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A new method for computing generalized surface harmonics of the second kind

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Abstract. Using the reflection properties of the spherical harmonics of the first kind for integer order and complex degree, $\mathrm{P}_n^\mu(z)$, it is shown, by taking an appropriate limit, that the surface harmonics of the second kind, $\mathrm{Q}_n^m(z)$, may be written in the form $\mathrm{Q}_n^m(z) = \frac{1}{2}\ln\left(\frac{z+1}{z-1}\right)\mathrm{P}_n^m(z) + (z^2-1)^{-m/2}\mathrm{S}_n^m(z)$, where $\mathrm{S}_n^m(z)$ is a terminating (generalized) hypergeometric function. This formula is valid for all z not on the real axis between $x = \pm 1$, this case being covered by the usual phase relationships between the factors $(z \pm 1)$ and $(1 \pm x)$. In particular, this formula permits a rapid and very accurate numerical calculation of $\mathrm{Q}_n^m(z)$, avoiding both the use of the recurrence relations and the necessity of analytic continuation for different $|z|$.

1. Introduction

First published in 1785 in his *Mémoires par divers savans*, the properties of the solutions of Legendre's differential equation

$$\left(1-z^2\right)\frac{\mathrm{d}^2w}{\mathrm{d}z^2} - 2z\frac{\mathrm{d}w}{\mathrm{d}z} + \left(\nu(\nu+1) - \frac{\mu^2}{1-z^2}\right)w = 0 \tag{1}$$

have long ago been documented (see, for example, Whittaker and Watson (1935), Abramowitz and Stegun (1965), Gradshteyn and Ryzhik (1980), Erdélyi *et al* (1953)). The solutions of this equation are the associated Legendre functions (spherical harmonics) of the first and second kind, $\mathrm{P}_\nu^\mu(z)$ and $\mathrm{Q}_\nu^\mu(z)$ respectively†. When ν and μ are both integers and z is real $\in [-1, +1]$, the solutions are known as surface harmonics because of their relation to the lines of latitude on the unit circle, z being the cosine of the angle of latitude (that is, the polar angle in spherical coordinates). We shall refer to *generalized* surface harmonics when z takes values not in this range, and is in general complex. The spherical harmonics and, in particular the surface harmonics, are ubiquitous in mathematical physics, being the angular part of the solutions of many of its equations, for example Laplace's equation and the wave equation (see, for example, Morse and Feschbach (1953), Lebedev (1972)).

The spherical harmonics are closely related to Gauss' hypergeometric series, indeed the hypergeometric differential equation may be reduced to Legendre's equation (1) in the case where the hypergeometric series admits of a quadratic transformation. For this reason the spherical harmonics are most elegantly expressed as hypergeometric functions. The

† In what follows, μ and ν denote complex numbers and m and n integers, z a complex argument and x a real one.

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transformation formulae for the hypergeometric functions may then be used to analytically continue the generalized spherical harmonics to cover the entire z plane. Due to the quadratic nature of the transformations there are 72 independent such forms (Olbricht 1887). For the surface harmonics of the first kind the solution in this form is particularly simple because the hypergeometric function terminates after $n-m$ terms, thus†

$$\begin{aligned} \mathrm{P}_n^m(z) &= \frac{1}{\Gamma(1-m)}\left[\frac{z+1}{z-1}\right]^{m/2} {}_2F_1\left(-n\,,\ n+1\,;\ 1-m\,;\ \frac{1-z}{2}\right) \\ &= \left[\frac{z+1}{z-1}\right]^{m/2} \sum_{k=m}^{n} \frac{(-n)_k(n+1)_k}{\Gamma(1-m+k)\,k!}\left(\frac{1-z}{2}\right)^k . \end{aligned} \tag{2}$$

The equivalent forms for $\mathrm{Q}_n^m(z)$ are not so simple since they involve either a limiting process or a hypergeometric series which does not terminate. Thus, for $\mathrm{Q}_\nu^\mu(z)$ given by

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}\mu\pi}\mathrm{Q}_\nu^\mu(z) &= \frac{\Gamma(1+\nu+\mu)\Gamma(-\mu)(z-1)^{\mu/2}(z+1)^{-\mu/2}}{2\Gamma(1+\nu-\mu)} \\ &\quad \times {}_2\mathrm{F}_1\left(-\nu\,,\ 1+\nu\,;\ 1+\mu\,;\ \frac{1-z}{2}\right) + \tfrac{1}{2}\Gamma(\mu)(z+1)^{\mu/2}(z-1)^{-\mu/2} \\ &\quad \times {}_2\mathrm{F}_1\left(-\nu\,,\ 1+\nu\,;\ 1-\mu\,;\ \frac{1-z}{2}\right) \qquad |1-z|<2 \end{aligned} \tag{3}$$

while it is true that for $\nu = n$ the hypergeometric series always terminate and we may lift the restriction $|1-z|<2$, clearly $\mu = m$ requires a limit to be taken.

Alternatively, in the formula

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}\mu\pi}\mathrm{Q}_\nu^\mu(z) &= \pi^{\frac{1}{2}}2^\mu\left(z^2-1\right)^{-\mu/2} \\ &\quad \times \left\{ \frac{\Gamma\left(\frac{1}{2}+\frac{\nu}{2}+\frac{\mu}{2}\right)}{2\Gamma\left(\frac{1}{2}+\frac{\nu}{2}-\frac{\mu}{2}\right)} \mathrm{e}^{\pm\frac{1}{2}\mathrm{i}\pi(\mu-\nu-1)}\, {}_2\mathrm{F}_1\left(-\frac{\nu}{2}-\frac{\mu}{2}\,,\ \frac{1}{2}+\frac{\nu}{2}-\frac{\mu}{2}\,;\ \frac{1}{2}\,;z^2\right)\right. \\ &\quad \left. + \frac{z\Gamma\left(1+\frac{\nu}{2}+\frac{\mu}{2}\right)}{\Gamma\left(\frac{1}{2}+\frac{\nu}{2}-\frac{\mu}{2}\right)} \mathrm{e}^{\pm\frac{1}{2}\mathrm{i}\pi(\mu-\nu)}\, {}_2\mathrm{F}_1\left(\frac{1}{2}-\frac{\nu}{2}-\frac{\mu}{2}\,,\ 1+\frac{\nu}{2}-\frac{\mu}{2}\,;\ \frac{3}{2}\,;z^2\right)\right\} \\ &\quad |z|<1 \end{aligned} \tag{4}$$

one of the hypergeometric functions does not terminate and (4) is then necessarily restricted to $|z|<1$. For $|z|>1$ it is then necessary to use either the formula

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}\mu\pi}\mathrm{Q}_\nu^\mu(z) &= \pi^{\frac{1}{2}}2^{-\mu-1}z^{-\nu-\mu-1}\left(z^2-1\right)^{\mu/2}\frac{\Gamma\left(1+\nu+\mu\right)}{\Gamma\left(\nu+\frac{3}{2}\right)} \\ &\quad \times {}_2\mathrm{F}_1\left(1+\frac{\nu}{2}+\frac{\mu}{2}\,,\ \frac{1}{2}+\frac{\nu}{2}+\frac{\mu}{2}\,;\ \nu+\frac{3}{2}\,;\frac{1}{z^2}\right) \qquad |z|>1 \end{aligned} \tag{5}$$

or another appropriate analytic continuation of the hypergeometric function to obtain sufficiently fast convergence of the infinite series. Thus an algorithm to calculate $\mathrm{Q}_n^m(z)$ for all possible m, n and z rapidly becomes very complicated and necessarily involves the calculation of other special functions, for example the digamma function.

† We shall use the convention that if the lower index in the summation is greater than the upper one, then the sum is zero. Thus $\mathrm{P}_n^m(z) = 0$ for $m > n$ as it should be.

It is possible, however, to write the $Q_n^m(z)$ in a form similar to (2), that is in a way which involves only terminating series which are defined for all m and n. Indeed, one only has to generate the first few to see that they may be written as

$$Q_n^m(z) = \tfrac{1}{2}\ln\left(\frac{z+1}{z-1}\right)P_n^m(z) + (z^2-1)^{-m/2}S_n^m(z) \tag{6}$$

where $S_n^m(z)$ is a terminating polynomial of degree $n+m-1$ at the most. Surprisingly none of the literature gives the analytic form of $S_n^m(z)$†. This paper supplies this lacuna. A further *raison d'etre* is that (6) provides a very fast and efficient algorithm for the numerical calculation of $Q_n^m(z)$ for either a real or a complex argument, in contrast to present algorithms which use the recurrence relations (Braithwaite 1973, Press *et al* 1992). The drawback of this type of algorithm is that upwards recurrance becomes unstable when $|z|$ is large. It then becomes necessary to use one of the hypergeometric forms to calculate $Q_n^m(z)$ for some large order followed by downwards recurrance to the value required. The difficulty here, as we have sought to highlight above, is that this will usually involve summing an infinite series, the convergence of which may be very slow. Another problem with such an algorithm is that it is inherently neither vectorizable nor parallelizable, that is, the parameters in the computer code are loop-dependent and therefore the program cannot be used to calculate a large number of $Q_n^m(z)$'s simultaneously. These difficulties are overcome by using (2) and (6), since both $P_n^m(z)$ and $S_n^m(z)$ require a fixed number of terms in the summations and each of these terms may be calculated independently of all the others‡.

2. Derivation

In order to derive the form of $S_n^m(z)$ we use the reflection formula for the Legendre polynomials of the first kind

$$P_\nu^\mu(-z) = e^{\mp i\nu\pi}P_\nu^\mu(z) - \frac{2}{\pi}e^{-i\mu\pi}\sin(\pi(\nu+\mu))\,Q_\nu^\mu(z) \tag{7}$$

so that the surface harmonics are then given by the limit

$$Q_n^m(z) = \frac{\pi}{2}(-1)^m \lim_{\mu\to m}\frac{(-1)^n P_n^\mu(z) - P_n^\mu(-z)}{\sin(\pi(n+\mu))}. \tag{8}$$

Clearly a limit does exist since

$$P_n^m(-z) = (-1)^n P_n^m(z) \tag{9}$$

so that L'Hôpital's rule gives

$$Q_n^m(z) = \frac{1}{2}\frac{\partial}{\partial\mu}\left[P_n^\mu(z) + (-1)^{n+1}P_n^\mu(-z)\right]_{\mu=m}. \tag{10}$$

Using (2) with μ replacing m, we find that

$$\frac{\partial}{\partial\mu}P_n^\mu(z)\bigg|_{\mu=m} = \tfrac{1}{2}\ln\left(\frac{z+1}{z-1}\right)P_n^m(z) + \left(\frac{z+1}{z-1}\right)^{m/2}\sum_{k=0}^{n}\frac{(-n)_k(n+1)_k}{k!}\frac{\psi(1-m+k)}{\Gamma(1-m+k)}\left(\frac{1-z}{2}\right)^k \tag{11}$$

† Hobson (1931) does give a formula for $Q_\nu^m(z)$ which is similar in form to (6); however, not all the series involved terminate and as $\nu \to n$ a limit must still be taken.

‡ Other possible numerical methods for calculating $Q_n^m(z)$ (other than explicitly solving Legendre's differential equation (1)) are restricted to certain values of n and m, for example Christoffel's formula (see below) or Neumann's integral representation (Neumann 1881, and generalizations, Wrinch 1930, Gormley 1934). However, these methods involve at least one numerical integration and a consequent loss of accuracy over efficiency.

so that $Q_n^m(z)$ is given by (6), with

$$S_n^m(z) = \sum_{k=0}^{n} \frac{(-n)_k (n+1)_k}{k!} \frac{\psi(1-m+k)}{\Gamma(1-m+k)} \frac{(-1)^k}{2^{k+1}} R_{nk}^m(z) \tag{12}$$

and

$$R_{nk}^m(z) = (z+1)^m (z-1)^k + (-1)^{n+k+1} (z-1)^m (z+1)^k. \tag{13}$$

Clearly $R_{nk}^m(z)$ is a terminating polynomial in z. It is also clear that $S_n^m(z)$ is defined for all m and n since for $k \leqslant m-1$

$$\lim_{\mu \to m} \frac{\psi(1-\mu+k)}{\Gamma(1-\mu+k)} = (-1)^{m+k} (m-k-1)! \tag{14}$$

therefore we have the required power series. We can eliminate the digamma function from (12) by distinguishing the following two cases.

Case (1): $m > n$. In this case $k \leqslant m-1$ for all k, therefore using (14)

$$S_n^m(z) = (-1)^m \sum_{k=0}^{n} \frac{(-n)_k (n+1)_k}{k!} \frac{(m-k-1)!}{2^{k+1}} R_{nk}^m(z). \tag{15}$$

We note at this point that it is possible to resum (15) to get the more conventional form of $Q_n^m(z)$ (4). Thus, writing (13) as

$$\begin{aligned} R_{nk}^m = 2(z^2-1)^k \Bigg\{ & z(m-k)(\mathrm{i})^{m+n} \cos\left(\frac{\pi}{2}(m+n)\right) \\ & \times {}_2F_1\left(\frac{-m+k+1}{2}, \frac{-m+k+2}{2}; \frac{3}{2}; z^2\right) \\ & + (\mathrm{i})^{m+n-1} \sin\left(\frac{\pi}{2}(m+n)\right) \; {}_2F_1\left(\frac{-m+k}{2}, \frac{-m+k+1}{2}; \frac{1}{2}; z^2\right) \Bigg\} \end{aligned} \tag{16}$$

then, for example, with $n+m =$ odd, we use

$${}_2F_1\,(a\,,\,b\,;\,c\,;\,z) = (1-z)^{c-a-b}\,{}_2F_1\,(c-a\,,\,c-b\,;\,c\,;\,z) \tag{17}$$

and reverse the order of the summations, so that from (15) we find

$$S_n^m(z) = (-1)^m (1-z^2)^m \sum_{s=0}^{\infty} \frac{\Gamma(m+2s)}{\left(\frac{1}{2}\right)_s \, s!} \left(\frac{z}{2}\right)^{2s} \; {}_2F_1\left(-n, n+1; 1-m-2s; \tfrac{1}{2}\right). \tag{18}$$

The simplification comes because we can use (2) to sum the hypergeometric function in (18), that is

$${}_2F_1\left(-n, n+1; 1-m-2s; \tfrac{1}{2}\right) = 2^{m+2s} \pi^{-\frac{1}{2}} \frac{\Gamma\left(\frac{m+n+1}{2}+s\right)\Gamma\left(\frac{m-n}{2}+s\right)}{\Gamma\,(m+2s)}. \tag{19}$$

We can repeat this for $m+n =$ even and, substituting into (15), equation (4) follows.

Case (2): $m \leqslant n$. In this case $S_n^m(z)$ has two parts depending on whether or not $k \leqslant m-1$ or $k > m-1$. Thus

$$S_n^m(z) = (-1)^m \sum_{k=0}^{m-1} \frac{(-n)_k (n+1)_k}{k!} \frac{(m-k-1)!}{2^{k+1}} R_{nk}^m(z)$$

$$+ \sum_{k=m}^{n} \frac{(-n)_k (n+1)_k}{k!} \frac{\psi(1-m+k)}{\Gamma(1-m+k)} \frac{(-1)^k}{2^{k+1}} R_{nk}^m(z). \tag{20}$$

Given

$$\psi(n+1) = -\gamma + \sum_{s=1}^{n} \frac{1}{s} \tag{21}$$

where γ is Euler's constant, we then find that

$$S_n^m(z) = (-1)^m \sum_{k=0}^{m-1} \frac{(-n)_k (n+1)_k}{k!} \frac{(m-k-1)!}{2^{k+1}} R_{nk}^m(z)$$

$$+ \sum_{k=m+1}^{n} \frac{(-n)_k (n+1)_k}{(k-m)!\, k!} \frac{(-1)^k}{2^{k+1}} R_{nk}^m(z) \sum_{s=1}^{k-m} \frac{1}{s}. \tag{22}$$

In this case it is not possible to sum analytically the series in (22) since they are related to generalized forms of the hypergeometric function. Thus the first term in is related to a ${}_3F_2$, since

$$\sum_{k=0}^{r} \frac{(-n)_k (n+1)_k (r-k)!}{k!} z^k$$

$$= \frac{(-n)_r (n+1)_r}{r!} z^r \, {}_3F_2\left(-r\,,\ 1\,,\ 1\,;\ -n-r\,,\ 1+n-r\,;\ -\frac{1}{z}\right)$$

with $r < n$, and the second to a limit of the derivative of this with respect to the second argument.

We can now combine the two cases, and the result is

$$Q_n^m(z) = \tfrac{1}{2} \ln\left(\frac{z+1}{z-1}\right) P_n^m(z) + (-1)^m (z^2-1)^{-m/2}$$

$$\times \sum_{k=0}^{[n,m-1]} \frac{(-n)_k (n+1)_k}{k!} \frac{(m-k-1)!}{2^{k+1}} R_{nk}^m(z)$$

$$+ (z^2-1)^{-m/2} \sum_{k=m+1}^{n} \frac{(-n)_k (n+1)_k}{(k-m)!\, k!} \frac{(-1)^k}{2^{k+1}} R_{nk}^m(z) \sum_{s=1}^{k-m} \frac{1}{s} \tag{23}$$

where by $[n, m-1]$ we mean the smaller of n and $m-1$, and we make use of the convention referred to in the second footnote.

Finally, we note that (23) is not valid for z real $\in [-1, +1]$, and the appropriate formulae may be found by applying the usual prescription, namely replace $(z-1)$ by $(1-x)\mathrm{e}^{\pm i\pi}$, (z^2-1) by $(1-x^2)\mathrm{e}^{\pm i\pi}$ and $(z+1)$ by $(1+x)$, for $z = x + \mathrm{i}0$, thus

$$Q_n^m(x) = \tfrac{1}{2} \ln\left(\frac{1+x}{1-x}\right) P_n^m(x) + (-1)^m (1-x^2)^{-m/2} \times$$

$$\times \sum_{k=0}^{[n,m-1]} \frac{(-n)_k(n+1)_k}{k!} \frac{(m-k-1)!}{2^{k+1}} R_{nk}^m(x)$$

$$+(1-x^2)^{-m/2} \sum_{k=m+1}^{n} \frac{(-n)_k(n+1)_k}{(k-m)!\,k!} \frac{(-1)^k}{2^{k+1}} R_{nk}^m(x) \sum_{s=1}^{k-m} \frac{1}{s}. \tag{24}$$

Hence for a given m and n, the sums in (23) and (24) are quickly and easily computed and thereby the surface harmonics of the second kind. Moreover these sums immediately lend themselves to computation in highly vectorized loops.

As a corollary to (23) and (24) it is clear that, for example, on the cut

$$\mathrm{Q}_n(x) = \tfrac{1}{2}\ln\left(\frac{1+x}{1-x}\right)\mathrm{P}_n(x) + \sum_{k=1}^{n} \frac{(-n)_k(n+1)_k}{(1)_k\,k!\,2^{k+1}} \left[(1-x)^k + (-1)^{n+1}(1+x)^k\right] \sum_{s=1}^{k} \frac{1}{s}. \tag{25}$$

For afficianados of generalized hypergeometric functions we show in the appendix how, using Saalshutz's theorem (Slater 1966), equation (25) may be used to prove Christoffel's formula, namely

$$\mathrm{Q}_n(x) = \tfrac{1}{2}\ln\left(\frac{1+x}{1-x}\right)\mathrm{P}_n(x) - \sum_{q=1}^{[n/2]} \frac{2n-4q+3}{(2q-1)(n-q+1)} \mathrm{P}_{n-2q+1}(x) \tag{26}$$

where $[n/2] = n/2, n$ even, $= (n+1)/2, n$ odd.

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Appendix

In this appendix we give a proof of Christoffel's formula using equation (25), that is, we are required to prove that

$$\sum_{k=1}^{n} \frac{(-n)_k(n+1)_k}{(1)_k\,k!\,2^{k+1}} \left[(1-x)^k + (-1)^{n+1}(1+x)^k\right] \sum_{s=1}^{k} \frac{1}{s}$$
$$= -\sum_{q=1}^{[n/2]} \frac{2n-4q+3}{(2q-1)(n-q+1)} \mathrm{P}_{n-2q+1}(x). \tag{A1}$$

Suppose n is odd, then let

$$\sum_{k=1}^{n} \frac{(-n)_k\,(n+1)_k}{(1)_k\,k!\,2^{k+1}} \left[(1-x)^k + (1+x)^k\right] \sum_{s=1}^{k} \frac{1}{s} = \sum_{q=0}^{(n-1)/2} A_{n,2q} \mathrm{P}_{2q}(x) \tag{A2}$$

where $A_{n,2q}$ is some coefficient (dependent only on n and q) to be determined. Writing

$$\tfrac{1}{2}\left[(1-x)^k + (1+x)^k\right] = {}_2\mathrm{F}_1\left(-\frac{k}{2}, -\frac{k}{2}+\frac{1}{2}; \frac{1}{2}; x\right) \tag{A3}$$

multiply both sides of (A2) by $P_{2q'}(x)$ and integrate over $x \in [-1, +1]$. Using the othogonality relationship

$$\int_{-1}^{+1} P_{2q}(x)P_{2q'}(x)\,dx = \frac{2}{4q+1}\delta_{qq'} \tag{A4}$$

and the result

$$\int_{-1}^{+1} x^{2r}P_{2q}(x)\,dx = \frac{\pi^{\frac{1}{2}}\Gamma(1+2r)}{4^r\,\Gamma(1+r-q)\Gamma(r+q+3/2)} \tag{A5}$$

we obtain, using Gauss' theorem,

$$A_{n,2q} = \frac{(L+4q)!}{L!\,4q!}\sum_{p=1}^{L}\frac{(-L)_p(L+4q+1)_p}{(4q+2)_p\,p!}\sum_{s=2q+1}^{p+2q}\frac{1}{s} \tag{A6}$$

where $L = n - 2q \geqslant 1$, and we have used the fact that

$${}_2F_1(\,-L\,,\;L+4q+1\,;\;4q+2\,;\;1\,) = 0 \qquad \forall\, L. \tag{A7}$$

The double sum on the right-hand-side of (A6) may be evaluated using Saalshutz's theorem (Slater 1966), that is

$${}_3F_2(a\,,\;b\,,\;-n\,;\;c\,,\;1+a+b-c-n\,;\;1) = \frac{(c-a)_n(c-b)_n}{(c)_n(c-a-b)_n}. \tag{A8}$$

Thus, taking $n = L$, $a = L+4q+1$, $b = 2q+1+x$ and $c = 4q+2+x$ we have

$$\sum_{p=0}^{L}\frac{(-L)_p(L+4q+1)_p(2q+1+x)_p}{(4q+2+x)_p(2q+1)_p\,p!} = \frac{(1+x-L)_L(2q+1)_L}{(4q+2+x)_L(-L-2q)_L}. \tag{A9}$$

If we now take the derivative of (A9) with respect to x and evaluate the result at $x = 0$ we find

$$\sum_{p=1}^{L}\frac{(-L)_p(L+4q+1)_p}{(4q+2)_p\,p!}\sum_{s=2q+1}^{p+2q}\frac{1}{s} - \sum_{p=1}^{L}\frac{(-L)_p(L+4q+1)_p}{(4q+2)_p\,p!}\sum_{s=4q+2}^{p+4q+1}\frac{1}{s}$$
$$= -\frac{(L-1)!(4q+1)!}{(L+4q+1)!} \tag{A10}$$

where we have used the reflection formula for the digamma function. The second term on the left-hand-side of (A10) may be summed by replacing $4q+2$ by $4q+2+x$ in the third argument of the hypergeometric function in (A7), differentiating with respect to x and letting $x = 0$. Then the final result is

$$\sum_{p=1}^{L}\frac{(-L)_p(L+4q+1)_p}{(4q+2)_p\,p!}\sum_{s=2q+1}^{p+2q}\frac{1}{s} = -2\frac{(L-1)!(4q+1)!}{(L+4q+1)!} \tag{A11}$$

so that from (A6) we have

$$A_{n,2q} = -2\frac{4q+1}{(n-2q)(n+2q+1)} \qquad n \text{ odd}. \tag{A12}$$

The appropriate result for n even is

$$A_{n,2q+1} = -2\frac{4q+3}{(n-2q-1)(n+2q+2)} \qquad n \text{ even}. \tag{A13}$$

If we now substitute equations (A12) and (A13) into (A2), and sum in the opposite direction, equation (A1) follows. QED.

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