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Lattice Green function (at 0) for the 4D hypercubic lattice

M L Glasser† and A J Guttmann‡

† Department of Physics, Clarkson University, Parkville, Victoria 3052, Australia
‡ Department of Mathematics, the University of Melbourne, Potsdam, NY 13699-5820, USA

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Abstract. The generating function for recurrent Polya walks on the four-dimensional hypercubic lattice is expressed as a Kampé–de Fériet function. Various properties of the associated walks are enumerated.

1. Introduction

Lattice statistics play an important role in many areas of chemistry and statistical physics. Random lattice walks have been investigated extensively, both numerically and analytically, and explicit analytic expressions for recurrent lattice walks (those that end where they began) are available for several lattices in one, two and three dimensions [1, 2]. The interest in this problem follows from the numerous connections between random walks and other problems in mathematical physics. They form the basis of certain proofs in the problem of self-avoiding walks [3], they are a key component in the study of lattice dynamics [4], and they have an extensive following in the mathematical literature [1, 3]. Furthermore, d-dimensional lattice Green functions have recently [5] been shown to underlie the theory of d-dimensional staircase polygons and to be related to the generating function for d-dimensional multinomial coefficients.

The aim of this note is to extend this list to four dimensions by summarizing a study of the lattice Green function

$$P(z) = P_4(z) = \frac{1}{\pi^4}\iiiint_0^{\pi} \frac{\mathrm{d}^4k}{1-\frac{z}{4}\sum_{j=1}^{4}\cos(k_j)} \qquad |z| \leqslant 1 \tag{1}$$

which generates the statistics for recurrent Polya walks (uniform step probabilities) on the 4D hypercubic lattice.

From (1) it is clear that $P(z)$ is an analytic function of z^2 within the unit circle and has a branch point at $z^2 = 1$. It is representable as a single integral in a variety of ways. From the relations in [6], for example, we have

$$P(z) = \int_0^{\infty} \mathrm{e}^{-x} I_0^4(\tfrac{1}{4}xz)\mathrm{d}x \tag{2}$$

and

$$P(z) = \frac{8}{\pi^3}\int_0^1 \frac{K(k_+)K(k_-)}{\sqrt{1-x^2}}\mathrm{d}x \tag{3}$$

where

$$k_{\pm}^2 = \tfrac{1}{2}[1 \pm x^2z^2\sqrt{1-\tfrac{1}{4}x^2z^2} - (1-\frac{1}{2}x^2z^2)\sqrt{1-x^2z^2}] \tag{4}$$

and K denotes the complete elliptic integral of the first kind.

In terms of the variables $u = z^2$ and $p(u) = P(z)$, $P(z)$ satisfies the Fuchsian differential equation

$$\begin{aligned}4u^3(u-4)(u-1)p^{(iv)}(u) + 8u^2(5u^2-20u+12)p'''(u) + u(99u^2-293u+112)p''(u) \\ + (57u^2-106u+16)p'(u) + (3u-2)p(u) = 0.\end{aligned} \tag{5}$$

Asymptotic analysis of (2) and series analysis show that near $z^2 = 1$

$$\begin{aligned}&P(z) \cong C_0 + C_1(1-z^2)\ln(1-z^2) \\ &C_0 = 1.23946712\ldots \\ &C_1 = 2/\pi^2.\end{aligned} \tag{6}$$

Upon expanding (1) in powers of z^2, one has

$$P(z) = \sum_{n=0}^{\infty} a_n z^{2n} \tag{7}$$

where

$$a_n = \frac{1}{\pi^4}\iiiint_0^{\pi}\left[\frac{1}{4}\sum_{j=1}^{4}\cos(k_j)\right]^{2n} \mathrm{d}^4k. \tag{8}$$

On the other hand, by expanding the Bessel function in (2), integrating term by term, and proceeding as in the appendix in [6], we find

$$a_n = \left[\frac{(1/2)_n}{n!}\right]^3 {}_4F_3\left[\begin{matrix}-n/2 & (1-n)/2 & -n & 1/2; \\ 1/2-n & 1/2-n & 1; & \end{matrix}\; 1\right]. \tag{9}$$

Next, by using the identity [6]

$$\begin{aligned}&{}_4F_3(-n, (1-n)/2, -n/2; 1/2-n, 1/2-n, 1; 1) \\ &\quad = \frac{(1/2)_n}{n!}\, {}_4F_3(-n, 1/2, 1/2, 1/2; 1/2-n, 1/2-n, 1/2-n; 1)\end{aligned} \tag{10}$$

expressing the latter ${}_4F_3$ in terms of its series, and noting that

$$(-n)_k = (-1)^k n!/(n-k)! \qquad (1/2-n)_k = (-1)^k (1/2)_n/(1/2)_{n-k} \tag{11}$$

we arrive at the double hypergeometric series

$$P(z) = \sum_{m,n=0}^{\infty} \frac{(1/2)_{m+n}(1/2)_n^3(1/2)_m^3}{(1)_{m+n}^3}\,\frac{z^{2m}z^{2n}}{n!m!} \tag{12}$$

Table 1. Number of $2n$-step recurrent walks.

n	r_n
1	8
2	168
3	5120
4	190120
5	7939008
6	357713664
7	16993726464
8	839358285480
9	42714450658880
10	2225741588095168

which defines a Kampé–de Fériet function [7]:

$$P(z) = F^{1:3:3}_{3:0:0}\left[1,1,1;\quad -;\quad -; z^2, z^2\right] = F^{2:1:1}_{0:2:2}\left[\begin{matrix}1/2,1; & 1/2; & 1/2 \\ -; & 1,1; & 1,1;\end{matrix} z^2/4, z^2/4\right]. \quad (13)$$

The quantity a_n in (8) is the probability that the random walker ends at its starting point in 2n steps (not necessarily for the first time). The number of such walks is therefore $r_n = 8^{2n}a_n$, which obeys the recursion relation

$$n^4 r_n - 4(20n^4 - 40n^3 + 33n^2 - 13n + 2)r_{n-1} + 256(4n^4 - 16n^3 + 23n^2 - 14n + 3)r_{n-2} = 0. \quad (14)$$

The first ten values are given in the table.

For large n, for the d-dimensional hypercubic lattice [8]

$$r_n^{(d)} \sim 2(2d)^{2n}(d/4\pi n)^{d/2}$$

so in the present case $a_n \sim 2/\pi^2 n^2$ and $r_n \sim 64^n(2/n^2\pi^2)$. (For example, this yields $a_{500} \sim 8.10569 \times 10^{-7}$, compared to the exact value $a_{500} = 8.0976 \times 10^{-7}$, a difference of less than 0.1%).

To our knowledge, the only previous studies of $P_4(z)$ were by Bender *et al* [8], who examined $P_d(1)$ as a function of d and by a $1/d$ expansion obtained a value consistent with (6), and by Mayer and Nuttall [9], who derived a differential equation consistent with (5). We have not examined $P(z)$ outside the unit circle, although it is clearly analytic in the z^2 plane cut along the real axis from $z^2 = 1$ to infinity. While it is doubtful that $P(z)$ can be expressed in terms of elliptic integrals as for the three dimensional cubic lattices [2], it is hoped that further analysis of (13) will lead to a more transparent representation of its analytic properties.

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