Some Square Lattice Green Function Formulas

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Abstract

We derive formulas for the matrix elements of the two dimensional square lattice Green function along the diagonal, and along the coordinate axes. We also give an asymptotic formula for the diagonal elements.
I. INTRODUCTION

In some recent papers [1, 2] Cserti showed how a lattice Green function (LGF) can be used to find the resistance between two points in an infinite lattice of resistors. Cserti gives an expression for the matrix elements of the LGF in the form of an integral. In this paper we will show how to solve this integral for the case of a two dimensional square lattice along the diagonal and the coordinate axes. This allows any arbitrary diagonal or coordinate axis LGF matrix element to be calculated directly. Formulas for these elements were first derived by McCrea and Whipple [3][4] using a different procedure than that presented here. We will also give an asymptotic formula for the diagonal matrix elements that converges to Cserti’s asymptotic limit formula for large values of \( n \).

The LGF with which we are concerned here can in general be used to solve the discrete two dimensional Poisson equation with boundary conditions at infinity. Therefore it will be useful in solving two dimensional electrostatics problems [5] as well as many other problems that can be modeled by a Poisson equation.

II. DIAGONAL MATRIX ELEMENTS

The matrix elements of the two dimensional square lattice Green function can be expressed in terms of an integral as

\[
g(n, m) = \frac{1}{2\pi^2} \int_0^\pi d\phi \int_0^{2\pi} d\theta \, \cos n\theta \cos m\phi \cos \theta \cos \phi
\]

This is essentially the same as Cserti’s [1] eq. B1. We will begin by looking at the diagonal elements where \( m = n \). First note that for \( m = n \) eq. 1 can be rewritten in the following form

\[
g(n, n) = \frac{1}{4\pi^2} \int_0^\pi d\phi \int_0^{2\pi} d\theta \, \cos^2 n\theta \cos \phi \cos \theta
\]

By symmetry the two cosine terms in the numerator of the integrand can be combined to give

\[
g(n, n) = \frac{1}{2\pi^2} \int_0^\pi d\phi \int_0^{2\pi} d\theta \, \frac{1}{2} \cos n(\phi + \theta) \cos \phi \cos \theta
\]

In terms of new variables \( \phi^0 = \frac{1}{2}(\phi - \theta), \theta^0 = \frac{1}{2}(\phi + \theta) \) eq. 3 becomes

\[
g(n, n) = \frac{1}{4\pi^2} \int_0^\pi d\phi \int_0^{2\pi} d\theta \, \frac{1}{4\pi} \frac{1}{\cos \phi \cos \theta} \cos 2n\theta
\]
The integration over $\phi$ can now be done to give

$$g(n; n) = \frac{1}{4\pi} \int_0^\pi d\theta \frac{\cos 2n\theta}{\sin \theta}$$  \hspace{1cm} (5)$$

Using the identity $\cos 2\theta = 2\sin^2 \theta$, eq. (5) can be written as

$$g(n; n) = \frac{1}{2\pi} \int_0^\pi d\theta \frac{\sin^2 n\theta}{\sin \theta} = \frac{1}{2\pi} \int_0^\pi d\theta \frac{\sin n\theta}{\sin \theta}^2 \sin \theta$$  \hspace{1cm} (6)$$

Now if we let $x = \cos \theta$ then this becomes the integral of a type II Chebyshev polynomial [6]

$$g(n; n) = \frac{1}{2\pi} \int_1^1 U_{2n-1}^2(x) \, dx = \frac{1}{\pi} \int_0^\pi U_{2n-1}^2(\cos \theta) \, d\theta$$  \hspace{1cm} (7)$$

The square of a type II Chebyshev polynomial can be expressed as

$$U_n^2(x) = \sum_{k=0}^n U_{2k}(x)$$  \hspace{1cm} (8)$$

To prove this identity it is sufficient to show that $U_n^2(x) = U_{2n-1}^2(x) = U_{2n}(x)$. With $x = \cos \theta$ we have $U_n(x) = \sin(n+1)\theta = \sin \theta$ and

$$U_n(x) U_{n-1}(x) = \frac{\sin(n+1)\theta}{\sin \theta} \frac{\sin n\theta}{\cos 1/2 \theta} = \frac{\cos(n+1/2)\theta}{\cos 1/2 \theta}$$

$$U_n(x) + U_{n-1}(x) = \frac{\sin(n+1)\theta + \sin n\theta}{\sin \theta} = \frac{\sin(n+1/2)\theta}{\sin 1/2 \theta}$$

$$U_n^2(x) U_{n-1}^2(x) = \frac{\cos(n+1/2)\theta \sin(n+1/2)\theta}{\cos 1/2 \theta \sin 1/2 \theta} = \frac{\sin(2n+1)\theta}{\sin \theta} = U_{2n}(x)$$

So using eq. (8) eq. (7) can be written as

$$g(n; n) = \frac{1}{\pi} \sum_{k=0}^n U_{2k}(x) \, dx$$  \hspace{1cm} (9)$$

Letting $x = \cos \theta$, the integrals in eq. (9) become

$$\int_0^\pi U_{2k}(x) \, dx = \frac{1}{2k+1} \int_0^{2k+1} \sin(2k+1)\theta \, d\theta = \frac{1}{2k+1}$$  \hspace{1cm} (10)$$

Substituting this into eq. (9) and changing the summation index gives

$$g(n; n) = \frac{1}{\pi} \sum_{k=1}^n \frac{1}{2k-1}$$  \hspace{1cm} (11)$$
Note that \( g(n; n) \) also obeys a difference equation and that the solution for \( g(n; n) \) given in eq. (11) could also be arrived at by solving the difference equation. The difference equation for \( g(n; n) \) is the same as that given by Cserti [1] eq. 32 for the resistances along the diagonal

\[
\frac{Q(n + 1)}{Q(n)} g(n + 1; n + 1) = 4n g(n; n) + \frac{Q(n)}{Q(n + 1)} g(n + 1; n) - g(n - 1; n - 1) = 0
\]  
(12)

Since the coefficients of this equation add up to zero, if we substitute \( g(n; n) = \sum_{k=1}^{n} f(k) \), \( g(n - 1; n - 1) = g(n; n) f(n) \), \( g(n + 1; n + 1) = g(n; n) + f(n + 1) \) into the equation, we will get a first order equation for \( f(n) \).

\[
\frac{Q(n + 1)}{Q(n)} f(n + 1) = f(n) - \frac{Q(n)}{Q(n + 1)} f(n) = 0
\]  
(13)

With the initial condition \( f(1) = \frac{1}{\pi} \) the solution to this equation is \( f(k) = \frac{1}{\pi} \frac{1}{2k+1} \) which once again gives us eq. (11) as the solution for \( g(n; n) \).

We will now derive an asymptotic formula for \( g(n; n) \). First note that the \( g(n; n) \) elements are proportional to the partial sums of a generalized harmonic series. They can also be expressed in terms of the standard harmonic series as follows

\[
g(n; n) = \frac{1}{\pi} \sum_{k=1}^{n} \frac{1}{k} \sum_{k=1}^{n} \frac{1}{k} = \frac{1}{\pi} \frac{H_{2n}}{2n}
\]  
(14)

where we have introduced the notation

\[
H_n = \sum_{k=1}^{n} \frac{1}{k}
\]  
(15)

for the \( n \)th partial sum of the standard harmonic series. The asymptotic formula for the \( n \)th partial sum of the harmonic series is [7] p. 338

\[
H_n = \ln n + \gamma + \frac{1}{2n} \sum_{k=1}^{n} \frac{B_{2k}}{2k n^{2k}}
\]  
(16)

where \( \gamma = 0.5772156649 \ldots \) is the Euler-Mascheroni constant and \( B_{2k} \) is a Bernoulli number. Using this in eq. (14) results in the following asymptotic formula for \( g(n; n) \)

\[
g(n; n) = \frac{1}{2\pi} \ln(n) + \gamma + 2 \ln(Q) + \sum_{k=1}^{\infty} \frac{B_{2k} Q^{2k} 1}{k (Q n)^{2k}}
\]  
(17)

Without the Bernoulli sum, this is essentially the same as Cserti’s [1] eq. 33 for the asymptotic limit of the resistance.
III. THE ON-Axis ELEMENTS

We now turn to the on-axis elements where \( m = 0 \) and eq. 1 becomes

\[
g(n; 0) = \frac{1}{2\pi^2} \int_0^{\pi} d\phi \int_0^{\pi} d\theta \frac{1}{2} \frac{\cos n\theta}{\cos \theta \cos \phi}  
\]

(18)

The integral with respect to \( \phi \) can be carried out to give

\[
g(n; 0) = \frac{1}{2\pi} \int_0^{\pi} \frac{1}{d\theta} \frac{\cos n\theta}{(\cos \theta)^2}  
\]

(19)

Now note that \( \cos n\theta = 2\sin^2\left(\frac{n\theta}{2}\right) \) and \( \cos \theta = 1 + 2\sin^2\left(\frac{\theta}{2}\right) \) so that the denominator of the integrand in eq. 19 becomes \( (1 + 2\sin^2\left(\frac{\theta}{2}\right))^2 = 1 + 2\sin^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right) \). Eq. 19 then becomes

\[
g(n; 0) = \frac{1}{2\pi} \int_0^{\pi} \frac{\sin n\theta}{\sin \theta} \sin^2\left(\frac{d\theta}{2}\right) \left(1 + \sin^2\left(\frac{d\theta}{2}\right)\right)  
\]

(20)

Making the change in variable \( \theta^0 = \frac{\theta}{2} \), we write eq. 20 as

\[
g(n; 0) = \frac{1}{\pi} \int_0^{\pi} \frac{\sin n\theta}{\sin \theta} \frac{\sin^2\left(\frac{\theta}{2}\right)}{1 + \sin^2\left(\frac{\theta}{2}\right)} d\theta  
\]

(21)

With \( x = \cos \theta \) we then have an integral involving the Chebyshev polynomial \( U_{n-1}(x) \)

\[
g(n; 0) = \frac{1}{\pi} \int_0^{\pi} \frac{U_{n-1}^2(x)}{2} dx  
\]

(22)

Now if we let \( x = \frac{p}{1 - \cos \theta} \) then

\[
g(n; 0) = \frac{1}{2\pi} \int_0^{\pi} U_{n-1}^2 \left(\frac{p}{1 - \cos \theta}\right) d\theta  
\]

(23)

\[
g(n; 0) = \frac{1}{2\pi} \sum_{k=0}^{n} \int_0^{\pi} U_{2k} \left(\frac{p}{1 - \cos \theta}\right) d\theta  
\]

(24)

If the type I and type II Chebyshev polynomials are expressed in the following forms [6]

\[
T_n(x) = \frac{1}{2} x + \frac{p}{x^2} \left(\frac{n}{1} + \frac{x}{\sqrt{1 - x^2}}\right)  
\]

(25)

\[
U_n(x) = \frac{x + \frac{p}{x^2} \left(\frac{n+1}{1} + \frac{x}{\sqrt{1 - x^2}}\right)}{2}  
\]

then it is straightforward to prove the identity

\[
U_{2k} \left(\frac{p}{1 - x}\right) = \left(\frac{1}{2}\right)^k \frac{p}{x} T_{2k+1} \left(\frac{p}{x}\right)  
\]

(26)
Using this identity eq. 24 becomes

\[ g(n; 0) = \frac{1}{2\pi} \sum_{k=0}^{n-1} (1)^k \int_0^{\pi/2} T_{2k+1}(x) \exp(-j\theta) \cos^k \theta \, d\theta \]

(27)

\( T_{2k+1}(x) \) can be expressed in series form as

\[ T_{2k+1}(x) = \sum_{j=0}^{k} (1)^k \binom{2k+1}{2j+1} x^{2j+1} \]

(28)

so that we have

\[ (1)^k \frac{T_{2k+1}(x)}{x} = \sum_{j=0}^{k} (4)^j \binom{2k+1}{2j+1} x^j \]

(29)

and eq. 27 can be written as

\[ g(n; 0) = \frac{1}{2\pi} \sum_{k=0}^{n-1} \sum_{j=0}^{k} a(k;j) b(j) \]

(30)

where

\[ a(k;j) = (4)^j \binom{2k+1}{2j+1} \frac{k+j}{2j} \]

(31)

\[ b(j) = \frac{\pi}{2} \cos^j \theta d\theta = \begin{cases} \frac{\pi}{2} & j = 0; 2; 4; 6; \cdots \\ \frac{(j-1)!}{j!!} & j = 1; 3; 5; 7; \cdots \end{cases} \]

Eq. 30 can be used to directly calculate \( g(n; 0) \) for arbitrary values of \( n \).

IV. CONCLUSION

We have derived equations by which \( g(n;n) \) and \( g(n;0) \) can be calculated for arbitrary values of \( n \). For the case of \( g(n;n) \) we have an asymptotic formula eq. 17 that allows for a quick and efficient calculation. In the case of \( g(n;0) \) we have eq. 30 whose evaluation can be optimized for large values of \( n \). A complete asymptotic formula for \( g(n;0) \) has not yet been found. A formula very similar to eq. 17 for \( g(n;n) \) has been found for \( g(n;0) \) but only the first few terms in the Bernoulli sum have so far been determined. Formulas for the general matrix elements \( g(n;m) \) have been found by us. These formulas are found by solving the partial difference equation for \( g(n;m) \). This equation can only be solved after a formula for the diagonal elements, \( g(n;n) \) has been found.
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[1] J. Cserti, Amer. J. Phys. 68, 896 (2000), cond-mat/9909120.

[2] J. Cserti, G. David, and A. Piroth, Amer. J. Phys. 70, 153 (2002), cond-mat/0107362.

[3] This was brought to our attention by L. Raymond and S. Schaefer after the first version of this paper appeared. We thank them for making us aware of this fact.

[4] W. H. McCrea and F. J. W. Whipple, Proc. Roy. Soc. Edinburgh 60, 281 (1940).

[5] http://www.exstrom.com/lgf/lgfpe/lgfpe.html.

[6] J. Mason and D. Handscomb, *Chebyshev Polynomials* (Chapman and Hall/CRC, 2003).

[7] G. Arfken, *Mathematical Methods for Physicists* (Academic Press, 1985), 3rd ed.