The Coulomb potential of a line of charges

J.F. HARPER

Mathematics Department, Victoria University, Wellington, New Zealand
e-mail: `John.Harper@vuw.ac.nz`

Recently Lekner gave formulae for the total Coulomb force and potential on a charged particle due to a line of other charged particles, and showed how to use it for a regular array of charges in two or three dimensions. His method involves a series in terms of the Bessel function K_0 which converges fast for points sufficiently far from the line. This paper gives an integral which can be evaluated faster for points close to the line.

1. Introduction

In the context of speeding up computer simulations of a set of ions in a central cell which is repeated to infinity in two or three spatial dimensions, Lekner [1] found the electrostatic potential of an infinite set of equal point charges at regular intervals L along a line, in terms of the function $I(\alpha, \beta)$ defined as

$$I(\alpha, \beta) = \sum_{n=0}^{\infty} \cos(\alpha n) K_0(\beta n). \tag{1}$$

where K_0 denotes the usual Bessel function [2, equation 8.407], α and β measure distance along and perpendicular to the line with $L/2\pi$ being used as the unit of length, and $\alpha = 0$ at one of the charges. His formula holds because [2, equation 8.526.1]

$$\begin{aligned} \frac{2}{\pi} I(\alpha, \beta) &= \frac{1}{\pi}\left(\mathbf{C} + \ln\left(\frac{\beta}{4\pi}\right)\right) + \frac{1}{(\alpha^2 + \beta^2)^{1/2}} + \\ &+ \sum_{l=1}^{\infty}\left(\frac{1}{[(\alpha - 2l\pi)^2 + \beta^2]^{1/2}} - \frac{1}{2l\pi}\right) \\ &+ \sum_{l=1}^{\infty}\left(\frac{1}{[(\alpha + 2l\pi)^2 + \beta^2]^{1/2}} - \frac{1}{l\pi}\right), \end{aligned} \tag{2}$$

where $\mathbf{C}$ is Euler's constant $0.5772\ldots$

The series (2) always converges slowly. Lekner [1] pointed out that the series (1) converges rapidly if β is large but slowly if β is small. It is the purpose of this paper to give an integral representation of the function $I(\alpha, \beta)$ which can be evaluated rapidly if β is small.

2. The integral

Lekner [1] showed that equation (1) is equivalent to

$$I(\alpha, \beta) = \int_0^{\infty} \frac{\exp(\beta \cosh t)\cos\alpha - 1}{\exp(2\beta \cosh t) - 2\exp(\beta\cosh t)\cos\alpha + 1}\, dt. \tag{3}$$

The limits of integration may be changed from $(0, \infty)$ to $(-\infty, 0)$ because the integrand is an even function of t, and then the transformation $x = \mathrm{e}^t$ converts the integral into

$$I(\alpha, \beta) = \int_0^1 \frac{E(\cos\alpha - E)}{1 - 2E\cos\alpha + E^2}\frac{dx}{x}, \tag{4}$$

where

$$E = \exp\left[-\frac{\beta}{2}(x + \frac{1}{x})\right]. \qquad (5)$$

3. Results

Numerical experiments were performed with Lekner's sum (1), the finite integral (4), and the equivalent integral with the same integrand but limits $(1, \infty)$, using the NAG [3] routines S18ACF to find K_0, D01ARF for the finite integration (with lower limit 0.01 if $\beta \geq 2$, 0.005β if $\beta < 2$ to avoid the essential singularity at 0 where $E = 0$), and D01AMF for the integration over a semi-infinite domain.

No case was found in which the semi-infinite domain of integration was better than the finite one. With a maximum relative error of 10^{-6} the integral (4) was found to converge faster than Lekner's series (1) to the same answer if β is less than 0.5 to 0.6, i.e. if the potential was calculated at a point nearer to the line of charges than about 0.1 unit cell sizes.

References

[1] J. Lekner, Physica A 176 (1991) 485.

[2] I.S. Gradshteyn and I.M. Ryzhik, Table of Integrals, Series and Products (Academic Press, New York, 1980)

[3] NAG Fortran Library Manual, Mark 14 (Numerical Algorithms Group, Oxford, 1990).