Explicit bounds for the return probability of simple random walk

(The running head should be the same as the title.)

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Abstract

We give an exact computation of the second order term in the asymptotic expansion of the return probability, $P^d_{2n}(0,0)$, of a simple random walk on the d-dimensional cubic lattice. We also give an explicit bound on the remainder. In particular, we show that $P^d_{2n}(0,0) < 2\left(\frac{d}{4\pi n}\right)^{d/2}$ where $n \geqslant M$ is explicitly given.

Key words and phrases. simple random walk, random walk, return probability, asymptotic probability

1 Introduction

We study here the asymptotic properties of the simple random walk on a d–dimensional lattice. That is, the single step probability is given by the formula:

$$P^d_1(i,j) \;=\; \begin{cases} \frac{1}{2d}\;, & \text{if } |i-j| = 1\;; \\ 0\;, & \text{otherwise.} \end{cases}$$

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Using this notation, one can write the probability of starting at lattice point i and ending at j after n steps of the random walk as the convolution of P^d_1 with itself n times:

$$P^d_n(i,j) \ = \ [P^d_1]^{*n}(i,j) \ .$$

In particular, the probability of starting at and returning to the origin after $2n$ steps is given by the formula:

$$P^d_{2n}(0,0) \ = \ \frac{1}{(2d)^{2n}} \frac{(2n)!}{n! \cdot n!} \sum_{k_1+\ldots+k_d=n} \left(\frac{n!}{k_1! \cdot \ldots \cdot k_d!} \right)^2 \ .$$

This is easily seen by a counting argument, or by evaluating the constant term in the series:

$$[\widehat{P^d_{(1)}}(0,\cdot)]^{2n}(\Theta) \ = \ \left[\frac{1}{2d} \sum_{i=1}^{d} \left(e^{i\theta_i} + e^{-i\theta_i} \right) \right]^{2n} \ . \qquad (1.1)$$

By orthogonality, one can also compute the constant term on the right hand side of (1.1) by integration of the entire expression over the d dimensional torus $\mathbb{T}^d$. That is, evaluation of the integral:

$$P^d_{2n}(0,0) \ = \ \frac{1}{(2\pi)^d} \int_{\Theta \in [0,2\pi]^d} \left(\frac{1}{d} \sum_i \cos\, \theta_i \right)^{2n} \ d\Theta \ . \qquad (1.2)$$

By Taylor expanding the integrand of (1.2), one can show that one has the asymptotic:

$$P^d_{2n}(0,0) \ \sim \ 2 \left(\frac{d}{4\pi n} \right)^{d/2} \ .$$

This result is originally due to Pólya, and an account can be found, for instance, in [4]. Recently, C. Ritzmann [3] has given a local central limit theorem for the distribution $P^d_{2n}(x,y)$ in the case of fairly general random walks with bounded step size on $\mathbb{Z}^d$. The method of proof is to again Taylor expand integrals of the form (1.2) which arise from the Fourier transform of the distribution function. Our purpose here is to give a simple and explicit calculation of (a bound for) the integral (1.2), which includes bounds for all the constants involved. This is partial progress on a conjecture of Russ Lyons, that in fact the following bound holds:

$$P^d_{2n}(0,0) \ \leq \ 2 \left(\frac{d}{4\pi n} \right)^{d/2} \ \text{for all } d \geq 1, n \geq 0 \ . \qquad (1.3)$$

This is not difficult to show for $d = 1, 2$, so we concentrate on the case where $d \geq 3$.

We prove here that for each fixed d, if $n \geqslant M$, for M sufficiently large, the inequality in (1.3) is satisfied. Computer calculation can be then be used to check (1.3) for the first $(M-1)$ terms for a fixed dimension d. Indeed, we have verified this for dimensions up to and including $d = 6$.

This work is used by Felker and Lyons in [1] to prove rigorous lower bounds for the following thermodynamic limit. Let G_n be the graph induced by the cube of side length n in the d-dimensional hypercubic lattice $\mathbb{Z}^d$ and let $\tau(G_n)$ be the number of spanning trees of G_n. Then define

$$h_d = \lim_{n\to\infty} \frac{1}{n^d} \ln\left[\tau(G_n)\right] \,.$$

Felker and Lyons estimate h_d using the following formula:

$$h_d = \ln(2d) - \sum_{n=1}^{\infty} P_n^d(0,0)/n \,.$$

Since the terms of the summation are all nonnegative, a proof of inequality 1.3 gives a method for computing a rigorous lower bound for h_d. Thus, our results can be used to provide a lower bound up to $d = 6$.

In this paper, we will use the following "strict–O" notation:

$$h(x) \;=\; O_M(f(x)) \,,$$

to mean that

$$|h(x)| \;\leqslant\; M|f(x)| \,.$$

This notation follows obvious rules for additions and multiplications. We will show that:

Proposition 1. *For all $2 \leqslant n$ and $d \leqslant n$, one has the bound:*

$$P_{2n}^d(0,0) \;\leqslant\; 2\left(\frac{d}{4\pi n}\right)^{d/2}\left[1 \;-\; \frac{d}{8n} \;+\; \frac{7}{2}d(d+2)\left(\frac{d}{4n}\right)^2\right] \;+\; \left(1+\frac{1}{\sqrt{n}}\right)e^{-\frac{2n}{d}} \,. \quad (1.4)$$

Remark 1. In particular, the expansion (1.4) shows that one has $P_{2n}^d(0,0) < 2\left(\frac{d}{4\pi n}\right)^{d/2}$ when $n \geqslant M$ for an M which can be read off from the above formula. Ignoring the exponential error for a moment, we see that we need to at least take $n \geq \frac{7}{4}d^2(d+2)$. Hence, M is of the order d^3. When $d = 3$, one sees that the top term in the asymptotic is guaranteed to take over at the point $n \approx 79$. It is likely that this number can be improved by at least a factor of 2 by tweaking the analysis, and will indicate how this can be done as we go along. Of course we also need to regard the exponential error term in the expansion (1.4), but it is easily seen that this falls away quickly.

In fact, it suffices to tack on one more unit to get $n \geq \frac{7}{4}d^2(d+2)+1$ to cover the exponential error. This can be seen as follows. We need to show that for $n \geq \frac{7}{4}d^2(d+2)+1$, we have:

$$2\left(\frac{d}{4\pi n}\right)^{d/2}\left[-\frac{d}{8n}+\frac{7}{2}d(d+2)\left(\frac{d}{4n}\right)^2\right]+\left(1+\frac{1}{\sqrt{n}}\right)e^{-\frac{2n}{d}} \leq 0.$$

Multiplying through by $\frac{4n^2}{d}\left(\frac{4\pi n}{d}\right)^{d/2}$, estimating $(1+1/\sqrt{n})$ by 2, and using the assumtion that $n \geq \frac{7}{4}d^2(d+2)+1$, we get that it suffices to show that for appropriate d and n,

$$\frac{8n^2}{d}\left(\frac{4\pi n}{d}\right)^{d/2} e^{-2n/d} \leq 1. \tag{1.5}$$

By taking a derivative, it is easy to show that for fixed d this is a decreasing function of n for n in our range. Therefore, it is enough to prove the inequality in (1.5) when $n = d^3$ (since $d^3 < \frac{7}{4}d^2(d+2)+1$, which is the smallest value of n in our range) :

$$8d^5(4\pi d^2)^{d/2}e^{-2d^2} \leq 1. \tag{1.6}$$

To prove this, we take another derivative and show that the left-hand side is decreasing in d when $d \geq 3$. Therefore, it suffices to check that (1.6) holds when $d = 3$, which it does.

As we have already mentioned, for $n < \frac{7}{4}d^2(d+2)+1$, computer calculation can be used to verify (1.3) for a fixed dimension. We have done this for $d = 3, 4, 5, 6$.

In our analysis, we do not try to directly compute the integral (1.2), but instead employ a carefully chosen substitute which is a one dimensional integral that bounds (the relevant part of) (1.2) while at the same time it preserves the first two terms in the asymptotic expansion of (1.2). It should be observed that it is also possible to obtain an equality in (1.4) by directly dealing with (1.2), but the computations required would become quite a bit more involved.

2 The main computation

We start with the integral:

$$I_1 \;=\; \frac{1}{(2\pi)^d}\int_{\Theta\in[-\pi,\pi]^d}\left(\frac{1}{d}\sum_i \cos\,\theta_i\right)^{2n} d\Theta\;.$$

The main contributions to this integral come from near where the integrand is equal to 1. That is, modulo an exponential error, we need only concern ourselves with the points $(0,\dots,0)$ and $(\pi,\dots,\pi)$. In fact, by symmetry, we need only concern ourselves with the interval $[-\frac{\pi}{2},\frac{\pi}{2}]^d$. This allows us to write:

$$I_1 \;=\; \frac{2}{(2\pi)^d}\int_{\Theta\,\in\,\mathcal{N}\cap[-\frac{\pi}{2},\frac{\pi}{2}]^d}\left(\frac{1}{d}\sum_i \cos\,\theta_i\right)^{2n} d\Theta + O_1\left(\left(\frac{d-1}{d}\right)^{2n}\right)\;, \quad (2.1)$$

where $\mathcal{N}$ is a neighborhood of the point $(0,\dots,0)$ which we will explain in a moment. Rearranging the first term on the right hand side of (2.1) above, using the trigonometric identity $\cos\theta_i = 1-2\sin^2\frac{1}{2}\theta_i$, and a rescaling, we may write the integral as:

$$I_2 \;=\; \frac{2}{\pi^d}\int_{\Theta\,\in\,\frac{1}{2}\cdot\mathcal{N}\cap[-\frac{\pi}{4},\frac{\pi}{4}]^d}\left(1-\frac{2}{d}\sum_i \sin^2\,\theta_i\right)^{2n} d\Theta\;.$$

Now, performing the substitution $u_i=\sin\theta_i$, we may write:

$$I_2 \;=\; \frac{2}{\pi^d}\int_{u\,\in\,\mathcal{N}'\cap[-\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}]^d}\left(1-\frac{2}{d}|u|^2\right)^{2n}\prod_i\frac{1}{\sqrt{1-u_i^2}}\,du\;,$$

where $\mathcal{N}'$ is the image of $\frac{1}{2}\mathcal{N}$ under this change of variable. We now choose $\mathcal{N}$ so that $\mathcal{N}'$ is the ball of radius $\frac{1}{\sqrt{2}}$ centered at the origin. Notice that this is consistent with the remainder (second term) on the right hand side of (2.1).

The choice of radius of integration is the single most important factor in obtaining bound constants in Proposition 1. In particular, the constant of $\frac{7}{2}$ in the third order asymptotics of (1.4) can probably be improved by at least a factor of 2 by taking the radius of integration to be smaller. This will of course increase the size of the exponential error.

Now, a simple induction shows that in the range we consider:

$$\prod_i\frac{1}{\sqrt{1-u_i^2}} \;\leqslant\; \frac{1}{\sqrt{1-|u|^2}}\;.$$

This allows us to bound:

$$I_2 \;<\; |\mathbb{S}^{d-1}|\cdot\frac{2}{\pi^d}\int_0^{\frac{1}{\sqrt{2}}}\left(1-\frac{2}{d}u^2\right)^{2n}\frac{u^{d-1}}{\sqrt{1-u^2}}\,du\;,$$

where $|\mathbb{S}^{d-1}|$ denotes the volume of the standard unit sphere in $\mathbb{R}^d$. Therefore, modulo an exponential error and some constants, we have reduced the problem of bounding $P^d_{2n}(0,0)$ to that of studying the one dimensional the integral:

$$I_3 \;=\; \int_0^{\frac{1}{\sqrt{2}}}\left(1-\frac{2}{d}u^2\right)^{2n}\frac{u^{d-1}}{\sqrt{1-u^2}}\,du\;.$$

It is important for us to point out that, although we do not make it explicit here, the asymptotic expansion for I_3 matches the asymptotic expansion of the original multidimensional integral I_1 in the first two terms. Therefore, the integral I_3 incorporates the mechanism which is responsible for the bound (1.3) (at least for n sufficiently large), i.e. a negative second asymptotic, while at the same time it eliminates many of the error terms that would come up by trying to treat I_1 directly. This is the important point of the analysis here. The bounds we will produce are as follows:

Lemma 1. *For $n > 0$ and $d \geqslant 3$, one has that:*

$$I_3 \;=\; \int_0^{\sqrt{-\frac{d}{2}\ln(1-\frac{1}{d})}} e^{-2n\cdot\frac{2}{d}s^2} s^{d-1} \cdot \Big(1 - \frac{1}{d}s^2 + O_{14}(s^4)\Big)\, ds \;. \tag{2.2}$$

Proof of Lemma 1. The identity (2.2) is a straight forward consequence of Taylor's theorem with remainder and the following implicit change of variables:

$$1 - \frac{2}{d}u^2 \;=\; e^{-\frac{2}{d}s^2} \;.$$

Explicitly, one has the formulas:

$$s \;=\; \sqrt{-\frac{d}{2}\ln(1 - \frac{2}{d}u^2)} \;, \tag{2.3}$$

$$u \;=\; \sqrt{\frac{d}{2}(1 - e^{-\frac{2}{d}s^2})} \;. \tag{2.4}$$

With this change of variables and the help of the Taylor expansion:

$$\frac{1}{\sqrt{1-u^2}} \;=\; 1 + \frac{1}{2}u^2 + O_{\frac{3}{\sqrt{2}}}(u^4) \;, \qquad\qquad u \in [0, \frac{1}{\sqrt{2}}] \;,$$

we may write:

$$I_3 \;=\; \int_0^{\sqrt{-\frac{d}{2}\ln(1-\frac{1}{d})}} e^{-2n\cdot\frac{2}{d}s^2} s^{d-1} \cdot e^{-\frac{2}{d}s^2} \cdot \Big(\frac{u}{s}\Big)^{d-2} \cdot \Big(1 + \frac{1}{2}u^2 + O_{\frac{3}{\sqrt{2}}}(u^4)\Big)\; ds \;.$$

Our task is now to give a Taylor with remainder formula for the product of the last three functions in the integrand above. For this, it is useful to note that by the formula (2.3), one has the bound $\frac{2}{d}s^2 \leqslant \frac{3}{2d}$ over the range of integration. This follows from he estimate:

$$-\ln\big(1 - \frac{1}{d}\big) \;\leqslant\; \frac{1}{d} + \frac{1}{2(d-1)^2} \;,$$

which can be proved with th the help of Taylors formula with remainder. Therefore, we have that $s \leqslant \sqrt{\frac{3}{4}}$. This fact will be used implicitly in all the "strict–O" notation that follows. We first compute the Taylor expansions:

$$e^{-\frac{2}{d}s^2} \; = \; 1 - \frac{2}{d}s^2 + O_{\frac{1}{2}\cdot(\frac{2}{d})^2}(s^4) \; , \tag{2.5}$$

$$e^{-\frac{2}{d}s^2} \; = \; 1 - \frac{2}{d}s^2 + \frac{1}{2}\left(\frac{2}{d}\right)^2 s^4 + O_{\frac{1}{3!}(\frac{2}{d})^3}(s^6) \; . \tag{2.6}$$

Next, we substitute (2.6) into the change of variable formula (2.4) to see that we may write:

$$u^2 \; = \; s^2 \cdot \left(1 - \frac{1}{d}s^2 + O_{\frac{1}{3!}\cdot(\frac{2}{d})^2}(s^4)\right) \; , \tag{2.7}$$

where the expression $\frac{1}{d}s^2 - O_{\frac{1}{3!}\cdot(\frac{2}{d})^2}(s^4)$ comes from an alternating–decreasing series that is dominated by $\frac{1}{d}s^2$. In particular, we have that this expression lies in the interval $[0, \frac{1}{2}]$. This allows us to use the Taylor expansion:

$$(1-x)^{\frac{d-2}{2}} \; = \; 1 - \frac{d-2}{2}x + O_{\frac{1}{2}(\frac{d-2}{2})(\frac{d-4}{2})\max\{1, 2^{\frac{6-d}{2}}\}}(x^2) \; , \quad x \in [0, \frac{1}{2}] \; , \tag{2.8}$$

as well as the identity:

$$\left(\frac{1}{d}s^2 - O_{\frac{1}{3!}\cdot(\frac{2}{d})^2}(s^4)\right)^2 \; = \; O_{\frac{3}{2d^2}}(s^4) \; ,$$

to set:

$$x \; = \; \frac{1}{d}s^2 + O_{\frac{1}{3!}\cdot(\frac{2}{d})^2}(s^4) \; ,$$

in (2.8) and expand things out and collect terms together to write:

$$\left(\frac{u}{s}\right)^{d-2} \; = \; 1 - \frac{d-2}{2d}s^2 + O_1(s^4) \; . \tag{2.9}$$

Finally, we can again use the identity (2.7) as well as the fact that $u = O_1(s)$ to write:

$$1 + \frac{1}{2}u^2 + O_{\frac{3}{\sqrt{2}}}(u^4) \; = \; 1 + \frac{1}{2}s^2 + O_3(s^4) \; . \tag{2.10}$$

The desired result now follows from multiplying through the expressions on lines (2.5), (2.9), and (2.10) and then using some direct computations to show the identity:

$$\left(1-\frac{2}{d}s^2+O_{\frac{1}{2}\cdot(\frac{2}{d})^2}(s^4)\right)\cdot\left(1-\frac{d-2}{2d}s^2+O_1(s^4)\right)\cdot\left(1+\frac{1}{2}s^2+O_3(s^4)\right)$$
$$= \ 1-\frac{1}{d}s^2+O_{14}(s^4)\ .$$

This completes the proof of formula (2.2). □

2.1 Wrapping things up

To get bounds on each of the integrals on the right hand side of (2.2), we use the fact that:

$$\int_0^{\sqrt{-\frac{d}{2}\ln(1-\frac{1}{d})}} e^{-2n\cdot\frac{2}{d}s^2}s^{d-1}\,ds \ < \ \int_0^\infty e^{-2n\cdot\frac{2}{d}s^2}s^{d-1}\,ds\ ,$$

and

$$\int_0^{\sqrt{-\frac{d}{2}\ln(1-\frac{1}{d})}} e^{-2n\cdot\frac{2}{d}s^2}s^{d-1}\cdot O_{14}(s^4)\,ds \ = \ O_{14}(\int_0^\infty e^{-2n\cdot\frac{2}{d}s^2}s^{d+3}\,ds)\ ,$$

as well as the fact that:

$$\begin{aligned}
&\frac{1}{d}\int_{\sqrt{-\frac{d}{2}\ln(1-\frac{1}{d})}}^\infty e^{-2n\cdot\frac{2}{d}s^2}s^{d+1}\,ds\\
<\ &\frac{1}{d}e^{-\frac{2n}{d}}\int_{\frac{1}{\sqrt{2}}}^\infty e^{-2n\cdot\frac{2}{d}(s^2-\frac{1}{2})}s^{d+1}\,ds\\
<\ &\frac{1}{d}e^{-\frac{2n}{d}}\int_0^\infty e^{-2n\cdot\frac{2}{d}s^2}(s+\frac{1}{\sqrt{2}})^{d+1}\,ds\\
<\ &\frac{1}{d}e^{-\frac{2n}{d}}\left(2^{(d-1)/2}\int_0^\infty e^{-2n\cdot\frac{2}{d}s^2}\,ds\ +\ 2^d\int_0^\infty e^{-2n\cdot\frac{2}{d}s^2}s^{d+1}\,ds\right)\ .
\end{aligned} \tag{2.11}$$

A little further computation shows that we now have:

$$\begin{aligned}
\frac{2}{\pi^d}\cdot|\mathbb{S}^{d-1}|\cdot I_3\ <\ &2(\frac{d}{4\pi n})^{d/2}\ -\ (\frac{d}{4\pi n})^{d/2}\cdot(\frac{d}{4n})\ +\\
&0_{\,7d(d+2)}\left((\frac{d}{4\pi n})^{d/2}\cdot(\frac{d}{4n})^2\right)\ +\ \frac{2}{\pi^d}\cdot|\mathbb{S}^{d-1}|\cdot(R.H.S.)(2.11)\ .
\end{aligned} \tag{2.12}$$

We recall the gamma formulas:

$$\int_0^\infty e^{-s^2} s^l \, ds \ = \ \frac{1}{2}\Gamma\left(\frac{l+1}{2}\right) \ ,$$

$$|\mathbb{S}^{d-1}| \ = \ \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \ ,$$

and use the following bound (which for instance follows easily from the integral formula (8.13) on p. 87 of [2]):

$$\frac{1}{\Gamma(x)} \ < \ 2(2\pi)^{-1/2} x^{-x} e^x x^{1/2} \ , \qquad\qquad 1 \leqslant x \ ,$$

to compute that:

$$\begin{aligned}
&\frac{2}{\pi^d} \cdot |\mathbb{S}^{d-1}| \cdot (R.H.S.)(2.11) \\
= \ &\frac{4}{\pi^{\frac{d}{2}}} \cdot \frac{1}{\Gamma(\frac{d}{2})} \cdot \frac{1}{d} e^{-\frac{2n}{d}} \cdot \left(2^{\frac{d-3}{2}} \left(\frac{d}{4n}\right)^{1/2} \cdot \Gamma\left(\frac{1}{2}\right) \ + \ 2^{d-2} \left(\frac{d}{4n}\right)^{d/2+1} \cdot d \cdot \Gamma\left(\frac{d}{2}\right) \right) \\
< \ &e^{-\frac{2n}{d}} \left(\left(\frac{4e}{\pi d}\right)^{d/2} \cdot \frac{1}{2\sqrt{2n}} \ + \ \left(\frac{d}{\pi n}\right)^{d/2} \cdot \frac{d}{\sqrt{n}} \cdot \frac{1}{4\sqrt{n}} \right) \ , \\
< \ &e^{-\frac{2n}{d}} \cdot \frac{1}{\sqrt{n}} \ , \qquad\qquad d \leqslant n \ \ .
\end{aligned}$$

Substituting this last inequality into the right hand side of (2.12), and using the inequality:

$$\frac{d-1}{d} \ < \ e^{-\frac{1}{d}} \ ,$$

to tack on the exponential error from line (2.1), we obtain the result of Proposition 1.

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