_j(z) \rho_l(z) - \rho_j(z) g_l(z)] P_j(\mu_0).\end{aligned}\quad (10)$$

To conform to conventional definitions of Chandrasekhar polynomials, let

$$\begin{aligned}g_l(z) &\rightarrow (-1)^l g_l(z) \\ \rho_l(z) &\rightarrow (-1)^l \rho_l(z)\end{aligned}$$

to give for Eq(10)

$$\bar{\psi}_l(k; \mu_0) = g_l(-z) \bar{\psi}_0(k; \mu_0) - \chi_l(-z, \mu_0), \quad (11a)$$

with  $\chi_l$

$$\chi_l(z, \mu) \equiv \sum_{j=0}^l (2j+1) P_j(\mu) [ \rho_l(z) g_j(z) - g_l(z) \rho_j(z) ]. \quad (11b)$$

### 3.1.1 Transport closure

To continue, we need  $\bar{\psi}_0(k; \mu_0)$  or, in other words, closure of the moments equations [Eq(8)].

To apply the exact ‘‘transport closure’’ one sets  $j$  to zero in Eq(4),

$$\sum_{l=0}^L [\delta_{0,l} - c \omega_l L_{0,l}(z)] \bar{\psi}_l(k; \mu_0) = \frac{z}{z + \mu_0}, \quad (12)$$

to give on substitution of Eq(11a)

$$\bar{\psi}_0(k; \mu_0) = \frac{1}{\Lambda_L(z)} \left[ \frac{z}{z + \mu_0} - cz \sum_{l=0}^L \omega_l Q_l(-z) \chi_l(-z, \mu_0) \right] \quad (13)$$

with the dispersion relation

$$\Lambda_L(z) \equiv 1 - cz \sum_{l=0}^L \omega_l Q_l(z) g_l(z),$$

also written as

$$\Lambda_L(z) = (L+1) \left[ g_{L+1}(z) Q_L(z) - g_L(z) Q_{L+1}(z) \right].$$

### 3.2 The Fourier Transform of the Angular Flux

We can conveniently express the angular flux transform as the Legendre polynomial expansion

$$\psi_L(k, \mu; \mu_0) = \sum_{l=0}^{\infty} \frac{(2l+1)}{2} \bar{\psi}_{l,L}(k; \mu_0) P_l(\mu), \quad (14)$$

where the moments  $\bar{\psi}_{l,L}(k; \mu_0)$  are from Eqs(11). The subscript  $L$  indicates truncated scattering. When the moments are introduced into Eq(14) with  $k$  replaced by  $-k$  (for notational convenience), there results

$$\psi_L(-k, \mu; \mu_0) = \phi(z, \mu) \bar{\psi}_{0,L}(-k; \mu_0) - T(z, \mu; \mu_0) \quad (15a)$$

with

$$\phi(z, \mu) \equiv \sum_{l=0}^{\infty} \frac{(2l+1)}{2} g_l(z) P_l(\mu) \quad (15b)$$

and

$$T(z, \mu; \mu_0) \equiv \sum_{l=0}^{\infty} \frac{(2l+1)}{2} \chi_l(z, \mu_0) P_l(\mu). \quad (15c)$$

The sums in Eq(15b,c) require further clarification whereby a generalized singular eigenfunction will emerge.

#### 3.2.1 Generalized singular eigenfunctions

To proceed, consider the limit

$$\phi(z, \mu) = \lim_{N \rightarrow \infty} \sum_{l=0}^N \frac{(2l+1)}{2} g_l(z) P_l(\mu),$$

along with the Christoffel-Darboux formula,

$$\sum_{l=0}^N \frac{(2l+1)}{2} g_l(z) P_l(\mu) = \frac{1}{z - \mu} \left\{ (N+1) \left[ g_{N+1}(z) P_N(\mu) - g_N(z) P_{N+1}(\mu) \right] + \right. \\ \left. + cz g_L^*(z, \mu) \right\},$$

where

$$g_l^*(z, \mu) \equiv \begin{cases} \sum_{j=0}^l \omega_j g_j(z) P_j(\mu), & l \leq L \\ g_L^*(z, \mu), & l \geq L+1. \end{cases}$$

For  $N \geq L+1$ , one can show [with some effort]

$$g_l(z) = \Lambda_L(z) P_l(z) + \tilde{\psi}_L(z) Q_l(z),$$

and

$$\tilde{\psi}_l(z) = (l+1) [g_l(z) P_{l+1}(z) - g_{l+1}(z) P_l(z)].$$

As a consequence, formally

$$\begin{aligned} & \sum_{l=0}^{\infty} \frac{(2l+1)}{2} P_l(z) P_l(\mu) = \\ & = \lim_{N \rightarrow \infty} \left\{ \frac{N+1}{2} \left[ \frac{P_{N+1}(z) P_N(\mu) - P_N(z) P_{N+1}(\mu)}{z - \mu} \right] \right\} = \delta(z - \mu) \end{aligned}$$

and

$$\begin{aligned} & \sum_{l=0}^{\infty} \frac{(2l+1)}{2} Q_l(z) P_l(\mu) = \\ & = \lim_{N \rightarrow \infty} \left\{ \frac{N+1}{2} \left[ \frac{Q_N(z) P_{N+1}(\mu) - Q_{N+1}(z) P_N(\mu)}{z - \mu} \right] \right\} = 0 \end{aligned}$$

to conveniently give (after some manipulation)

$$\phi_L(z, \mu) = \frac{cz}{2} \frac{g_L^*(z, \mu)}{z - \mu} + \Lambda_L(z) \delta(z - \mu). \quad (16a)$$

Similarly, the second kind polynomials generate the generalized singular eigenfunction



$$\Theta(z, \mu) \equiv \sum_{l=0}^{\infty} \frac{(2l+1)}{2} \rho_l(z) P_l(\mu),$$

or

$$\Theta_L(z, \mu) = \frac{z}{2} \frac{[ch_L^*(z, \mu) - 1]}{z - \mu} + \gamma_L(z) \delta(z - \mu), \quad (16b)$$

where

$$h_l^*(z, \mu) \equiv \sum_{j=0}^l \omega_j \rho_j(z) P_j(\mu).$$

$$\gamma_l(z) \equiv (l+1) [\rho_{l+1}(z) Q_l(z) - \rho_l(z) Q_{l+1}(z)].$$

The expression  $\delta(z - \mu)$  reduces to the delta function and Eqs(16) become the Case singular eigenfunctions on the branch cut in the complex  $z$ -plane as shown below.

### 3.2.2 Evaluation of $T(z, \mu; \mu_0)$

With some manipulation, the evaluation of  $T(z, \mu; \mu_0)$  follows from Eqs(11b) and (15c)

$$T(z, \mu; \mu_0) = 2S_L(z, \mu; \mu_0) + \frac{z}{z - \mu} [\delta(z - \mu) - \delta(\mu - \mu_0)], \quad (17)$$

where

$$S_L(z, \mu; \mu_0) = \Theta_L(z, \mu) \phi_L(z, \mu_0) - \Theta_L(z, \mu_0) \phi_L(z, \mu) -$$

$$- \sum_{l=0}^L \frac{(2l+1)}{2} \left\{ \begin{array}{l} \rho_l(z) [\phi_l(z, \mu_0) - \phi_l(z, \mu)] - \\ -g_l(z) [\Theta_l(z, \mu_0) - \Theta_l(z, \mu)] \end{array} \right\} P_l(\mu).$$

### 3.2.3 Alternative expression for $\bar{\psi}_{0,L}(k; \mu_0)$

Exploiting the following symmetry:

$$\bar{\psi}_L(k, \mu; \mu_0) = \bar{\psi}_L(k, \mu_0; \mu),$$

one can show

$$\bar{\psi}_{0,L}(k; \mu_0) = 2\phi_L(-z, \mu_0) \frac{\gamma_L(z)}{\Lambda_L(z)} - \Theta_L(-z, \mu_0). \quad (18)$$

We are now in position to invert the transform of Eq(15a).

### 3.3 Fourier transform inversion

By introducing  $\bar{\psi}_{0,L}(k; \mu_0)$  from Eq(18) into Eq(15a) with  $T(z, \mu; \mu_0)$  from Eq(17),  $\bar{\psi}_L(k, \mu; \mu_0)$  becomes

$$\bar{\psi}_L(k, \mu; \mu_0) = 2\phi_L(-z, \mu) \phi_L(-z, \mu_0) \frac{\gamma_L(z)}{\Lambda_L(z)} - H_L(-z, \mu; \mu_0) \quad (19)$$

with

$$H_L(z, \mu; \mu_0) \equiv 2 \left\{ \begin{aligned} & \Theta_L(z, \mu) \phi_L(z, \mu_0) + \\ & + \sum_{l=0}^L \frac{(2l+1)}{2} \left\{ \begin{aligned} & \rho_l(z) [\phi_l(z, \mu_0) - \phi_L(z, \mu_0)] - \\ & - g_l(z) [\Theta_l(z, \mu_0) - \Theta_L(z, \mu_0)] \end{aligned} \right\} P_l(\mu) + \\ & + \frac{1}{2} \frac{z}{z - \mu} [\delta(z - \mu_0) - \delta(\mu - \mu_0)] \end{aligned} \right\}.$$

A brief description of the Fourier transform inversion follows.

The poles and branch points of the integrand are

$$\Lambda_L(\pm \nu_{0m}) = 0, \quad m = 1, \dots, \mathcal{M}_L,$$

and  $\pm i$  (from the logarithm in the Legendre functions) respectively. Then, for the contour of Fig. 1:

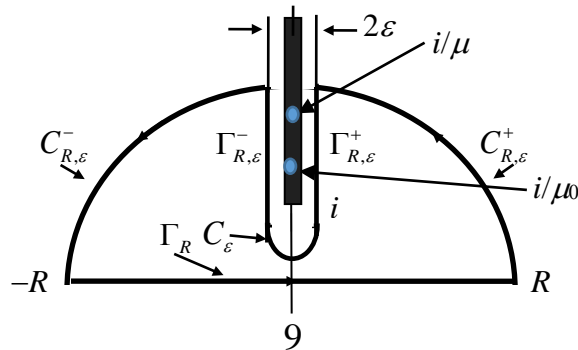


Fig. 1. Complex  $k$ -plane:  $C_{R,\varepsilon} \equiv \Gamma_R + C_{R,\varepsilon}^- + \Gamma_{R,\varepsilon}^- + C_\varepsilon + \Gamma_{R,\varepsilon}^+ + C_{R,\varepsilon}^+$

contributions from the pole singularities and along the branch cut give

$$\psi_L(x, \mu; \mu_0) = I_L(x, \mu; \mu_0) - I_{L, \Gamma^+ + \Gamma^-}(x, \mu; \mu_0), \quad (20a)$$

where the first term is

$$I_L(x, \mu; \mu_0) = \sum_{m=1}^{\mathcal{M}_L} \frac{\phi_L(v_{0m}, \mu) \phi_L(v_{0m}, \mu_0)}{M_L(v_{0m})} e^{-x/v_{0m}}. \quad (20b)$$

The second term in Eq(20a) is from the branch cut, which is an integration over the discontinuity of the boundary values of the sectionally analytic integrand and becomes

$$I_{L, \Gamma^+ + \Gamma^-}(x, \mu; \mu_0) = -\frac{i}{2\pi} \int_0^1 dv \frac{e^{-x/v}}{v^2} \text{Disc} \left[ \bar{\psi}_L(-k(v), \mu; \mu_0) \right]$$

with

$$\begin{aligned} \text{Disc} \left[ \bar{\psi}_L(-k(v), \mu; \mu_0) \right] &\equiv \\ &\equiv \bar{\psi}_L^+(-k(v), \mu; \mu_0) - \bar{\psi}_L^-(-k(v), \mu; \mu_0). \end{aligned}$$

The boundary values of  $\bar{\psi}_L$  are

$$\bar{\psi}_L^\pm(-k(v), \mu; \mu_0) \equiv \lim_{\varepsilon \rightarrow 0} \bar{\psi}_L(-k(v \pm i\varepsilon), \mu; \mu_0).$$

With some extensive manipulation and noting  $H_L(-z, \mu; \mu_0)$  is analytic, allows the entire branch cut contribution to derive from the first term of Eq(15a) to give

$$I_{L, \Gamma^+ + \Gamma^-}(x, \mu; \mu_0) = -\int_0^1 dv \frac{e^{-x/v}}{M_L(v)} \phi_L(v, \mu) \phi_L(v, \mu_0) \quad (20c)$$

with

$$M_L(v) \equiv v\Lambda_L^+(v)\Lambda_L^-(v).$$

Also noting that the contributions from the contours  $C_\varepsilon$  and  $C_{R,\varepsilon}^\pm$  vanish in their respective limits, Eqs(20) give the final solution for truncated scattering for  $x \geq 0$  as

$$\begin{aligned}\psi_L(x, \mu; \mu_0) &= \sum_{m=1}^{\mathcal{M}_L} \frac{\phi_L(v_{0m}, \mu) \phi_L(v_{0m}, \mu_0)}{M_L(v_{0m})} e^{-x/v_{0m}} + \\ &+ \int_0^1 dv \frac{e^{-x/v}}{M_L(v)} \phi_L(v, \mu) \phi_L(v, \mu_0).\end{aligned}\quad (21a)$$

From reciprocity

$$\psi_L(-|x|, \mu; \mu_0) = \psi_L(|x|, -\mu; -\mu_0)$$

and  $\phi_L(-v, \mu) = \phi_L(v, -\mu)$ , Eq(21a) also is

$$\begin{aligned}\psi_L(-|x|, \mu; \mu_0) &= \sum_{m=1}^{\mathcal{M}_L} \frac{\phi_L(-v_{0m}, \mu) \phi_L(-v_{0m}, \mu_0)}{M_L(v_{0m})} e^{-|x|/v_{0m}} + \\ &+ \int_0^1 dv \frac{e^{-|x|/v}}{M_L(v)} \phi_L(-v, \mu) \phi_L(-v, \mu_0).\end{aligned}\quad (21b)$$

Eliminating scattering truncation by letting  $L \rightarrow \infty$ , gives the classical singular eigenfunction expansion for  $x \gtrless 0$  as found by Case

$$\begin{aligned}\psi(x, \mu; \mu_0) &= \sum_{m=1}^{\mathcal{M}_L} \frac{\phi(\pm v_{0m}, \mu) \phi(\pm v_{0m}, \mu_0)}{M(v_{0m})} e^{-|x|/v_{0m}} + \\ &+ \int_0^1 dv \frac{e^{-|x|/v}}{M(v)} \phi(\pm v, \mu) \phi(\pm v, \mu_0),\end{aligned}\quad (22)$$

where

$$\phi(v, \mu) \equiv \lim_{L \rightarrow \infty} \phi_L(v, \mu) = \frac{cv}{2} \mathbf{P} \frac{g^*(v, \mu)}{v - \mu} + \Lambda^*(v) \delta(v - \mu)$$

with

$$g^*(v, \mu) \equiv \sum_{l=0}^{\infty} \omega_l g_l(v) P_l(\mu)$$

$$\Lambda^*(\nu) \equiv 1 - c\nu \sum_{l=0}^{\infty} \omega_l Q_l(\nu) g_l(\nu),$$

and  $\mathcal{P}$  is the principal value of the expression following when under an integral.

### FINAL REMARKS

The above derivation merits additional comment. While the result is not new, the steps getting to it are. The primary reason the approach succeeds is that it is a consequence of the solution to the moments recurrence coming from an analytical closure. This is novel since an analytical solution to a recurrence is not common in analytical solutions to the transport equation. Recurrences generally find use in numerical, not theoretical evaluations. It is also obvious that the approach works because we know what to look for—the singular eigenfunction expansion. Thus, it is not too surprising that, without Case’s guidance, the singular eigenfunction expansion was not first discovered from the Fourier transforms. Additionally, no orthogonality or completeness is required as the eigenfunction expansion simply emerges from manipulation in the complex plane. For this reason, the Fourier transform derivation, while less elegant than Case’s solution, is more classically mathematical.

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