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Portent of Heine's Reciprocal Square Root Identity

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Abstract. Precise efforts in theoretical astrophysics are needed to fully understand the mechanisms that govern the structure, stability, dynamics, formation, and evolution of differentially rotating stars. Direct computation of the physical attributes of a star can be facilitated by the use of highly compact azimuthal and separation angle Fourier formulations of the Green's functions for the linear partial differential equations of mathematical physics.

1. Introduction

Solutions to the three dimensional inhomogeneous linear partial differential equations of mathematical physics are expressible in terms their appropriate Green's functions (Duffy 2001). Single, double, and triple eigenfunction integration and summation expressions for Green's functions are obtainable in the coordinate systems that allow for separation of variables (Morse & Feshbach 1953). Separation of variables maps the linear three dimensional homogeneous partial differential equations into three decoupled ordinary differential equations (Miller 1977). Important linear 3D partial differential equations of mathematical physics include the Laplace equation, the Helmholtz equation, the biharmonic equation, the wave equation, the diffusion equation, and the Schroedinger equation. The properties of R-separability for these partial differential equations are reflected in the Green's function expansions. In the rotationally invariant coordinate systems that R-separably solve these equations, new discrete Fourier representations exist for the Green's functions for the Laplace equation (Cohl et al. 2000). Discrete Fourier expansions, given in terms of the azimuthal and separation angles, must exist for the rest of the linear partial differential equations of mathematical physics. The coefficients of these discrete Fourier representations will be given in terms of identifiable transcendental functions obtained by reversing and collapsing Green's function expansions for these partial differential equations. The fundamental mathematical tools required in order to complete this investigation are commonly available in the mathematics and physics literature.

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The Green's function for Laplace's equation is

$$\mathcal{G}_L(\mathbf{x},\mathbf{x}') = \frac{1}{|\mathbf{x}-\mathbf{x}'|}, \tag{1}$$

where $\mathbf{x}$ and $\mathbf{x}'$ are given by the Cartesian coordinates (x, y, z) and (x', y', z'). Traditionally, the Green's function is expanded in terms of spherical harmonics

$$\mathcal{G}_L = \frac{1}{\sqrt{rr'}} \sum_{\ell=0}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+\frac{1}{2}} P_\ell(\cos\gamma), \tag{2}$$

in spherical (r, ϕ, θ) coordinates, where $r_<$ $(r_>)$ is the smaller (larger) of the distances r and r', $\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi')$, and P_ℓ is the Legendre polynomial of the first kind. [1]

By utilizing Heine's toroidal identity (Cohl & Tohline 1999, Cohl et al. 2000, Cohl et al. 2001):

$$\frac{1}{\sqrt{\zeta-\cos\psi}} = \frac{\sqrt{2}}{\pi} \sum_{m=-\infty}^{\infty} Q_{m-\frac{1}{2}}(\zeta)\, e^{im\psi}, \tag{3}$$

where $|\zeta| \geq 1$, and, $0 \leq \psi \leq 2\pi$, one can derive two highly compact Fourier series representations for the Green's function of Laplace's equation

$$\mathcal{G}_L = \frac{1}{\pi\sqrt{rr'}} \sum_{n=-\infty}^{\infty} Q_{n-\frac{1}{2}}\left(\frac{r^2+r'^2}{2rr'}\right) e^{in\gamma}, \tag{4}$$

$$\mathcal{G}_L = \frac{1}{\pi\sqrt{RR'}} \sum_{m=-\infty}^{\infty} Q_{m-\frac{1}{2}}\left(\frac{R^2+R'^2+(z-z')^2}{2RR'}\right) e^{im(\phi-\phi')}, \tag{5}$$

in spherical and cylindrical (R, ϕ, z) coordinates respectively. Similar discrete Fourier transform expressions must exist for the linear partial differential equations of mathematical physics. Algorithmic implementation of compact Fourier representations for the Green's functions of mathematical physics significantly improves the accuracy of the solution for these partial differential equations.

2. The Biharmonic, Triharmonic, and Higher Harmonic Equations

One may also express potential problems in terms of an inhomogeneous biharmonic equation whose source is proportional to the Laplacian of the density. The solution is expressible in terms of an integral of it's Green's function, $|\mathbf{x}-\mathbf{x}'|$, convolved with source. The resulting inhomogeneous biharmonic equation

$$\nabla^4\Phi(\mathbf{x}) = 4\pi\ \nabla^2\rho(\mathbf{x}), \tag{6}$$

[1] "...The set of six coordinates $\{\mathbf{x},\mathbf{x}'\}$ may be viewed either as defining two points relative to the origin or as the coordinates of a three-body system once the center of mass has been separated. In the *body frame,* three out of the six coordinates are dynamical variables, the potential energy depending on them." (Cohl et al. 2001)

where ∇^2 is the Laplacian, represents the solution to the potential problem over the infinite three-dimensional domain. The Green's function for the biharmonic equation (Vautherin 1972)

$$\mathcal{G}_{2L}(\mathbf{x},\mathbf{x}') = \frac{1}{2}|\mathbf{x}-\mathbf{x}'|, \tag{7}$$

is a much better behaved integration kernel than for Laplace's equation because the singularity has been moved to infinity through

$$\Phi(\mathbf{x}) = -\frac{1}{2}\int d^3\mathbf{x}'\ \nabla'^{\,2}\rho(\mathbf{x}')\ |\mathbf{x}-\mathbf{x}'|. \tag{8}$$

One can generalize Heine's reciprocal square root identity using (Abramowitz & Stegun, 1965; Gradshteyn & Ryzhik 1994–to within a sign)

$$\int_\zeta^\infty \cdots \int_\zeta^\infty Q_{m-\frac{1}{2}}(\zeta)(d\zeta)^n = (-1)^n \frac{\Gamma(m-n+\frac{1}{2})}{\Gamma(m+n+\frac{1}{2})}(\zeta^2-1)^{n/2} Q^n_{m-\frac{1}{2}}(\zeta), \tag{9}$$

and by integrating both sides of eq. (2) with respect to ζ. Performing the integrations over ζ we obtain the following general result for *any* integer n - generalizing the last expression at the bottom of p. 182 in Magnus, Oberhettinger, & Soni (1966) (see also eqs. (26) & (30) in Cohl et al. 2000)

$$(\zeta-\cos\psi)^{n-\frac{1}{2}} = \sqrt{\frac{2}{\pi}}\frac{(\zeta^2-1)^{\frac{n}{2}}}{\Gamma(\frac{1}{2}-n)} \sum_{m=-\infty}^{\infty} \frac{\Gamma(m-n+\frac{1}{2})}{\Gamma(m+n+\frac{1}{2})}\ Q^n_{m-\frac{1}{2}}(\zeta)\ e^{im\psi}, \tag{10}$$

which reduces for $n=1$ to

$$\sqrt{\zeta-\cos\psi} = \frac{\sqrt{\zeta^2-1}}{\sqrt{2}\pi}\sum_{m=-\infty}^{\infty}\left(m^2-\frac{1}{4}\right)^{-1} Q^1_{m-\frac{1}{2}}(\zeta)\ e^{im\psi}. \tag{11}$$

Using this expression, we can rewrite the Green's function for the biharmonic equation in two different ways

$$2\mathcal{G}_{2L} = |\mathbf{x}-\mathbf{x}'| = \frac{r_>^2-r_<^2}{2\pi\sqrt{rr'}}\sum_{n=-\infty}^{\infty}\left(n^2-\frac{1}{4}\right)^{-1} Q^1_{n-\frac{1}{2}}\left(\frac{r^2+r'^2}{2rr'}\right)e^{in\gamma}, \tag{12}$$

and

$$2\mathcal{G}_{2L} = \Psi\sum_{m=-\infty}^{\infty}\left(m^2-\frac{1}{4}\right)^{-1} Q^1_{m-\frac{1}{2}}\left(\frac{R^2+R'^2+(z-z')^2}{2RR'}\right)e^{im(\phi-\phi')}, \tag{13}$$

where

$$\Psi \equiv \frac{[(R^2-R'^2)^2+2(R^2+R'^2)(z-z')^2+(z-z')^4]^{\frac{1}{2}}}{2\pi\sqrt{RR'}}. \tag{14}$$

This new formulation is amenable in analytic and computational physics applications on high-performance-computing architectures, since Laplacians can be readily computed on computational fluid dynamics meshes. Higher order harmonic Green's function expansions can be generated using this method. Boundary values can now be computed effectively along an arbitrarily chosen z-axis ($m = 0$) and at values chosen to lie within the outer-most extent of a chosen volumetric region ($m \geq 0$). Physical solution of the interior inhomogeneous problem can be obtained by proper boundary value treatment as described above. Accelerations can be obtained from the potential by performing a precise numerical gradient. In the case of cylindrical and spherical coordinates, the three dimensional Poisson solve can be further facilitated through the use of a discrete azimuthal Fourier transform. This decouples the three dimensional Poisson problem into a set of decoupled 2D problems that can be solved with second order accurate finite differencing using either direct or iterative methods.

3. Applications

Using highly compact representations of infinite domain Green's functions, solutions to the linear partial differential equations of mathematical physics can be more easily obtained. In this paper, and in recent papers, we treat the Green's function for the Laplace equation. Here we have extended this result to the three dimensional biharmonic and higher harmonic equations. Further variants are possible for the 3D Helmholtz, wave, and diffusion equations. In the future, we intend to investigate and more precisely describe these new Green's function expansions. Many areas of theoretical physics will benefit greatly from precise numerical implementations of these compact expansions.

Azimuthal Fourier identities for potentials such as Coulomb ($|\mathbf{x} - \mathbf{x}'|^{-1}$) or Yukawa ($e^{-k|\mathbf{x}-\mathbf{x}'|}|\mathbf{x} - \mathbf{x}'|^{-1}$) lead to new classical and quantum energy theorems. These allow for rapid and precise evaluation of the Coulomb or Yukawa direct and exchange interactions (Cohl et al. 2001). Classical Yukawa eigenfunctions are obtained through transcendental function identification of the Lamb-Sommerfeld integral (see Magnus et al. 1966). In quantum physics this is accomplished through the use of the azimuthal selection rule for the self-energies, namely for the direct and exchange Hamiltonian elements only the $m = 0$ and $m = m_1 - m_2$ terms survive respectively. The application of the selection rule allows for exact evaluation of the Hamiltonian matrix elements for two-electron interactions in atomic physics, molecular physics, condensed matter physics, physical chemistry, and biology. Two-electron interactions are critically important in obtaining opacities and correct equations of state in astrophysically dense atomic and molecular fluid media. Magnetohydrodynamic problems can now be easily handled with Heine expansions for the Green's functions of potential theory. By expressing the equations of fluid dynamics of a compressible media in terms of a velocity potential and a vector Poisson equation, one may compute precise velocity boundary values in vortex and shock flow regions (Lamb 1932) by solving the appropriate Poisson problem. Radiation transport, and classical and quantum scattering, will be greatly facilitated through compact Poisson formulations of the Green's function for the 3D diffusion and Helmholtz equations.

Precise Coulomb and Yukawa energies in the nuclear Hamiltonian allow for a higher degree of precision in obtaining nuclear structure.

4. Conclusion

The ultimate resolution of these analytical investigations will be efficient algorithmic implementations of these new schemes. We propose these methods to the three dimensional star community in hope that you may continue to enjoy significantly improved economical and precise boundary values for studies of analytical and numerical three dimensional stellar astrophysics.

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A Expressions for Unit Order Toroidal Functions

The unit order negative one half degree Legendre function of the second kind can be expressed as

$$Q^1_{-\frac{1}{2}}(\zeta) = \frac{-1}{\sqrt{2(\zeta-1)}} E\left(\sqrt{\frac{2}{\zeta+1}}\right), \tag{15}$$

where E is the complete elliptic integral of the second kind. The unit order, positive one half degree Legendre function can be expressed as

$$Q^1_{\frac{1}{2}}(\zeta) = -\frac{\zeta}{\sqrt{2(\zeta-1)}} E\left(\sqrt{\frac{2}{\zeta+1}}\right) + \sqrt{\frac{\zeta-1}{2}} K\left(\sqrt{\frac{2}{\zeta+1}}\right), \tag{16}$$

where K is the complete elliptic integral of the first kind. We can express this same function in terms of the complete elliptic integral D

$$Q^1_{\frac{1}{2}}(\zeta) = -\frac{1}{\sqrt{2(\zeta-1)}} E\left(\sqrt{\frac{2}{\zeta+1}}\right) + \frac{\sqrt{2(\zeta-1)}}{\zeta+1} D\left(\sqrt{\frac{2}{\zeta+1}}\right), \tag{17}$$

as well. Higher degree, unit order toroidal functions of the second kind can be easily derived using the following recurrence relation,

$$Q^1_{m+\frac{1}{2}}(\zeta) = \frac{4m\zeta}{2m-1}\, Q^1_{m-\frac{1}{2}}(\zeta) - \frac{2m+1}{2m-1}\, Q^1_{m-\frac{3}{2}}(\zeta). \tag{18}$$

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