

Discrete Fourier Inversion of Linear Inhomogeneity

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Solutions to tensor, vector, and scalar linear inhomogeneous partial differential equations can be obtained by discrete Fourier inversion of the linear system. The inverse (Green's function) problem can be cast into sets of single, double, and triple summation/integration expressions by using transcendental eigenfunction expansions in certain three-dimensional triply-orthogonal geometries whose solutions admit simple and R -separation of variables. By reversing and collapsing traditional ordering schemes for the inverse problem, one can derive new special function addition theorems for asymmetric, axisymmetric and cylindrical, orthogonal curvilinear coordinate geometries. In this paper, we introduce such important applications as inhomogeneous Laplace, Helmholtz, wave, Schrödinger, heat, Klein–Gordon, Laplace–Beltrami, biharmonic, triharmonic as well as mixed higher-order harmonic and linear inhomogeneous partial differential equations. Compact expressions are seen to exist in spherical geometries through the utilization of separation angle spherical linear system-function expansions.

1 Introduction

Inhomogeneity is defined as the presence of a source contribution to an otherwise homogeneous linear partial differential equation. Hereafter we refer to linear partial differential equations as linear systems and their solutions as linear system-functions. Inhomogeneity in linear systems is expressed as a non-zero scalar, vector, or tensor valued function ρ . The presence of inhomogeneity usually implies non-zero potential energies through assemblage and confinement. The precise influence due to specific inhomogeneity is often required in many different mathematical and physical contexts. Inhomogeneous variations are described below by adopting general curvilinear coordinate systems, such as spherical and cylindrical, which have been previously studied in the literature [1].

In coordinate systems which allow simple and R -separation of variables for linear systems, rearranging the orderings of multi-summation-integration expressions for infinite-extent Green's functions reveals new special function descriptions. Green's functions in spherical coordinates span an infinite two-dimensional space of quantum numbers (ℓ, m) [2]. Traditional precedent in spherical coordinates $\mathbf{x} = (r, \phi, \theta)$ and $\mathbf{x}' = (r', \phi', \theta')$ is to sum first over the orbital quantum number ℓ

$$\mathcal{G} = \sum_{\ell=0}^{\infty} \mathcal{G}_{\ell}, \quad (1)$$

where $\mathcal{G} = \mathcal{G}(\mathbf{x}, \mathbf{x}', t, t')$, and then to sum second over the azimuthal quantum number m

$$\mathcal{G}_{\ell} = \sum_{m=-\ell}^{\ell} \mathcal{G}_{\ell, m}. \quad (2)$$

Equation (2) represents an addition theorem for spherical system-functions. By rearranging the traditional ordering we obtain a separate algorithm for summing over the infinite two-

dimensional (ℓ, m) space, first over m

$$\mathcal{G} = \sum_{m=-\infty}^{\infty} \mathcal{G}_m e^{im(\phi-\phi')}, \quad (3)$$

and then over ℓ

$$\mathcal{G}_m = \sum_{\ell=|m|}^{\infty} \mathcal{G}_{\ell,m}. \quad (4)$$

The coefficients \mathcal{G}_m are a better basis than \mathcal{G}_ℓ since they represent an infinite series over $\mathcal{G}_{\ell,m}$ (equation (4)) rather than a finite series over $\mathcal{G}_{\ell,m}$ (equation (2)). This is also true for linear system-functions in oblate and prolate spheroidal coordinates.

Rotationally invariant coordinate systems possess the azimuthal coordinate ϕ and can therefore be described using Fourier analysis over the azimuthal quantum number m . The coefficients \mathcal{G}_m in cylindrical coordinates are given by the definite integral

$$\mathcal{G}_m = \int_0^{\infty} d\kappa \mathcal{G}_m(\kappa). \quad (5)$$

So, in cylindrical coordinates, the problem of obtaining the Fourier coefficients \mathcal{G}_m of a particular linear system is reduced to solving a definite integral which represents the Fourier coefficients [3, 4]. Definite integrals arise for \mathcal{G}_m in parabolic coordinates as well.

Since all linear systems admit solutions through Green's functions, higher-order linear systems represent excellent candidates for discrete azimuthal and separation angle Fourier Green's function analysis. Examples of higher-order linear systems include poly-operator systems such as the biharmonic and triharmonic equations. Poly-operator systems are generated by using integral products of specific linear operators. One can also construct higher-order, hybrid-operator linear systems by introducing different linear operators in a product formalism. There are an infinite number of combinations resulting in linear poly-operator or hybrid-operator inhomogeneous systems. One example which uses the poly-operator formalism has recently been treated by Cohl [5]. There, compact Fourier Green's function expansions are obtained for a biharmonic equation which is equivalent to Poisson's equation. One of the nice features of higher-order poly-operator systems is that the transformed kernel is converted to one which is no longer locally singular. Examples of higher-order inhomogeneous linear systems include the vector and scalar n -Laplace, n -Helmholtz, n -heat, n -wave, n -Schrödinger, n -Klein-Gordon, and n -Laplace-Beltrami equations.

For every linear system, there exist unique multi-summation-integration expressions for the appropriate Green's function in spherical and cylindrical coordinates [6]. The derivation of these addition theorems is critically important to our description and understanding of the properties of linear system-functions [7–10]. Other rearrangements are possible in asymmetric coordinate geometries such as ellipsoidal, paraboloidal, and conical.

2 Separation angle Fourier analysis

The separation angle in an orthogonal curvilinear coordinate system can be obtained by examining the dot product of the observation vector $\mathbf{x} = (r, \phi, \theta)$ with the source vector $\mathbf{x}' = (r', \phi', \theta')$,

$$\mathbf{x} \cdot \mathbf{x}' = rr' \cos \gamma, \quad (6)$$

where $\cos \gamma = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\phi - \phi')$ is called the separation angle. When $\gamma = 0$ both vectors have the same orientation, and the relative distances are determined by r and r' . As γ is

increased from zero (radial alignment) to π (radial anti-alignment), the surface of constant γ maps out an infinite cone in space. One may apply a discrete separation angle Fourier analysis of Green's system-functions \mathcal{G} , on a sphere, given by

$$\mathcal{G} = \sum_{n=-\infty}^{\infty} \mathcal{G}_n e^{in\gamma}, \quad (7)$$

where n is the separation angle quantum number [4, 5] and $\mathcal{G}_n = \mathcal{G}_n(r, r', t, t')$.

Ordinarily, Green's functions in spherical coordinates are expanded in spherical harmonics. One may directly compare the relative strengths of expansions in Legendre polynomials (spherical harmonics, see equation (1)) as compared to discrete Fourier expansions (equation (7)). Discrete separation angle Fourier analysis of functions on spheres is more compact than spherical harmonic analysis (which uses integer degree, integer order, associated Legendre functions). By using separation angle Fourier analysis, one can take advantage of the full spherical component, which is contained entirely within the $n = 0$ term in the expansion. Notice that the Fourier expansion is fully 2π -periodic and necessarily takes full advantage of this particular property of spheres. A second 2π -periodic angle is seen as an azimuthal coordinate about the line of centers which connects the two rays $\gamma = (0, \pi)$. The $n = 0$ term in the expansion represents the offset of a spherical density distribution which is constant at any (ϕ, θ) orientation. It requires an infinite sum over the orbital angular momentum quantum number ℓ to obtain the true spherically symmetric contribution in a modal analysis. For the Laplace equation, the separation angle Fourier coefficients are given by the odd-half-integer degree associated Legendre function of the second kind, which is a toroidal harmonic [11, 12]. We suggest that separation angle Fourier analysis represents a set of spherical linear system-functions which are more fundamental when solving physical problems, and even in pure mathematical contexts on spheres.

3 Newtonian/Coulomb potential self-energy

Here we introduce the potential self-energy W for the inhomogeneous Laplace equation (Poisson's equation)

$$W = \frac{1}{2} \int d^3 \mathbf{x} \Phi(\mathbf{x}) \rho(\mathbf{x}), \quad (8)$$

where \mathbf{x} is the observation vector. $\Phi(\mathbf{x})$ is the potential function generated by the source density function $\rho(\mathbf{x})$

$$\nabla^2 \Phi(\mathbf{x}) = 4\pi \rho(\mathbf{x}), \quad (9)$$

where ∇^2 is the Laplacian operator. An integral equivalent representation of equation (9) is given by

$$\Phi(\mathbf{x}) = -\frac{1}{2} \int d^3 \mathbf{x}' |\mathbf{x} - \mathbf{x}'| \nabla'^2 \rho(\mathbf{x}'), \quad (10)$$

where \mathbf{x}' is the source vector. The integral representation of equation (9) is preferable to the standard representation

$$\Phi(\mathbf{x}) = - \int d^3 \mathbf{x}' \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}, \quad (11)$$

because the kernel of integration (Green's function) is better behaved locally. Notice that the kernel of integration $\frac{1}{2}|\mathbf{x} - \mathbf{x}'|$ is the Green's function for the biharmonic equation [5].

The potential self-energy W is often required in energy minimization techniques in classical and non-classical physics. Due to the global nature of these types of problems, modest errors in the computation of the potential self-energy will often impede the ability of such algorithms, which otherwise yield satisfactory results.

This potential self-energy can be computed as a three-space integral, given that the potential functions are known. The process of obtaining the potential functions is obtained by solving the boundary value problem with the appropriate Dirichlet boundary conditions, which should be obtained by a modal analysis. The choice of a Fourier basis has clear advantages when viewed in terms of a total potential self-energy computation. The choice of expanding physical variables in separation angle or azimuthal angle Fourier bases affords two separate choices in the facility of the computation of the potential self-energy for different types of mass or charge distributions.

The separation distance [5] is given by

$$|\mathbf{x} - \mathbf{x}'| = \Psi \sum_{m=-\infty}^{\infty} \left(m^2 - \frac{1}{4}\right)^{-1} Q_{m-\frac{1}{2}}^1(\chi) e^{im(\phi-\phi')}, \quad (12)$$

where

$$\chi = \frac{R^2 + R'^2 + (z - z')^2}{2RR'}, \quad (13)$$

and

$$\Psi = \frac{\sqrt{(R^2 - R'^2)^2 + 2(R^2 + R'^2)(z - z')^2 + (z - z')^4}}{2\pi\sqrt{RR'}}. \quad (14)$$

The corresponding expression in spherical separation angle Fourier modes [5] is given by

$$|\mathbf{x} - \mathbf{x}'| = \frac{r_{>}^2 - r_{<}^2}{2\pi\sqrt{rr'}} \sum_{n=-\infty}^{\infty} \left(n^2 - \frac{1}{4}\right)^{-1} Q_{n-\frac{1}{2}}^1\left(\frac{r^2 + r'^2}{2rr'}\right) e^{in\gamma}. \quad (15)$$

In both cases, equations (12) and (15), one may take advantage of compact Fourier Green's function expansions. When applied to the azimuthal case, one may easily obtain the total potential self-energy for purely axisymmetric ($m = 0$) source distributions. In terms of the separation angle, one may also obtain the total potential self-energy for spherically symmetric ($n = 0$) source distributions. If the spherically symmetric ($n = 0$) contribution is used, the total energy is reduced to a one-dimensional integral over the r' variable. This contribution is easily gained by integrating over the appropriate complete elliptic integrals of the first and second kind (see below). If the axisymmetric ($m = 0$) contribution is needed, the total potential self-energy is reduced to a two-dimensional integral over the R' and z' variables.

3.1 Potential self-energy for axisymmetric source distributions

We now compute the potential self-energy for axisymmetric source distributions. In this case, only the ($m = 0$) term in the integral survives, therefore

$$W = \pi \int_0^\infty dR R \int_{-\infty}^\infty dz \rho_0(R, z) \Phi_0(R, z), \quad (16)$$

where (R, z) represent the radial and vertical circular cylindrical positions respectively. The axisymmetric ($m = 0$) Fourier component of a general nonaxisymmetric density distribution is given by

$$\rho_0(R, z) = \frac{1}{2\pi} \int_0^{2\pi} d\phi \rho(R, \phi, z), \quad (17)$$

and the azimuthal angle ($m = 0$) Fourier component of the potential is given by

$$\Phi_0(R, z) = -\frac{1}{2} \int d^3 \mathbf{x}' |\mathbf{x} - \mathbf{x}'|_{m=0} \nabla'^2 \rho_0(R', z'). \quad (18)$$

The azimuthal angle ($m = 0$) Fourier component of the separation distance is given by [5]

$$|\mathbf{x} - \mathbf{x}'|_{m=0} = -\frac{2Q_{-\frac{1}{2}}^1(\chi)}{\pi\sqrt{RR'}} \left[(R^2 - R'^2)^2 + 2(R^2 + R'^2)(z - z')^2 + (z - z')^4 \right]^{\frac{1}{2}}, \quad (19)$$

where $Q_{-\frac{1}{2}}^1$ is the unit order, negative one-half degree, associated Legendre function of the second kind. The azimuthal angle ($m = 0$) Fourier component can be simplified as

$$|\mathbf{x} - \mathbf{x}'|_{m=0} = \frac{2}{\pi} \alpha E \left(\sqrt{\frac{4RR'}{(R + R')^2 + (z - z')^2}} \right), \quad (20)$$

where E is the complete elliptic integral of the second kind [8] and

$$\alpha = \sqrt{\frac{(R^2 - R'^2)^2 + 2(R^2 + R'^2)(z - z')^2 + (z - z')^4}{(R - R')^2 + (z - z')^2}}. \quad (21)$$

Finally, the azimuthal angle ($m = 0$) Fourier component of the potential is given by

$$\Phi_0(R, z) = -2 \int_0^\infty dR' R' \int_{-\infty}^\infty dz' \alpha E \left(\sqrt{\frac{4RR'}{(R + R')^2 + (z - z')^2}} \right) \nabla'^2 \rho_0(R', z'). \quad (22)$$

3.2 Potential self-energy for spherically symmetric source distributions

We now compute the potential self-energy for spherically symmetric source distributions. In this case, only the ($n = 0$) term in the integral survives, therefore

$$W = 2\pi \int_0^\infty dr r^2 \rho_0(r) \Phi_0(r), \quad (23)$$

where r is the spherical radial coordinate and the spherically symmetric ($n = 0$) Fourier component of a general nonspherical density distribution is given by

$$\rho_0(r) = \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \rho(r, \phi, \theta). \quad (24)$$

The separation angle ($n = 0$) Fourier component of the potential is given by

$$\Phi_0(r) = -\frac{1}{2} \int d^3 \mathbf{x}' |\mathbf{x} - \mathbf{x}'|_{n=0} \nabla'^2 \rho_0(r'), \quad (25)$$

and the separation angle ($n = 0$) Fourier component of the separation distance is given by

$$|\mathbf{x} - \mathbf{x}'|_{n=0} = -2 \frac{r_{>}^2 - r_{<}^2}{\pi\sqrt{rr'}} Q_{-\frac{1}{2}}^1 \left(\frac{r^2 + r'^2}{2rr'} \right), \quad (26)$$

where the subscript notation $r_{>}$ and $r_{<}$ represents the greater and lesser of the spherical distances respectively. The separation angle ($n = 0$) Fourier component of the separation distance can be simplified to

$$|\mathbf{x} - \mathbf{x}'|_{n=0} = \frac{2}{\pi} (r + r') E \left(\frac{2\sqrt{rr'}}{r + r'} \right). \quad (27)$$

Finally, the separation angle ($n = 0$) Fourier component of the potential is given by

$$\Phi_0(r) = -4 \int_0^\infty dr' r'^2 (r + r') E \left(\frac{2\sqrt{rr'}}{r + r'} \right) \nabla'^2 \rho_0(r'). \quad (28)$$

4 Summary

In order for one to compute the solution of an arbitrary linear inhomogeneous problem, one has to first obtain the azimuthal Fourier component of the Green's function in question. The Fourier Green's function expansion has been obtained [3, 4, 12] for the Laplace and biharmonic equations. One must also look at the Fourier expansions of other important linear partial differential equations such as the Helmholtz, heat, wave, Schrödinger, Klein–Gordon, Laplace–Beltrami, triharmonic, and higher-order equations. There are an infinite number of product and sum combinations of separate linear operators which can represent even higher-order linear differential operators in space, time, and space-time. By obtaining these results, the integral inverse (Green's function) for that particular problem will have a highly-useful compact Fourier representation. Furthermore, these Green's function expansions will be expressible in all the coordinate systems which allow simple and R -separation of variables (see Moon and Spencer [9, 10] and Miller [7]). Relevant coordinate systems include spherical, cylindrical, parabolic, oblate and prolate spheroidal, and toroidal.

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