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Convergence acceleration of Fourier series by analytical and numerical application of Poisson's formula

Simon L Marshall†

Department of Chemistry, University of Natal, Private Bag X01, Scottsville, Pietermaritzburg 3209, South Africa

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Abstract. A form of the Poisson summation formula appropriate for the transformation of infinite Fourier series is derived and shown to be applicable to slowly converging series arising in the solution of Laplace's equation in a rectangular electrochemical cell. The result is a rapidly convergent Fourier series which is particularly useful in giving the potential close to the electrode surface. Results obtained from the analytical expression are found to be in close agreement with those resulting from numerical evaluation of the Fourier integrals (using Simpson's rule and the Euler transformation) and direct summation by using Goertzel's (1958) algorithm.

1. Introduction

The need for efficient and accurate convergence acceleration methods for Fourier series remains undiminished, despite recent extraordinary advances in computer power. Recently, Oleksy (1996) gave some striking examples of slowly converging Fourier series in which direct addition of the terms yields a result with only one or two significant figures. In this paper we consider the analytical and numerical application of the Poisson summation formula (PSF) to the evaluation of infinite Fourier series, we demonstrate this by application to solutions of Laplace's equation.

Two main problems must be addressed by numerical methods designed for the evaluation of Fourier series. These are: (1) the evaluation of N-term finite sums of the series, and (2) acceleration of the convergence of the sequence of partial sums as $N \to \infty$. The evaluation of finite Fourier sums arises in the approximation not only of the corresponding infinite series, but also of the Fourier expansion coefficients of a given function. Both of these tasks have been achieved by application of Clenshaw-type recursion schemes (Clenshaw 1955, Goertzel 1958; for analyses of error propagation in such algorithms see Elliott 1968, Gentleman 1969, Oliver 1977, Press *et al* 1992, pp 172–7), the discrete PSF (Lyness 1970), and fast Fourier transformation (Cooley and Tukey 1965, Dilts 1985).

Most of the published work on the convergence-acceleration of sequences of partial Fourier sums has been directed towards the construction of rapidly convergent trigonometric approximations for a given function. The pioneering work on this problem was that of Lanczos (1966, pp 119–58), who showed that a function could be approximated by a truncated series of Bernoulli polynomials with the remainder represented as a rapidly convergent Fourier series. The Lanczos method was subsequently extended and generalized

† Present address: Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6110, USA.

by Jones and Hardy (1970), Lyness (1974), Shaw *et al* (1976), Tasche (1979) and most recently by Baszenski *et al* (1995).

Since the Lanczos method and its elaborations require knowledge of the analytical properties of the function of interest, they are not useful for summing Fourier series of unknown functions. The first numerical methods developed for this purpose were based on Cesàro summation (Fejér 1904, see also Lanczos 1966, pp 55–61), and construction of moving averages (Lanczos 1966, pp 61–75). More recently, sequence transformations designed for slowly converging power series (Wynn 1956, Levin 1973) have been used to accelerate the convergence of exponential Fourier series (Smith and Ford 1982, Brezinski and Redivo Zaglia 1991, pp 282–4, Homeier 1993). The most recent developments of series transformations for Fourier series are due to Oleksy (1996), who described a preliminary transformation that considerably enhances the performance of the Levin and Homeier algorithms.

In favourable cases it is also possible to apply classical methods such as Kummer's transformation (Knopp 1956, pp 171–2), as in a recent article by Dillmann and Grabitz (1995) on the summation of a Fourier–Bessel series arising in supersonic potential-flow theory. This relies on the availability of a simpler series that converges at approximately the same rate, but which can be summed much more easily, preferably in closed form. Since such series are often hard to come by, this method is not widely applicable.

Completely analytical transformation methods for slowly converging series, such as those based on the application of residue theory and the use of the PSF, are generally very efficient, but suffer from the disadvantage of involving fairly intricate analytical manipulations. The residue method, which is usually discussed in books on complex analysis (e.g. Spiegel 1974, Mitrinović and Kečkić 1985), is most useful for Fourier sums of functions that have finitely many poles in the complex plane. On the other hand, the PSF is applicable to any convergent series of functions for which the Fourier transform exists, and converts a slowly converging series to a series of Fourier transforms that can either be summed in closed form or converges extremely rapidly. Some of the most spectacular applications of the PSF are to the evaluation of extremely slowly convergent sums of Coulomb potentials arising in solid-state physics (Wimp 1981, pp 237–42, Haug 1972, pp 249–56) and in theoretical models of ionic and molecular adsorption (Marshall 1986, Marshall and Conway 1992a, b). In this connection, the PSF invites comparison with methods based on other representations of the reciprocal distance in terms of Gaussian integrals (Ewald 1921) or gamma functions (van der Hoff and Benson 1953), both of which have been applied to problems of interfacial structure by Barlow and Macdonald (1964, 1965) and Macdonald and Barlow (1966).

Since the alternation of signs in an ionic lattice can be expressed in terms of a complex exponential, the evaluation of crystal lattice sums can be regarded as the summation of a particular class of Fourier series. The outstanding performance of the PSF in the evaluation of lattice sums in turn suggests that the PSF might be useful in the summation of Fourier series of more general form arising in other physical contexts. Examples of such applications include the calculation of Green functions arising in waveguide theory (Grzesik 1984), and in the description of electromagnetic scattering from periodic structures (Jorgenson and Mittra 1990). These papers are also somewhat germane to our interest in calculating current and potential distributions in electrochemical cells by solution of Laplace's equation. In previous work (Marshall 1991, 1992, Marshall and Wolff 1993, 1998) we evaluated the resulting Fourier series by application of the Lanczos (1966) method of local smoothing. The present study was undertaken primarily with the intention of developing a more efficient way of evaluating Fourier series solutions of Laplace's equation. We show not only that the PSF is extremely effective when applied analytically, but also that it is equally effective when the required Fourier transforms are evaluated numerically.

2. Poisson's formula for infinite series

The most familiar form of the PSF is

$$\sum_{n=-\infty}^{\infty} g(n) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} g(u) \mathrm{e}^{2m\pi \mathrm{i}u}\, \mathrm{d}u. \tag{1}$$

If the summand of the left-hand series is replaced by $f(n)\exp(\mathrm{i}cn)$, where c is a real number and f is an even function of n, the integrals in the imaginary parts vanish, resulting in

$$\sum_{n=-\infty}^{\infty} f(n)\mathrm{e}^{\mathrm{i}cn} = \int_{-\infty}^{\infty} f(u)\cos cu\, \mathrm{d}u + \sum_{m=1}^{\infty}\left[\int_{-\infty}^{\infty} f(u)\cos(2m\pi + c)u\, \mathrm{d}u + \int_{-\infty}^{\infty} f(u)\cos(2m\pi - c)u\, \mathrm{d}u\right]. \tag{2}$$

To illustrate the application of this result to solutions of Laplace's equation, we consider a rectangular electrochemical cell in which one face is maintained at zero potential, the current density is specified on the opposite face and the remaining boundary surfaces are insulators. This configuration might be encountered in certain types of plating operations. In the limiting case where kinetic and mass-transfer resistances are negligible, the current distribution is associated with a potential function that satisfies Laplace's equation

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0 \qquad 0 \leqslant x \leqslant H \qquad 0 \leqslant y \leqslant L \tag{3}$$

together with the boundary conditions

$$\frac{\partial V}{\partial y}(x, 0) = f(x) \tag{4}$$

$$V(x, L) = 0 \tag{5}$$

and

$$\frac{\partial V}{\partial x}(0, y) = \frac{\partial V}{\partial x}(H, y) = 0. \tag{6}$$

As shown in appendix A, the potential within the electrolyte is given by

$$V(x, y) = \int_0^H f(\xi) S(x, y|\xi)\, \mathrm{d}\xi \tag{7}$$

where S is the potential due to a unit current source on the boundary plane $y = 0$:

$$S(x, y|\xi) = \frac{1}{H}(y - L) - \frac{2}{H}\sum_{n=1}^{\infty} \frac{\sinh \frac{n\pi}{H}(L - y)}{\frac{n\pi}{H}\cosh \frac{n\pi L}{H}} \cos\frac{n\pi x}{H} \cos\frac{n\pi\xi}{H}. \tag{8}$$

(We refer to S as the source function to distinguish it from the Green and Neumann functions that are appropriate for Dirichlet or Neumann boundary conditions.) This Fourier series converges quite rapidly for values of y close to L, but for small values of y, for which it is of most interest to be able to calculate the potential, convergence becomes very slow. To calculate the potential in the vicinity of the smaller electrode, it is therefore desirable to develop a rapidly convergent form of equation (8). To apply the PSF to this series, we first observe that the summand is an even function of n, and that

$$\lim_{n\to 0}\left\{\frac{\sinh\frac{n\pi}{H}(L-y)}{\frac{n\pi}{H}\cosh\frac{n\pi L}{H}}\cos\frac{n\pi x}{H}\cos\frac{n\pi\xi}{H}\right\} = L-y \tag{9}$$

from which it follows that $n = 0$ corresponds to a removable singularity. We can therefore write

$$S(x, y|\xi) = -\frac{1}{H}\sum_{n=-\infty}^{\infty}\frac{\sinh\frac{n\pi}{H}(L-y)}{\frac{n\pi}{H}\cosh\frac{n\pi L}{H}}\cos\frac{n\pi x}{H}\cos\frac{n\pi\xi}{H} \tag{10}$$

where the summation operator is defined as

$$\sum_{n=-\infty}^{\infty} \equiv \lim_{n\to 0} + 2\sum_{n=1}^{\infty}. \tag{11}$$

From equation (2) it is seen that transformation of equation (10) requires evaluation of the integral

$$\int_{-\infty}^{\infty}\frac{\sinh au}{u\cosh bu}\mathrm{e}^{(2m\pi\pm c)\mathrm{i}u}\,\mathrm{d}u = \int_{-\infty}^{\infty}\frac{\sinh au}{u\cosh bu}\cos(2m\pi \pm c)u\,\mathrm{d}u \tag{12}$$

where

$$a \equiv \frac{\pi}{H}(L-y) \qquad b \equiv \frac{\pi L}{H} \qquad c \equiv \frac{\pi}{H}(x \pm \xi). \tag{13}$$

As shown in appendix B, the integrals in equation (12) can be evaluated by application of the residue theorem. The transformed series corresponding to equation (10) is

$$\begin{aligned} S(x, y|\xi) &= -\frac{2}{\pi}\sum_{k=0}^{\infty}\frac{(-1)^k\sin(k+\frac{1}{2})\pi(1-\frac{y}{L})}{k+\frac{1}{2}}\cdot\frac{\cosh(k+\frac{1}{2})\frac{\pi}{L}(H-x)\cdot\cosh(k+\frac{1}{2})\frac{\pi\xi}{L}}{\sinh(k+\frac{1}{2})\frac{\pi H}{L}} \\ &\quad (x > \xi) \\ &= -\frac{2}{\pi}\sum_{k=0}^{\infty}\frac{(-1)^k\sin(k+\frac{1}{2})\pi(1-\frac{y}{L})}{k+\frac{1}{2}}\cdot\frac{\cosh(k+\frac{1}{2})\frac{\pi}{L}(H-\xi)\cdot\cosh(k+\frac{1}{2})\frac{\pi x}{L}}{\sinh(k+\frac{1}{2})\frac{\pi H}{L}} \\ &\quad (x < \xi). \end{aligned} \tag{14}$$

2.1. Numerical application of the Poisson formula

The potential distribution considered here is simple enough that an explicit expression for the Fourier coefficients can be obtained. In certain problems, such as those involving calculation of the potential distribution in cells with porous (Marshall 1991) or resistive electrodes (Marshall 1992, Marshall and Wolff 1993, 1998), the Fourier coefficients are solutions of simultaneous linear equations, and explicit expressions for them are difficult to obtain. In this section we see how the PSF can be applied in such situations with direct numerical evaluation of the Fourier cosine transform integrals that appear on the right-hand side of equation (2).

The most widely used method for the numerical evaluation of Fourier transforms is the Cooley–Tukey (1965) fast Fourier transform algorithm. While in principle this can be applied here as well, it is evident from the calculations presented so far that values of the integral are usually required for only a few values of the transform (frequency) variable. It may therefore prove more efficient to use an alternative approach to the evaluation of improper integrals of oscillatory functions, recommended by Davis and Rabinowitz (1975, pp 118–30, 178–80). For the evaluation of a cosine transform, this involves the subdivision of the integration interval into the subintervals $(0, \pi/2]$, $[\pi/2, 3\pi/2]$, $[3\pi/2, 5\pi/2]$, ... The integral can be identified as a series of terms of alternating sign, decreasing in magnitude:

$$\begin{aligned}\int_0^\infty f(t)\cos xt\,\mathrm{d}t &= \frac{1}{x}\int_0^\infty f\left(\frac{u}{x}\right)\cos u\,\mathrm{d}u\\ &= \frac{1}{x}\left[\int_0^{\pi/2} f\left(\frac{u}{x}\right)\cos u\,\mathrm{d}u + \sum_{n=1}^{\infty}\int_{(n-\frac{1}{2})\pi}^{(n+\frac{1}{2})\pi} f\left(\frac{u}{x}\right)\cos u\,\mathrm{d}u\right]\\ &\equiv U_0 - U_1 + U_2 - \cdots. \end{aligned} \tag{15}$$

The convergence of this series of subintegrals can be accelerated by the application of the Euler transformation (Scheid 1968, pp 71, 160–1), which involves rearranging terms in clusters that tend to zero much more rapidly:

$$\begin{aligned}U_0 - U_1 + U_2 - U_3 + \cdots = \tfrac{1}{2}[U_0 - \tfrac{1}{2}(U_1 - U_0) + \tfrac{1}{4}(U_2 - 2U_1 + U_0)\\ -\tfrac{1}{8}(U_3 - 3U_2 + 3U_1 - U_0) + \cdots].\end{aligned} \tag{16}$$

In practice, best results are achieved if the first few terms (up to about 10) in the series are added directly, and the Euler transformation is applied to the remainder. The coefficients on the right-hand side of equation (16) can be generated recursively by constructing a triangular forward difference table from successive terms in the original series. Each segment in the integral can obviously be evaluated by any numerical quadrature technique, but Simpson's rule and other formulae using equally spaced points have the advantage that they may be combined with the recursion satisfied by $\cos nh$ so that each integral only requires evaluation of one sine and one cosine. The number of panels into which each subinterval must be divided depends on how rapidly the function varies with its argument: for functions of the type considered in this paper, about 30 panels give sufficient accuracy. Failure of the Euler transformation to converge is a sign that the number of panels might not be sufficient. The evaluation of the Fourier transforms by this type of method involves the combination of a quadrature method used to integrate between successive nodes, and a convergence acceleration algorithm used to sum up these contributions to the total integral. Although we chose Simpson's rule and the Euler transformation for the sake of simplicity, many other combinations are possible. A detailed comparison of the efficiency of these combinations is, however, beyond the scope of this paper.

3. Numerical results

In this section we consider the evaluation of the series

$$S(a, b, c) = a + 2\sum_{n=1}^{\infty}\frac{\sinh an}{n\cosh bn}\cos cn \tag{17}$$

by: (1) numerical (section 3.1) application; (2) analytical (section 3.2) application of the PSF, and (3) numerical summation of the original series by Goertzel's method (section 3.3). The results serve not only to illustrate the power of the transformation but also as a check on the operation of the three methods. We select the values $a = 1$, $b = 1.01$ and $c = 0.3$, for which the series converges very slowly. Physically, this would correspond to a point quite close to the plane $y = 0$, on which the current density is specified.

3.1. Numerical application of the PSF

$m = 0$

argument $= 0.300\,0000$ integral $= 2.945\,656$

$$\left[\int_{-\infty}^{\infty} \frac{\sinh au}{u \cosh au} \cos cu \, \mathrm{d}u\right].$$

Terms in the series as transformed by the PSF.

$m = 1$

argument $= 6.583\,185$ integral $= 7.153\,1220E - 05$

argument $= 5.983\,185$ integral $= 1.817\,5979E - 04$

$$\left[\int_{-\infty}^{\infty} \frac{\sinh au}{u \cosh bu} \cos(2\pi \pm c)u \, \mathrm{d}u\right]$$

term $= 5.065\,8203E - 04$.

$m = 2$

argument $= 12.866\,37$ integral $= 7.572\,8167E - 08$

argument $= 12.266\,37$ integral $= -2.433\,0802E - 08$

$$\left[\int_{-\infty}^{\infty} \frac{\sinh au}{u \sinh bu} \cos(4\pi \pm c)u \, \mathrm{d}u\right]$$

term $= 1.027\,9473E - 07$.

$m = 3$

argument $= 19.149\,56$ integral $= -1.688\,0222E - 09$

argument $= 18.549\,56$ integral $= 3.009\,3361E - 08$

$$\left[\int_{-\infty}^{\infty} \frac{\sinh au}{u \cosh bu} \cos(6\pi \pm c)u \, \mathrm{d}u\right]$$

term $= 5.681\,0677E - 08$

cosine series $= 2.946\,162$.

We see that the first term in the transformed series (corresponding to $m = 0$) accounts for nearly the entire value of the series, and that the higher terms are negligible beyond $m = 2$. This is typical of the behaviour of Poisson's formula for a slowly converging series.

3.2. Analytical application of the Poisson summation formula

The analytical transformation can be evaluated in two forms, as given by equations (B.5) or (B.6). We use equation (B.5), since this allows us to compare each term in the series of transforms with the corresponding values obtained by numerical integration.

Argument $= 0.300\,0000$

$m = 0$ term $= 2.945\,655$

$$\left[2\sum_{k=0}^{\infty} \frac{(-1)^k \sin(k+\frac{1}{2})\frac{\pi a}{b}}{k+\frac{1}{2}} \mathrm{e}^{-(k+\frac{1}{2})\frac{\pi c}{b}}\right]$$

argument $= 6.583\,185$

argument $= 5.983\,185$

$m = 1$ term $= 5.067\,6987E - 04$

$$\left[2\sum_{k=0}^{\infty}\frac{(-1)^k\sin(k+\frac{1}{2})\frac{\pi a}{b}}{k+\frac{1}{2}}\mathrm{e}^{-(k+\frac{1}{2})\frac{\pi}{b}(2\pi\pm c)}\right]$$

argument $= 12.866\,37$

argument $= 12.266\,37$

$m = 2$ term $= 2.890\,2445E - 08$

$$\left[2\sum_{k=0}^{\infty}\frac{(-1)^k\sin(k+\frac{1}{2})\frac{\pi a}{b}}{k+\frac{1}{2}}\mathrm{e}^{-(k+\frac{1}{2})\frac{\pi}{b}(4\pi\pm c)}\right]$$

sum $= 2.946\,162$.

The analytically and numerically determined Fourier transforms are seen to be in satisfactory agreement (to within single-precision machine error), considering the fact that the summation tolerance was taken to be 0.000 0001 for both the Poisson summation subroutine and the subroutine that implements the Euler transformation.

3.3. Numerical evaluation of original series

For a Fourier series in which the coefficients a_n decrease monotonically with increasing n, the summation limit required to make the leading term less than some predetermined number ε can be determined by iterative solution of the equation

$$\log|a_n| = \log\varepsilon \tag{18}$$

for n. For the Fourier series considered here and $\varepsilon = 0.000\,0001$, we find the value of n to be 929. This results in the estimates 0.973 0814 for the semi-infinite cosine series, and 2.946 163 for the infinite cosine series. The estimate of the series obtained by direct addition of the terms (i.e. without the use of Goertzel's algorithm) is 2.946 164, and the same result is produced if the sine and cosine factors are generated recursively according to equations (19):

$$\begin{aligned}\sin(n+1)h &= \sin(nh)\cos(h) + \cos(nh)\sin(h)\\ \cos(n+1)h &= \cos(nh)\cos(h) - \sin(nh)\sin(h).\end{aligned} \tag{19}$$

A comparison of these estimates with those obtained by using the other methods suggests that for this particular series, accumulation of round-off errors is only a minor problem.

It is to be observed that the transformed series does not always converge more rapidly than the original series; this depends on the relative values of the parameters a and b. If a was considerably smaller than b, as would be the case for a point far removed from the electrode, the original series would converge quite adequately and the transformation would not be necessary. It is therefore advisable to select which form of the series to use by comparing the number of terms required to produce a leading term of magnitude less than the given summation tolerance. For the transformed series, the ratio of hyperbolic functions can be written

$$\frac{\cosh(k+\frac{1}{2})\frac{\pi}{b}(\pi-c)}{\sinh(k+\frac{1}{2})\frac{\pi^2}{b}} = \mathrm{e}^{-(k+\frac{1}{2})\frac{\pi c}{b}}\cdot\frac{1+\mathrm{e}^{-(2k+1)\frac{\pi(\pi-c)}{b}}}{1-\mathrm{e}^{-(2k+1)\frac{\pi^2}{b}}} \to \mathrm{e}^{-(k+\frac{1}{2})\frac{\pi c}{b}} \tag{20}$$

for sufficiently large k. An estimate of the value of k for which this ratio is less than ε is

$$k > k_{\max} = -\frac{1}{2} - \frac{b}{\pi c}\ln\varepsilon. \tag{21}$$

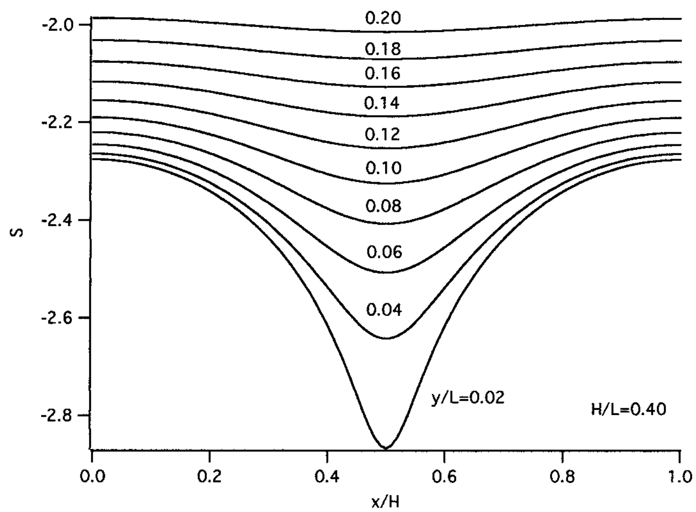

Figure 1. Potential due to a unit source at $\xi = 1$ in a rectangular cell with $L = 5$ and $H = 2$.

If $\varepsilon = 0.000\,0001$, $\ln \varepsilon \simeq -16$, so that the required number of terms in the transformed series is

$$k_{\max} \approx \frac{16b}{\pi c}. \tag{22}$$

An estimate for the summation limit of the original series can be derived by observing that for sufficiently large n, the general term can be approximated thus:

$$\frac{\sinh an}{n \cosh bn} \approx \frac{e^{a-b}}{n} \tag{23}$$

and the required value of $n_{\max}$ can be obtained easily by the iterative solution of the equation

$$a - b - \ln n_{\max} = \ln \varepsilon. \tag{24}$$

Experience shows that this iteration proceeds very rapidly, with at most four iterations being required to achieve an error of less than 1.

3.4. Behaviour of the source function

We next consider the potential variation in a rectangular cell with $L = 5$, $H = 2$, due to a unit source at $x = 1$. This is shown in figure 1 as a function of x, for different values of y. The potential becomes progressively more uniform as the grounded boundary plane $y = L$ is approached. The graphs are quite smooth, and betray no trace of the oscillatory behaviour of the terms in the original Fourier series and its transformation.

We finally consider the potential in an electrochemical cell consisting of one grounded electrode and another parallel electrode consisting of a conducting strip of width x_1 and (vertical) length w, across which the current density is assumed to be uniform. The arrangement of the electrodes is shown in figure 2. With this boundary condition, the integral of the source function is easily determined, and the dimensionless potential is found to be

$$\Phi \equiv \frac{H\kappa V}{I} = -J \cdot \frac{x_1}{H} \cdot \frac{y-L}{H} + \frac{2J}{\pi^2} \sum_{n=1}^{\infty} \frac{\sinh \frac{n\pi}{H}(L-y)}{n^2 \cosh \frac{n\pi L}{H}} \sin \frac{n\pi x_1}{H} \cos \frac{n\pi x}{H} \tag{25}$$

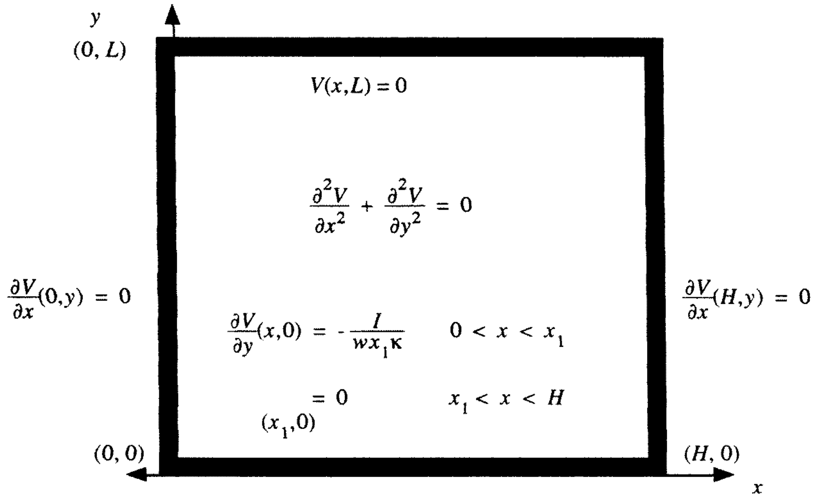

Figure 2. Rectangular electrochemical cell.

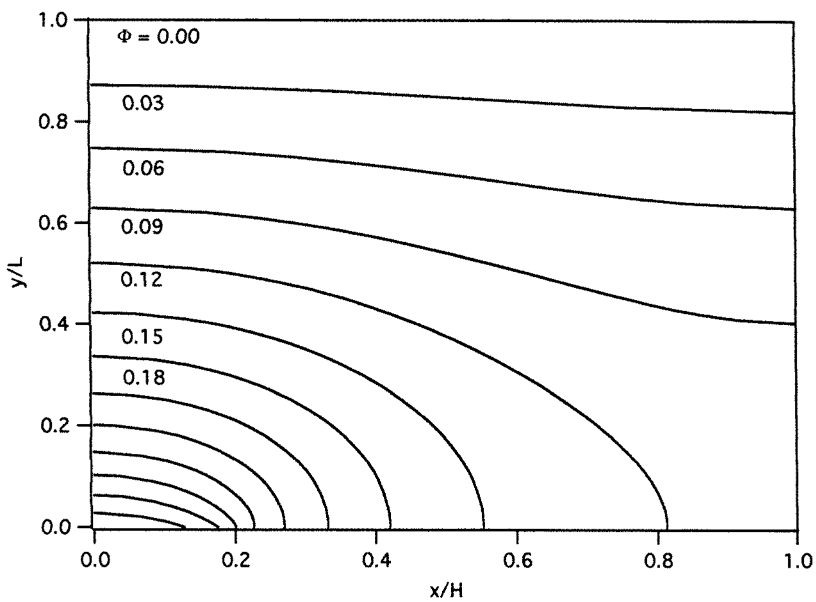

Figure 3. Equipotential contours for the cell of figure 2, with $x_1/H = 0.2$ and $J = 1$.

where J is defined by

$$J \equiv \frac{H^2}{w x_1}.$$

The equipotential contours for this cell are shown in figure 3, for $x_1/H = 0.2$ and $J = 1$.

Although in the above work we considered a boundary value problem for Laplace's equation in which the normal derivative of the function was specified on one part of the boundary and the value of the function on the other, it is to be observed that a precisely similar analysis could be applied to other situations, such as those in which either the normal derivative or the function is specified over the entire boundary. (Not all of these possibilities are equally useful in the description of electrochemical cells, however.) Further, the general approach can be expected to be applicable to conductors of any geometry for which Laplace's equation can be solved by separating variables, since in such cases the potential can always be expanded in terms of orthogonal functions. For example, in cylindrical cells with current density specified on the lateral surface, the potential is represented as a series of trigonometric and modified Bessel functions. This may be transformed by the methods described here into a more rapidly convergent series of exponentials and ordinary Bessel functions.

In some cases it is also possible to derive the source function in rectangular coordinates by application of the method of images, and to sum the resulting infinite series of logarithmic potentials in closed form by using the Weierstrass factorization theorem. The use of the PSF as described here has the advantage of greater generality, as it can be readily applied in the construction of rapidly convergent Green functions for problems that cannot be described physically in terms of images.

A further advantage becomes evident in the consideration of problems involving nonlinear boundary conditions, such as can be expected to result from appreciable kinetic resistance at the electrode surface. Such problems in general reduce to the solution of a nonlinear integral equation for the potential along the electrode, and require iteration. The representation of the source potential as a rapidly convergent series is clearly of benefit in these situations. The fact that the general term in the transformed series is a product of a function of x and a function of the source point ξ is of greater significance, since this results in an integral equation with a degenerate kernel. As we will show in a future paper, this integral equation can be solved analytically in the case of linear polarization, and can be reduced to a single nonlinear algebraic equation when nonlinear kinetics is assumed. In contrast, the equivalent logarithmic representation of the source function cannot be integrated analytically with respect to ξ, so that an iterative numerical solution is required even for linear boundary conditions.

4. Conclusions

In this paper we have demonstrated how the convergence of Fourier series solutions of Laplace's equation can be greatly accelerated by the application of the PSF, thereby providing an accurate and computationally efficient method for the evaluation of such analytical results. The general strategy involved constructing a rapidly converging expression for the source function or singularity solution, from which the potential due to an arbitrary boundary current distribution can be obtained by integration.

While the particular example considered here was simple enough that analytical expressions could be obtained for the required Fourier transforms, we also showed that the PSF could be applied equally well if these Fourier transforms were evaluated numerically by Simpson's rule in combination with the Euler transformation. The usefulness of the PSF as a method for accelerating the convergence of Fourier series does not, therefore, require extensive analytical manipulations.

Appendix A. Potential due to a unit current source

The potential distribution due to a unit current source can be derived by solving the boundary value problem defined by equations (3)–(6), with the boundary current distribution defined by

$$\begin{aligned} f(x) &= 0 \qquad 0 \leqslant x < \xi - \frac{\delta}{2} \\ &= Q \qquad \xi - \frac{\delta}{2} \leqslant x \leqslant \xi + \frac{\delta}{2} \\ &= 0 \qquad \xi + \frac{\delta}{2} < x \leqslant H. \end{aligned} \tag{A.1}$$

Separation of variables results in a solution of the form

$$V(x, y) = a_0(y - L) - \sum_{n=1}^{\infty} a_n \frac{\sinh \frac{n\pi}{H}(L - y)}{\frac{n\pi}{H} \cosh \frac{n\pi L}{H}} \cos \frac{n\pi x}{H}. \tag{A.2}$$

The coefficients can be determined by applying the boundary condition expressed by equation (4). From the theory of Fourier series and the definition of f given by equation (A.1),

$$a_0 = \frac{1}{H} \int_0^H f(x)\,\mathrm{d}x = \frac{Q\delta}{H} \tag{A.3}$$

$$a_n = \frac{2}{H} \int_0^H f(x) \cos \frac{n\pi x}{H}\,\mathrm{d}x = \frac{4Q}{n\pi} \cos \frac{n\pi\xi}{H} \sin \frac{n\pi\delta}{2H} \qquad (n = 1, 2, \ldots 0). \tag{A.4}$$

The coefficients corresponding to the unit source function are obtained by setting $\delta = 1/Q$ and considering the limit of equations (A.3) and (A.4) as $Q \to \infty$:

$$\lim_{Q\to\infty} a_n = \lim_{Q\to\infty} \left\{ \frac{4Q}{n\pi} \cos \frac{n\pi\xi}{H} \sin \frac{n\pi}{2HQ} \right\} = \frac{2}{H} \cos \frac{n\pi\xi}{H}. \tag{A.5}$$

Substitution into equation (A.2) then results in

$$S(x, y|\xi) = \frac{1}{H}(y - L) - \frac{2}{H} \sum_{n=1}^{\infty} \frac{\sinh \frac{n\pi\xi}{H}(L - y)}{\frac{n\pi}{H} \cosh \frac{n\pi L}{H}} \cdot \cos \frac{n\pi x}{H} \cos \frac{n\pi\xi}{H}.$$

Appendix B. Transformation of the source function

Assuming that $c > 0$, the integrals in the transformed series can be evaluated by integration of the function defined by

$$F(z) \equiv \frac{\sinh az}{z \cosh bz} \mathrm{e}^{(2m\pi \pm c)\mathrm{i}z} \tag{B.1}$$

around the contour shown in figure B1, where the radius of the semicircular arc is chosen so as not to coincide with any of the poles of the integrand on the positive imaginary axis. Application of Cauchy's theorem results in

$$\begin{aligned} \oint_C F(z)\,\mathrm{d}z &= \int_0^{\pi} F(R \cdot \mathrm{e}^{\mathrm{i}\theta})\mathrm{i}R \cdot \mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta + \int_{-\infty}^{\infty} F(u)\,\mathrm{d}u \\ &= 2\pi\mathrm{i} \sum \operatorname{res} F(z) \end{aligned} \tag{B.2}$$

where the sum is over all poles of the integrand (i.e. $(k + \frac{1}{2})\pi\mathrm{i}/b$) that lie within the contour. The residue is

$$\lim_{z\to(k+\frac{1}{2})\frac{\pi\mathrm{i}}{b}} \left\{ \frac{z - (k + \frac{1}{2})\frac{\pi\mathrm{i}}{b}}{\cosh bz} \right\} \cdot \frac{\sinh az}{z} \cdot \mathrm{e}^{(2m\pi\pm c)\mathrm{i}z} = \frac{(-1)^k \sin(k + \frac{1}{2})\frac{\pi a}{b}}{(k + \frac{1}{2})\pi\mathrm{i}} \mathrm{e}^{-(k+\frac{1}{2})\frac{\pi}{b}(2m\pi\pm c)} \tag{B.3}$$

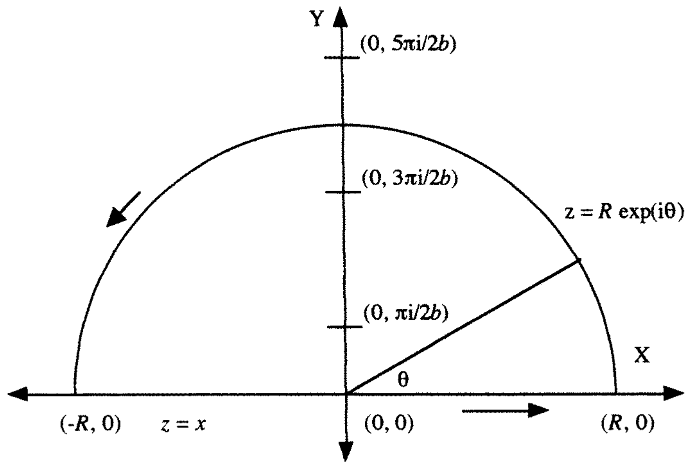

Figure B1. Integration contour C referred to in equation (B.2).

where we have used L'Hospital's rule. As the radius of the semicircular contour increases, the absolute value of the integrand diminishes exponentially, so that by Jordan's first lemma (see, for example, Mitrinović and Kečkić 1985, pp 35–8), the integral around this part of the contour vanishes. Therefore, in the limit as $R \to \infty$, equation (B.2) gives

$$\int_{-\infty}^{\infty} \frac{\sinh au}{u\cosh bu} \mathrm{e}^{(2m\pi \pm c)\mathrm{i}u}\, \mathrm{d}u = 2\sum_{k=0}^{\infty} \frac{(-1)^k \sin(k+\frac{1}{2})\frac{\pi a}{b}}{k+\frac{1}{2}} \mathrm{e}^{-(k+\frac{1}{2})\frac{\pi}{b}(2m\pi \pm c)}. \tag{B.4}$$

The transformed sum is therefore

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{\sinh au}{u\cosh bu} \cos cu\, \mathrm{d}u &+ \sum_{m=1}^{\infty}\left[\int_{-\infty}^{\infty} \frac{\sinh au}{u\cosh bu}\cos(2m\pi + c)u\, \mathrm{d}u\right. \\ &\left. + \int_{-\infty}^{\infty} \frac{\sinh au}{u\cosh bu}\cos(2m\pi - c)u\, \mathrm{d}u\right] \\ &= 2\sum_{k=0}^{\infty} \frac{(-1)^k \sin(k+\frac{1}{2})\frac{\pi a}{b}}{k+\frac{1}{2}}\left[\mathrm{e}^{-(k+\frac{1}{2})\frac{\pi a}{b}} + \sum_{m=1}^{\infty}\right. \\ &\left.\times\left\{\mathrm{e}^{-(k+\frac{1}{2})\frac{\pi}{b}(2m\pi+c)} + \mathrm{e}^{-(k+\frac{1}{2})\frac{\pi}{b}(2m\pi-c)}\right\}\right]\end{aligned} \tag{B.5}$$

where the order of summation has been reversed. This can be further simplified by expressing the geometric series of exponentials in braces in terms of reciprocal hyperbolic functions:

$$a + 2\sum_{n=1}^{\infty} \frac{\sinh an}{n\cosh bn}\cos cn = 2\sum_{k=0}^{\infty} \frac{(-1)^k \sin(k+\frac{1}{2})\frac{\pi a}{b}}{k+\frac{1}{2}} \cdot \frac{\cosh(k+\frac{1}{2})\frac{\pi}{b}(\pi - c)}{\sinh(k+\frac{1}{2})\frac{\pi^2}{b}}. \tag{B.6}$$

Since the argument of the hyperbolic sine in the denominator is always larger than the argument of the hyperbolic sine in the numerator, the summands behave approximately like exponentials for sufficiently large k, from which it is clear that the transformed series converges very rapidly. The transformed solution to the original boundary value problem follows from the appropriate identifications of a, b and c in terms of the cell geometrical parameters, so that

$$\frac{\pi a}{b} = \frac{\pi}{L}(L-y) \qquad \frac{\pi^2}{b} = \frac{\pi H}{L} \qquad \frac{\pi}{b}(\pi - c) = \frac{\pi}{L}(H - x \mp \xi). \tag{B.7}$$

Since it was assumed that $c > 0$, we can expect two different forms of the transformed series, corresponding to the cases $x > \xi$ and $x < \xi$. After application of the identity

$$\cosh\left(k = \frac{1}{2}\right)\frac{\pi}{L}(H - x + \xi) + \cosh\left(k + \frac{1}{2}\right)\frac{\pi}{L}(H - x - \xi)$$
$$= 2\cosh\left(k + \frac{1}{2}\right)\frac{\pi}{L}(H-x)\cdot\cosh\left(k + \frac{1}{2}\right)\frac{\pi\xi}{L} \tag{B.8}$$

the transformed source function is found to be

$$S(x, y|\xi) = \frac{1}{H}(y - L) - \frac{2}{H}\sum_{n=1}^{\infty}\frac{\sinh\frac{n\pi}{H}(L-y)}{\frac{n\pi}{H}\cosh\frac{n\pi L}{H}}\cos\frac{n\pi x}{H}\cos\frac{n\pi\xi}{H}$$
$$= -\frac{2}{\pi}\sum_{k=0}^{\infty}\frac{(-1)^k\sin(k+\frac{1}{2})\pi(1-\frac{y}{L})}{k+\frac{1}{2}}$$
$$\cdot\frac{\cosh(k+\frac{1}{2})\frac{\pi}{L}(H-x)\cdot\cosh(k+\frac{1}{2})\frac{\pi\xi}{L}}{\sinh(k+\frac{1}{2})\frac{\pi H}{L}} \qquad (x > \xi)$$
$$= -\frac{2}{\pi}\sum_{k=0}^{\infty}\frac{(-1)^k\sin(k+\frac{1}{2})\pi(1-\frac{y}{L})}{k+\frac{1}{2}}$$
$$\cdot\frac{\cosh(k+\frac{1}{2})\frac{\pi}{L}(H-\xi)\cdot\cosh(k+\frac{1}{2})\frac{\pi x}{L}}{\sinh(k+\frac{1}{2})\frac{\pi H}{L}} \qquad (x < \xi). \tag{B.9}$$

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