Generalized relations among N-dimensional Coulomb Green's functions using fractional derivatives

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Hostler [J. Math. Phys. **11**, 2966 (1970)] has shown that Coulomb Green's functions of different dimensionality N are related by $G^{(N+2)} = \mathscr{O}G^{(N)}$, where $\mathscr{O}$ is a first-order derivative operator in the variables x and y. Thus all the even-dimensional functions are connected, as are analogously the odd-dimensional functions. It is shown that the operations of functional differentiation and integration can further connect the even- to the odd-dimensional functions, so that Hostler's relation can be extended to give $G^{(N+1)} = \mathscr{O}^{1/2}G^{(N)}$.

I. INTRODUCTION

Hostler showed in 1970 that Coulomb Green's functions of varying dimension N were related as follows[1–3]:

$$G^{(N+2)}(x,y,k) = -\frac{1}{\pi(x-y)}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)G^{(N)}(x,y,k), \quad N=1,2,3,\ldots . \tag{1.1}$$

Here x and y are the two coordinate variables

$$x,y \equiv r_1 + r_2 \pm r_{12} \tag{1.2}$$

and k is the wave number variable, such that, in atomic units ($\hbar = \mu = e = 1$),

$$E = \frac{\hbar^2 k^2}{2\mu} = \frac{k^2}{2}, \quad \nu \equiv \frac{Z}{k}. \tag{1.3}$$

Thus the odd-dimensional functions $G^{(3)}, G^{(5)},\ldots$ are obtained by successive differentiation of $G^{(1)}$, while the even-dimensional functions follows analogously from $G^{(2)}$. We will show in this paper that the even- and odd-dimensional Coulomb Green's functions can be further connected to one another by the operations of fractional differentiation and integration.

By the N-dimensional Coulomb Green's function we understand the solution of the inhomogeneous differential equation:

$$\left(\frac{1}{2}k^2 + \frac{1}{2}\nabla_N^2 + \frac{Z}{\mathbf{r}_N}\right)G^{(N)}(\mathbf{r}_N, \mathbf{r}'_N, k) = \delta^{(N)}(\mathbf{r}_N - \mathbf{r}'_N), \tag{1.4}$$

which is not to be confused with the solution to Poisson's equation in N-dimensional space.

II. RESUME OF THE FRACTIONAL CALCULUS

The monograph of Oldham and Spanier[4] gives a definitive presentation of the fractional calculus. A brief heuristic account of some relevant results will suffice to make this paper self-contained.

Multiple differentiation in the complex plane can be represented by Cauchy's integral formula:

$$f^{(n)}(z) = \frac{n!}{2\pi i}\oint \frac{f(\zeta)d\zeta}{(\zeta - z)^{(n+1)}}, \tag{2.1}$$

for a contour enclosing $\zeta = z$. A possible generalization of (2.1) to derivatives of nonintegral order q defines

$$f^{(q)}(z) = \frac{\Gamma(q+1)}{2\pi i}\int_C \frac{f(\zeta)d\zeta}{(\zeta - z)^{q+1}}. \tag{2.2}$$

For $q \neq n$, $\zeta = z$ becomes a branch point. Let the contour C be taken counterclockwise around z and extending on both sides of a branch cut to a lower limit $\zeta = a$. The values $a = 0$ (Riemann) and $a = -\infty$ (Liouville) are the most common. For $q<0$, (2.2) reduces to the Riemann–Liouville definition of a fractional derivative, viz.,

$$f^{(q)}(z) = \frac{1}{\Gamma(-q)}\int_a^z \frac{f(\zeta)d\zeta}{(z-\zeta)^{q+1}} \equiv {}_aD_z^q f(z). \tag{2.3}$$

The case $q = -\frac{1}{2}$ is called the semi-integral:

$${}_aD_z^{-1/2} f(z) = \frac{1}{\sqrt{\pi}}\int_a^z \frac{f(\zeta)d\zeta}{(z-\zeta)^{1/2}}. \tag{2.4}$$

For $q>0$ (and $\neq n$) the singularity at $\zeta = z$ can be removed by integration by parts. Thus the semiderivative, with $q = \frac{1}{2}$, is given by

$${}_aD_z^{1/2} f(z) = \frac{1}{\sqrt{\pi}}\frac{f(a)}{(z-a)^{1/2}} + \frac{1}{\sqrt{\pi}}\int_a^z \frac{f'(\zeta)d\zeta}{(z-\zeta)^{1/2}}. \tag{2.5}$$

We will actually require the limit value $a = +\infty$. For appropriately behaved $f(z)$:

$${}_\infty D_z^{-1/2} f(z) = \frac{i}{\sqrt{\pi}}\int_z^\infty \frac{f(\zeta)d\zeta}{(\zeta - z)^{1/2}}, \tag{2.6}$$

and

$${}_\infty D_z^{1/2} f(z) = \frac{i}{\sqrt{\pi}}\int_z^\infty \frac{f'(\zeta)d\zeta}{(\zeta - z)^{1/2}}. \tag{2.7}$$

III. INTEGRAL REPRESENTATION OF N-DIMENSIONAL GREEN'S FUNCTION

The Coulomb Green's function in N-dimensional space can be expanded as a sum of partial waves as follows[5]:

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$$G^{(N)}=\frac{\Gamma(N/2)}{2\pi^{N/2}(N-2)}\sum_{L=0}^{\infty}(2L+N-2)C_L^{N/2-1}(\cos\theta)G_L^{(N)},\qquad(3.1)$$

where $C_L^\nu(z)$ is a Gegenbauer (ultraspherical) polynomial,

$$C_L^\nu(z)=(-)^L\frac{\Gamma(L+2\nu)}{L!\Gamma(2\nu)}\,{}_2F_1(-L,L+2\nu;\nu+1/2;(1+z)/2).\qquad(3.2)$$

The partial-wave retarded Green's functions are given by[6]

$$G_L^{(N)}(r_1,r_2,k)=(ik)^{-1}(r_1r_2)^{(1-N)/2}\Gamma(L+N/2-1/2-i\nu)$$
$$\times M_{i\nu}^{L+N/2-1}(-2ikr_<)W_{i\nu}^{L+N/2-1}(-2ikr_>),\quad N=3,4,5,...,\qquad(3.3)$$

where M and W are Whittaker functions as defined by Buchholz.[7,8]

Using Buchholz's integral representation for the above product of Whittaker functions,

$$G_L^{(N)}=-2(-i)^{2L+N-2}(r_1r_2)^{1-N/2}\int_0^\infty dq\,e^{2i\nu q}e^{ik(r_1+r_2)\coth q}J_{2L+N-2}(2k\sqrt{r_1r_2}\operatorname{csch}q),\qquad(3.4)$$

the summation in (3.1) can be carried out using the Neumann series[9]:

$$\left(\frac{kz}{2}\right)^{\mu-\nu}J_z(kz)=k^\mu\sum_{n=0}^{\infty}\frac{\Gamma(\mu+n)}{n!\Gamma(\nu+1)}\,{}_2F_1(\mu+n,-n;\nu+1;k^2)(\mu+2n)J_{\mu+2n}(z),\qquad(3.5)$$

with the identifications $n=L$, $k=\cos(\theta/2)$, $z=2k\sqrt{r_1r_2}\operatorname{csch}q$, $\mu=n-2$ and $\nu=(N-1)/2$. The result is the following integral representation for $G^{(N)}$ (see Ref. 10):

$$G^{(N)}(x,y,k)=(2\pi)^{1/2-N/2}(-i)^Nk^{N/2-1/2}\eta^{3/2-N/2}$$
$$\times\int_0^\infty dq(\operatorname{csch}q)^{N/2-1/2}e^{2i\nu q}e^{ik\xi\coth q}J_{N/2-3/2}(k\eta\operatorname{csch}q),\quad N=1,2,3,...,\qquad(3.6)$$

where

$$\xi\equiv r_1+r_2=(x+y)/2,\quad \eta\equiv 2r_1r_2\cos(\theta/2)=\sqrt{xy}.\qquad(3.7)$$

The above result for $N=2$ follows by a separate derivation. The case $N=1$ corresponds to Meixner's one-dimensional Coulomb system[11]

$$G^{(1)}=i\eta\int_0^\infty dq\operatorname{csch}q\,e^{2i\nu q}e^{ik\xi\coth q}J_1(k\eta\operatorname{csch}q)=(ik)^{-1}\Gamma(1-i\nu)M_{i\nu}^{1/2}(-iky)W_{i\nu}^{1/2}(-ikx),\qquad(3.8)$$

with the closed form following from Buchholz' integral representation. For $N=2$,

$$G^{(2)}=-\frac{1}{\pi}\int_0^\infty dq\operatorname{csch}q\,e^{2i\nu q}e^{ik\xi\coth q}\cos(k\eta\operatorname{csch}q),\qquad(3.9)$$

which can be reduced to a series of Whittaker functions,

$$G^{(2)}=-\frac{1}{i\pi k\eta}\sum_{m=-\infty}^{\infty}\Gamma\left(|m|+\frac{1}{2}-i\nu\right)M_{i\nu}^{|m|}(-iky)W_{i\nu}^{|m|}(-ikx),\qquad(3.10)$$

but no further reduction to a closed form is known.

IV. RELATIONS AMONG DIFFERENT DIMENSIONALITIES

Hostler's operator [cf. Eq. (1.1)], when applied to a function of ξ and η [cf. Eq. (3.7)], reduces as follows:

$$\mathcal{O}\equiv-\frac{1}{\pi(x-y)}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)=\frac{1}{2\pi\eta}\left(\frac{\partial}{\partial\eta}\right)_\xi=\frac{1}{\pi}D_{\eta^2}.\qquad(4.1)$$

By the well-known derivative formula for Bessel functions,[12]

$$\left(\frac{1}{z}\frac{d}{dz}\right)^n z^{-\nu}J_\nu(z)=(-)^nz^{-\nu-n}J_{\nu+n}(z).\qquad(4.2)$$

Identifying z with $k\eta\operatorname{csch}q$, we have

$$D_{\eta^2}^n\eta^{-\nu}J_\nu(k\eta\operatorname{csch}q)$$
$$=(-k\operatorname{csch}q/2)^n\eta^{-\nu-n}J_{\nu+n}(k\eta\operatorname{csch}q).\qquad(4.3)$$

Applying Hostler's operator succesively to the integral representation (3.6) then gives the odd-dimensional Green's function

$$G^{(2N+1)} = \mathscr{O}^N G^{(1)} \tag{4.4}$$

and analogously, for even N,

$$G^{(2N+2)} = \mathscr{O}^N G^{(2)}. \tag{4.5}$$

The identity (4.2) can be reexpressed as follows (with $z \to \sqrt{z}$):

$$D_z^n z^{-\nu/2} J_\nu(\sqrt{z}) = (-\tfrac{1}{2})^n z^{-(\nu+n)/2} J_{\nu+n}(\sqrt{z}). \tag{4.6}$$

Taking $n = 1$ and integrating between the limits a and z, we find

$$\zeta^{-\nu/2} J_\nu(\sqrt{\zeta})\Big]_a^z = -\frac{1}{2}\int_a^z \zeta^{-(\nu+1)/2} J_{\nu+1}(\sqrt{\zeta}). \tag{4.7}$$

For $\nu \geqslant 0$, the lower boundary term in (4.7) vanishes for $a = +\infty$. Thus the analog of (4.6) for negative n (multiple integration) can be written

$${}_\infty D_z^{-n} z^{-\nu/2} J_\nu(\sqrt{z}) = (-2)^n z^{-(\nu-n)/2} J_{\nu-n}(\sqrt{z}). \tag{4.8}$$

It is now suggested that (4.6) and (4.8) might be generalized to fractional n. For the semi-integral, Eq. (4.8) with $n = \frac{1}{2}$, use (2.6) and evaluate the integral.[13] The result is

$$\begin{aligned} {}_\infty D_z^{-1/2} z^{-\nu/2} J_\nu(\sqrt{z}) &= \frac{i}{\sqrt{\pi}} \int_z^\infty \frac{\zeta^{-\nu/2} J_\nu(\sqrt{\zeta})}{(\zeta - z)^{1/2}} d\zeta \\ &= i\sqrt{2} z^{-\nu/2+1/4} J_{\nu-1/2}(\sqrt{z}). \end{aligned} \tag{4.9}$$

Likewise, Eq. (4.6) works for $n = \frac{1}{2}$. One can therefore write the square root of Hostler's operator as

$$\mathscr{O}^{1/2} = -(1/\sqrt{\pi})\, {}_\infty D_{\eta^2}^{1/2} \tag{4.10}$$

such that

$$\mathscr{O}^{1/2} G^{(N)} = G^{(N+1)}, \quad \mathscr{O}^{N/2} G^{(1)} = G^{(N+1)}, \quad N = 1,2,3,\ldots. \tag{4.11}$$

This does not, incidentally, provide a closed form for $G^{(2)}$ since the semiderivative still involves either an integral or an infinite sum.

For $Z = 0$, the above reduce to free-particle Green's functions. In particular,

$$\begin{aligned} G_{\mathrm{FP}}^{(1)} &= (ik)^{-1}[e^{ik(x-y)/2} - e^{ik(x+y)/2}], \\ G_{\mathrm{FP}}^{(2)} &= -(i/2) H_0^{(1)}(kR), \\ G_{\mathrm{FP}}^{(3)} &= -e^{ikR}/2\pi R, \end{aligned} \tag{4.12}$$

where $R \equiv r_{12} = (x-y)/2$. It can be verified that the Hostler operator and its square root also transform among the functions (4.12) in accord with (4.11).

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[5] See Ref. 1, Eq. (3).

[6] S. M. Blinder, J. Math. Phys. **25**, 905 (1984), Eq. (4.4).

[7] H. Buchholz, *The Confluent Hypergeometric Function* (Springer, New York, 1969). See especially the integral representation, p. 86, Eq. (5c).

[8] For compactness of notation, we write $M_\kappa^{\mu/2}(z)$ in place of $\mathscr{M}_{\kappa,\mu/2}(z)$ and $W_\kappa^{\mu/2}(z)$ in place of $W_{\kappa,\mu/2}(z)$. See S. M. Blinder, J. Math. Phys. **22**, 306 (1981).

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[10] An equivalent result is given in Ref. 1, Eq. (5).

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