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Sharp Spectral Zeta Asymptotics on Graphs of Quadratic Growth

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Abstract. We investigate the spectral properties of the Dirichlet Laplacian on large finite metric balls within *irregular* infinite graphs of quadratic volume growth. We consider an exhaustion $G_n = B_{R_n}(x_0)$ and the spectral zeta value $Z_n(1) = \operatorname{tr}(\mathcal{L}_n^{-1})$ of the killed generator $\mathcal{L}_n$.

We establish a sharp asymptotic law under the assumptions that the graph satisfies uniform quadratic volume growth (VG(2)) and a Poincaré inequality (PI). These analytic–geometric hypotheses imply large-scale regularity. We further assume a standard quantitative homogenisation property (a uniform local central limit theorem with polynomial rate), which holds in the principal example classes, and implies the existence of a global heat-kernel constant $\mathcal{G} > 0$ (independent of x) such that the lazy simple random walk (LSRW) satisfies

$$p_t(x,x) \sim \frac{\mathcal{G}}{t} \qquad (t \to \infty).$$

Our main theorem establishes the sharp asymptotic

$$Z_n(1) = \mathcal{G}\, N_n \log N_n + O(N_n), \qquad N_n := |V(G_n)| \xrightarrow[n\to\infty]{} \infty.$$

This implies a relative error of $O(1/\log N_n)$, with constants depending only on the structural parameters of G. This result extends far beyond homogeneous lattices. For $\mathbb{Z}^2$, this yields the constant identification $\mathcal{G} = 2/\pi$, providing a new limit formula that recovers π without π appearing in the input (a "π-free” limit). Our techniques highlight the robustness of spectral asymptotics under homogenisation in this critical, recurrent setting.

1. Introduction

The relationship between the geometry of a space and the spectrum of its associated Laplacian is a fundamental area of study. In Riemannian geometry, Weyl’s law and the Minakshisundaram–Pleijel heat trace expansion provide deep connections between

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volume, curvature, and eigenvalue asymptotics. In the discrete setting, analogous investigations explore how the combinatorial and geometric structure of a graph influences the spectrum of the graph Laplacian (see [8]).

This paper focuses on the spectral zeta function on graphs. For a finite graph H, we consider the Laplacian associated with the lazy simple random walk (see Section 2). With Laplacian eigenvalues $0 < \lambda_1 \le \lambda_2 \le \cdots$, the spectral zeta function is defined as $\zeta_H(s) = \sum_k \lambda_k^{-s}$. We are interested in the value at $s = 1$, $Z_H(1) := \zeta_H(1)$, which corresponds to the trace of the inverse Laplacian (the Green operator).

Remark 1.1 (Connection to Kirchhoff Index). The value $Z_H(1) = \sum_k \lambda_k^{-1}$ is closely related to the Kirchhoff index $K(H)$, which is the sum of effective resistances $R_{\text{eff}}(x, y)$ between all pairs of vertices. We primarily use the probabilistic Laplacian $\mathcal{L} = I - P$. For the closely related normalized Laplacian $\mathcal{L}_{\text{norm}}$ (which is similar to $\mathcal{L}$ on graphs with bounded degree, see Theorem 2.5), there is an exact identity relating the trace of the inverse (starting from the second eigenvalue) to $K(H)$ weighted by the stationary distribution m (see [20, Chapter 9]):

$$K(H) = \sum_{x,y} R_{\text{eff}}(x, y) = m(V(H)) \sum_{k \ge 2} \frac{1}{\lambda_k(\mathcal{L}_{\text{norm}})}.$$

While we work with Dirichlet eigenvalues (killed walk), the asymptotics of $Z_H(1)$ studied here directly relate to the asymptotics of the Kirchhoff index for the corresponding finite graph when the walk is recurrent. We emphasize the distinction from the combinatorial Laplacian $D - A$.

We investigate the asymptotic behaviour of $Z_n(1)$ for large finite subgraphs G_n exhausting an infinite graph G. We focus on the critical case of *quadratic volume growth* ($|B_R| \asymp R^2$), corresponding to an effective dimension of $d = 2$. This dimension is critical, leading to distinct asymptotic behaviour compared to other dimensions, as summarized in Table 1. This class includes the lattice $\mathbb{Z}^2$ but also encompasses irregular structures that behave two-dimensionally on a large scale, such as lattices with random bounded conductances or certain planar graphs with uniform properties.

1.1. Main Result and Assumptions

We establish a precise asymptotic formula for $Z_n(1)$. Our foundational assumptions on the graph G are uniform quadratic volume growth (VG(2)) and a Poincaré inequality (PI). These ensure strong large-scale geometric regularity.

To achieve a sharp first-order asymptotic involving a global constant, we must ensure that the random walk on G homogenises uniformly to a Brownian motion. While VG(2) and PI imply qualitative homogenisation, we explicitly assume a quantitative version: a uniform Local Central Limit Theorem (LCLT) with a polynomial rate of convergence (see Theorem 2.9).

Definition 1.2 (Heat-kernel constant). Under the assumption of quantitative homogenisation, the LSRW on G satisfies

$$p_t(x,x) = \frac{\mathcal{G}}{t} + O(t^{-1-\delta})$$

as $t \to \infty$, for constants $\mathcal{G} > 0$ and $\delta > 0$ independent of x. We call $\mathcal{G}$ the *heat-kernel constant* of G.

Remark 1.3 (Explicit form of $\mathcal{G}$). In many standard cases, such as random walks on $\mathbb{Z}^d$ driven by a mean-zero, finite-variance step distribution with covariance matrix Σ, the LCLT yields an explicit formula (see, e.g., [19, Ch. 2]). In $d = 2$:

$$\mathcal{G} = \frac{1}{2\pi\sqrt{\det \Sigma}}.$$

For irregular media (like the RCM), Σ represents the effective homogenized diffusivity.

This assumption is standard and known to hold in many canonical examples of irregular media (see Theorem 2.10).

Theorem 1.4. *Let G be an infinite, connected graph of bounded degree satisfying quadratic volume growth (VG(2)) and a Poincaré inequality (PI). Assume further that G satisfies the quantitative homogenisation assumption (Theorem 2.9) with heat-kernel constant $\mathcal{G}$. For any exhaustion $\{G_n\}$ of G by metric balls $G_n = B_{R_n}(x_0)$ with volume $N_n = |V(G_n)| \to \infty$, we have*

$$Z_n(1) = \mathcal{G} N_n \log N_n + O(N_n).$$

1.2. Context, Significance, and Novelty

The $N_n \log N_n$ divergence is characteristic of the critical dimension $d = 2$, where the random walk is recurrent, contrasting sharply with other dimensions (see Table 1 and Section A for comparisons).

Table 1. Asymptotics of $Z_n(1)$ under polynomial volume growth $V(R) \asymp R^d$.

Dimension d	**Growth Rate**	**Walk Behaviour**	$G_{G_n}(v,v)$ **Behaviour**	$Z_n(1)$ **Asymptot**
$d = 1$	Linear (R)	Strongly recurrent	$\asymp N_n$ (interior)	$Z_n(1) \asymp N_n^2$
$d = 2$	**Quadratic** (R^2)	**Recurrent (Critical)**	$\asymp \log N_n$	$Z_n(1) \asymp N_n \log N$
$d \geq 3$	Polynomial (R^d)	Transient	Bounded ($O(1)$)	$Z_n(1) \asymp N_n$

Theorem 1.5 generalizes classical results known for regular structures. For Euclidean domains and tori, similar asymptotics for spectral zeta functions have been studied

(cf. [9, 13]). In the graph setting, results on the trace of the Green function have been established for highly regular graphs (e.g., results discussed in [18, 22]).

Our contribution lies in extending this connection to a broad class of potentially highly irregular graphs characterized by large-scale geometric (VG(2)) and analytic (PI) properties, supplemented by the quantitative homogenisation assumption. The novelty is the demonstration that this sharp asymptotic holds without requiring local uniformity or translational invariance. The approach is modular, isolating the roles of geometry (VG(2)+PI), stochastic homogenisation (LCLT with rate), and boundary regularity (CDC/IU).

1.3. Examples and Scope

The assumptions capture a wide variety of graphs that are metrically two-dimensional but may be combinatorially irregular.

Example 1.5 (The case of $\mathbb{Z}^2$ and spectral recovery of π). Consider the standard lattice $\mathbb{Z}^2$. The LSRW (defined in Section 2) has a step distribution covariance matrix $\Sigma = \frac{1}{4} I_2$. Using Theorem 1.4:

$$\mathcal{G} = \frac{1}{2\pi\sqrt{\det(\Sigma)}} = \frac{1}{2\pi(1/4)} = \frac{2}{\pi}.$$

Theorem 1.5 implies $\lim_{n\to\infty} Z_n(1)/(N_n \log N_n) = 2/\pi$.

Example 1.6 (Irregular Structures). Beyond $\mathbb{Z}^2$, the main examples satisfying all assumptions (including quantitative homogenisation, see Theorem 2.10 for details and references) are:

(1) **Periodic graphs:** Graphs with a co-compact $\mathbb{Z}^2$ action.

(2) **Random Conductance Model (RCM) on $\mathbb{Z}^2$:** If the conductances are i.i.d., uniformly bounded, and elliptic, the resulting graph satisfies VG(2) and PI almost surely, and the required uniform quantitative homogenisation holds [1, 7].

(3) **Supercritical Percolation on $\mathbb{Z}^2$:** The infinite cluster (for $p > p_c(\mathbb{Z}^2) = 1/2$) satisfies VG(2) and PI almost surely [3]. Quantitative homogenization results have also been established in this setting (see Theorem 2.10).

1.4. Methodology Overview and Structure

We employ a time-domain, fully discrete approach based on an interior-boundary decomposition strategy. By analyzing the sums of the heat kernel directly (rather than using Tauberian theorems on the spectral measure), we cleanly isolate the required inputs. The proof relies heavily on techniques derived from Volume Doubling (VD) and the Poincaré inequality (PI).

The lower bound relies on showing that the killed walk starting in the interior rarely reaches the boundary within the relevant timescale, using maximal inequalities derived from Gaussian bounds.

The upper bound uses a short/long time split. The short time uses the full-space LCLT sum. The long-time contribution is controlled sharply using Intrinsic Ultracontractivity (IU) for metric balls. This technique is pivotal as it avoids spurious $\log\log$ terms that would arise from using cruder estimates (see **??**). Both bounds crucially depend on the assumed quantitative homogenisation rate (Theorem 2.9) to sum the LCLT error terms.

Structure of the paper. Section 2 covers the preliminary definitions, assumptions, and key analytic tools, including a detailed discussion of the justification for IU under VD+PI. Section 3 introduces the interior-boundary decomposition method. Section 4 and Section 5 detail the proofs of the lower and upper bounds. Finally, Section 6 concludes the proof of Theorem 1.5 and discusses the assumptions and extensions. The appendices provide context on other growth regimes and explore numerical examples of the π-identities.

2. Preliminaries and Analytic Tools

Notation. We use $C, c, c_1, \ldots$ to denote positive constants depending only on the structural properties of the graph (e.g., constants in VG(2), PI, the maximum degree Δ) and the parameters of the quantitative homogenisation (QH) assumption (e.g., $\mathcal{G}, \delta, C_{QH}, t_0$); their values may change line by line. We write $A \lesssim B$ if $A \le CB$, and $A \asymp B$ if $cA \le B \le CA$. All logarithms (log) are natural logarithms.

Let $G = (V, E)$ be an infinite, connected graph with bounded maximum degree $\Delta < \infty$. We define metric balls as closed: $B_R(x) = \{y \in V : d_G(x, y) \le R\}$. We denote $V(x, R) = |B_R(x)|$.

2.1. Geometric and Analytic Assumptions

Definition 2.1 (Quadratic Volume Growth (VG(2))). G has (uniform) quadratic volume growth if there exist $c_1, c_2 > 0$ such that for all $x \in V$ and $R \ge 1$,

$$c_1 R^2 \le V(x, R) \le c_2 R^2. \tag{2.1}$$

This implies the Volume Doubling (VD) property: $V(x, 2R) \le C_D V(x, R)$.

Definition 2.2 (Poincaré Inequality (PI)). G satisfies a (scaled) Poincaré inequality if there exists $C_P > 0$ such that for any ball $B_R = B_R(x_0)$ and any function $f : V \to \mathbb{R}$,

$$\sum_{x \in B_R} (f(x) - \bar{f}_{B_R})^2 \le C_P R^2 \, \mathcal{E}_{B_{2R}}(f, f),$$

where $\bar{f}_{B_R}$ is the average of f over B_R (w.r.t. counting measure), and the local Dirichlet form $\mathcal{E}_U(f, f)$ is defined as

$$\mathcal{E}_U(f, f) = \sum_{\substack{\{x,y\} \in E \\ x,y \in U}} (f(x) - f(y))^2.$$

Remark 2.3. Under the VD condition, this formulation of PI is equivalent to the local version (see [17]). The combination of VD and PI (VD+PI) is central to analysis on graphs (see [16]).

Standing assumptions. We assume G is infinite, connected, has bounded degree $\Delta < \infty$, satisfies VG(2) (and thus VD), and PI.

2.2. Random Walk and the Analytic Framework

We consider the *lazy* simple random walk (LSRW) $(X_t)_{t \ge 0}$. This is a discrete-time Markov chain where at each step, the walk stays put with probability $1/2$ or moves to a uniformly chosen neighbor with probability $1/2$. The transition matrix is $P = \frac{1}{2}(I + P_{SRW})$, where $P_{SRW}(x, y) = 1/\deg(x)$ if $y \sim x$. The heat kernel is $p_t(x, y) = \mathbb{P}_x[X_t = y]$. The generator (Laplacian) is $\mathcal{L} = I - P$.

Laziness ensures the walk is aperiodic, simplifying spectral analysis. It also relates the generators: $\mathcal{L}_{\text{LSRW}} = \frac{1}{2}\mathcal{L}_{\text{SRW}}$ (see Theorem 6.6).

Remark 2.4 (Measures and Operators). The LSRW is reversible w.r.t. the degree measure $m(x) = \deg(x)$. The Laplacian $\mathcal{L}$ is self-adjoint on the Hilbert space $\ell^2(m)$. Due to the assumption of bounded degree ($\Delta < \infty$), the counting measure $|\cdot|$ and the degree measure m are comparable: $m(A) \asymp |A|$. This allows seamless transition between analytic results formulated w.r.t. m (such as those in Theorem 2.13) and geometric properties formulated w.r.t. $|\cdot|$ (see [10]).

On a finite subgraph H, the Dirichlet Laplacian $\mathcal{L}_H$ acting on $\ell^2(m|_H)$ is similar to the operator acting on $\ell^2(|\cdot||_H)$ (via the transformation induced by the square root of the measure densities, $M^{1/2}$). Since the trace is similarity-invariant in finite dimensions, $Z_H(1) = \operatorname{tr}(\mathcal{L}_H^{-1})$ is independent of the chosen (comparable) inner product.

We emphasize that we work with the probabilistic Laplacian $\mathcal{L} = I - P$ (or its similar normalized form), not the combinatorial Laplacian $D - A$.

Unless otherwise stated, all heat-kernel quantities (p_t, p_t^H, etc.) are those of the LSRW probability kernel. We often suppress the graph index in the Green function (e.g., writing $G_H(v, v)$ instead of $G_H(v, v)$) when clear from context.

The combination of VD and PI is fundamental:

Theorem 2.5 ([12]). *The combination of VD and PI is equivalent to the Parabolic Harnack Inequality (PHI).*

PHI provides strong regularity for solutions to the heat equation, which translates to precise estimates on the random walk.

2.3. Heat Kernel Toolbox

We summarize the crucial analytic tools.

2.3.1. Maximal Inequality and Gaussian Bounds.

Proposition 2.6 (Consequences of PHI, [12, 15]). *Under VD+PI:*

(1) *(Gaussian Bounds) There exist $C_G, c_G > 0$ such that*

$$p_t(x, y) \le \frac{C_G}{\sqrt{V(x, \sqrt{t})V(y, \sqrt{t})}} \exp\left(-c_G \frac{d(x, y)^2}{t}\right).$$

Under the VG(2) assumption, this specializes to $p_t(x, y) \lesssim t^{-1} \exp(-c_G d(x, y)^2/t)$.

(2) *(Maximal Inequality) There exist $C_M, c_M > 0$ such that for any $v \in V$, $t \ge 0$, and $d \ge 1$,*

$$\mathbb{P}_v\left(\max_{0\le s\le t} d_G(v, X_s) \ge d\right) \le C_M \exp\left(-c_M \frac{d^2}{t+1}\right). \tag{2.2}$$

Note on derivation. The Gaussian upper bounds are a direct consequence of PHI (see [12] for the general form). The maximal inequality (exit time estimate) follows from the Gaussian upper bounds via standard arguments involving chaining and union bounds (see, e.g., [15, Theorem 5.5.3] or arguments in [12]). ■

2.3.2. Heat Kernel Asymptotics (LCLT) and Homogenisation. A crucial ingredient is the sharp, uniform homogenisation of the heat kernel. We state this as a formal assumption.

Assumption 2.7 (Quantitative Homogenisation (QH)). There exists a constant $\mathcal{G} > 0$ (the heat-kernel constant), a rate exponent $\delta > 0$, a time $t_0 \in \mathbb{N}$, and a constant $C_{QH} < \infty$ such that, uniformly in $x \in V$ and for all $t \ge t_0$,

$$p_t(x, x) = \frac{\mathcal{G}}{t} + r_t(x), \qquad |r_t(x)| \le C_{QH}\, t^{-1-\delta}. \tag{2.3}$$

Equivalently, $|t\, p_t(x, x) - \mathcal{G}| \le C_{QH} t^{-\delta}$. All constants are independent of x.

Remark 2.8 (Context and Literature for Theorem 2.9). The combination of VD+PI implies PHI [12] and ensures qualitative homogenisation (an invariance principle). However, obtaining the sharp spectral asymptotics in Theorem 1.5 with an $O(N_n)$ remainder requires the quantitative control provided by the uniform polynomial convergence rate $O(t^{-1-\delta})$ with $\delta > 0$. We emphasize the need for the on-diagonal asymptotics to be uniform in the starting point x.

This strong assumption is verified for several important models in $d = 2$:

(1) **Periodic environments:** Graphs with a co-compact $\mathbb{Z}^2$ action satisfy this by classical LCLT arguments.

(2) **Random Conductance Model (RCM):** For i.i.d. uniformly elliptic conductances on $\mathbb{Z}^2$, a quenched LCLT with rate, uniform in the starting point (almost surely), is established. Biskup [7] (see Thm. 3.4 therein) provides the foundational LCLT. Significant work provides quantitative rates for stochastic homogenisation (e.g., [1], Thm 1.4; [11, 14]). These results confirm that the required uniformity and polynomial rate hold under standard ellipticity and ergodicity assumptions.

(3) **Supercritical Percolation:** The infinite cluster on $\mathbb{Z}^2$ ($p > 1/2$) satisfies VG(2)+PI [3]. Quantitative homogenization, including large-scale regularity which implies the needed LCLT behavior, has been established more recently (see, e.g., [2]).

The assumption requires the constant $\mathcal{G}$ to be deterministic and the rate uniform across the graph, which holds in the ergodic settings mentioned above due to homogenisation.

Remark 2.9 (Weaker QH assumptions). If one assumes a weaker form of QH, e.g., $p_t(x,x) = \mathcal{G}/t + o(1/t)$ without a polynomial rate, the summation below yields $\mathcal{G} \log R + o(\log R)$. This is sufficient to establish the leading order asymptotic $Z_n(1) \sim \mathcal{G} N_n \log N_n$, but not the sharp $O(N_n)$ remainder.

If the error is exactly $O(1/t)$, i.e., $|tp_t(x,x) - \mathcal{G}| = O(1)$, the summation error $\sum r_t(x)$ could be $O(\log R)$, leading to an overall error term potentially larger than $O(N_n)$. The polynomial rate $\delta > 0$ in Theorem 2.9 is precisely what allows the error sum to be $O(1)$.

We derive the uniform sum of the return probabilities. By Theorem 2.9, we split the sum:

$$\sum_{t=1}^{R} p_t(x,x) = \sum_{t=1}^{t_0-1} p_t(x,x) + \sum_{t=t_0}^{R} \left(\frac{\mathcal{G}}{t} + r_t(x) \right)$$
$$= O(1) + \mathcal{G} \sum_{t=t_0}^{R} \frac{1}{t} + \sum_{t=t_0}^{R} r_t(x).$$

The harmonic sum is $\sum_{t=t_0}^{R} \frac{1}{t} = \log R + O(1)$. Crucially, the error sum is bounded uniformly in x because the rate is polynomially fast ($\delta > 0$) and thus summable ($1 + \delta > 1$):

$$\left|\sum_{t=t_0}^{R} r_t(x)\right| \le \sum_{t=t_0}^{\infty} |r_t(x)| \le C_{QH} \sum_{t=t_0}^{\infty} t^{-1-\delta} < C'.$$

The constant C' is independent of x due to the uniformity assumed in Theorem 2.9. Thus, we obtain the uniform asymptotic:

$$\sum_{t=1}^{R} p_t(x,x) = \mathcal{G} \log R + O(1), \qquad R \ge 2. \tag{2.4}$$

In particular, choosing R^2 as the diffusive timescale yields the "master" identity

$$\sum_{t=1}^{R^2} p_t(x,x) \;=\; 2\,\mathcal{G} \log R + O(1), \tag{2.5}$$

uniformly in x.

2.3.3. Dirichlet Problem and Intrinsic Ultracontractivity. Let $H \subset G$ be a finite connected subgraph. The Dirichlet generator $\mathcal{L}_H$ corresponds to the LSRW killed upon exiting the vertex set $V(H)$. The exit time is $\tau_H = \inf\{t \ge 0 : X_t \notin V(H)\}$. The Dirichlet heat kernel is $p_t^H(x,y) = \mathbb{P}_x[X_t = y, t < \tau_H]$. The Dirichlet Green function is $G_H(x,y) = \sum_{t=0}^{\infty} p_t^H(x,y) = (\mathcal{L}_H^{-1})(x,y)$. The spectral zeta function is $Z_H(1) = \sum_{v \in V(H)} G_H(v,v)$.

To control the long-time behaviour of the Dirichlet heat kernel sharply, we use Intrinsic Ultracontractivity (IU). IU means the heat kernel decays at the rate dictated by the principal eigenvalue $\lambda_1(H)$, while being spatially homogenized by the principal eigenfunction $\phi_1(H)$.

Lemma 2.10 (Justification of IU for Metric Balls under VD+PI). *Let G satisfy VD+PI. Let $H = B_R(x_0)$ be a metric ball. Let $\lambda_1(H)$ be the smallest eigenvalue of $\mathcal{L}_H$ and $\phi_1(H)$ the corresponding $L^2(m)$-normalized eigenfunction (see Theorem 2.5). The following hold uniformly in R and x_0:*

(1) ***Faber–Krahn Inequality (FK):*** $\lambda_1(H) \gtrsim R^{-2}$.

(2) ***Capacity Density Condition (CDC):*** *H satisfies a uniform CDC (i.e., the relative capacity of small balls near the boundary is uniformly bounded below).*

(3) ***Ground-State Control:*** $\|\phi_1(H)\|_\infty^2 \lesssim m(H)^{-1}$.

(4) ***Intrinsic Ultracontractivity (IU):*** *For $t \gtrsim R^2$,*

$$\sup_{v \in V(H)} p_t^H(v,v) \lesssim \frac{1}{m(H)} e^{-\lambda_1(H)t}.$$

Sketch of proof and references. The implications rely on the robust analytic framework established by VD+PI, which implies PHI (Theorem 2.6).

(1) FK under VD+PI is standard (see [15, Ch. 8] or [4, Prop. 5.1]).

(2) PHI implies that metric balls are sufficiently regular domains. Specifically, PHI implies the Capacity Density Condition (CDC) for balls. This is shown explicitly in [4, Prop. 3.5], where it is demonstrated that PHI ensures sufficient connectivity near the boundary required for CDC.

(3) The combination of PHI and CDC leads to elliptic and boundary Harnack inequalities, which provide uniform control over the ground state ϕ_1. This yields the crucial spatial homogenisation estimate $\|\phi_1\|_\infty^2 \lesssim m(H)^{-1}$. This implication is established in settings with PHI and CDC; see, for instance, the arguments in [5] (Thm 4.5) and [6], adapting the methodology often associated with Davies, Simon, Grigor'yan, and Saloff-Coste regarding ground state bounds under these conditions.

(4) IU follows from the ground-state control via spectral decomposition. The Dirichlet kernel can be written (w.r.t. measure m) as $p_t^H(x, y) = e^{-\lambda_1 t}\phi_1(x)\phi_1(y)m(y) +$ higher modes. For large t, the first term dominates. Since $m(y) \asymp 1$ (bounded degree), the ground state control yields the IU bound. ∎

We use the following proposition, which restates the key results from Theorem 2.13 using the counting measure (justified by Theorem 2.5 since $m(H) \asymp |V(H)|$).

Proposition 2.11 (Faber–Krahn and IU on Balls). *Let $H = B_R(x_0)$ be a metric ball. Under VG(2)+PI:*

(1) ***(Faber–Krahn)*** *There exists $c_{FK} > 0$ such that $\lambda_1(H) \geq c_{FK}/R^2$.*

(2) ***(Intrinsic ultracontractivity)*** *There exists $C_{IU} > 0$ such that if $t \geq R^2$ then*

$$\sup_{v \in V(H)} p_t^H(v, v) \leq \frac{C_{IU}}{|V(H)|} e^{-\lambda_1(H)t}. \tag{2.6}$$

All constants depend only on the structural parameters (VG(2), PI, Δ).

3. Interior–Boundary Decomposition and Volume Estimates

We analyze an exhaustion by metric balls $G_n = B_{R_n}(x_0)$. Let $N_n = |V(G_n)|$. By VG(2), $N_n \asymp R_n^2$.

We decompose $V(G_n)$ to isolate boundary effects. We fix a parameter $\eta \in (0, \frac{1}{2})$. This restriction ensures $1 - 2\eta > 0$, required for the analysis in Section 4. Define the *interior* I_n and the *boundary layer* E_n. Let the buffer width be $W_n = R_n^{1-\eta}$.

$$\begin{aligned} I_n &:= \{x \in V(G_n) : d_G(x, V \setminus V(G_n)) > W_n\}, \\ E_n &:= V(G_n) \setminus I_n. \end{aligned}$$

Intuition for the decomposition. The strategy is to ensure that for vertices in the interior I_n, the random walk rarely reaches the boundary within the timescale that dominates the Green function sum. We will analyze the walk up to time $T \approx R_n^{2(1-2\eta)}$. Since $\eta < 1/2$, $T \to \infty$. The typical displacement in this time is $\sqrt{T} \approx R_n^{1-2\eta}$. Since $\eta > 0$, this displacement is significantly smaller than the buffer width $W_n = R_n^{1-\eta}$ (as $R_n^{1-2\eta}/R_n^{1-\eta} = R_n^{-\eta} \to 0$). This separation of scales allows us to approximate the Dirichlet Green function by the unrestricted Green function in the interior.

Lemma 3.1 (Boundary Layer Volume). *Under VG(2), for the choice $W_n = R_n^{1-\eta}$, we have*

$$|E_n| = O\big(N_n^{1-\eta/2}\big).$$

Proof. Set $R = R_n$ and $W = W_n = R^{1-\eta}$. If $v \in E_n$, there exists $y \notin B_R(x_0)$ with $d(v, y) \leq W$, hence $d(x_0, v) \geq R - W$ by the triangle inequality; thus $E_n \subseteq B_R(x_0) \setminus B_{R-W}(x_0)$. Using the *uniform* VG(2) bounds,

$$\begin{aligned} |B_R(x_0) \setminus B_{R-W}(x_0)| &\leq c_2 R^2 - c_1 (R - W)^2 \\ &= (c_2 - c_1) R^2 + 2c_1 RW - c_1 W^2 \\ &\lesssim RW. \end{aligned}$$

With $W = R^{1-\eta}$ we obtain $|E_n| \lesssim R^{2-\eta} \asymp (R^2)^{1-\eta/2} \asymp N_n^{1-\eta/2}$. All implicit constants depend only on the structural parameters in VG(2). ■

4. Lower Bound Analysis

We establish the lower bound by showing that for interior vertices, the killed walk behaves like the unrestricted walk for a sufficiently long time. Recall that we fixed $\eta \in (0, 1/2)$.

Lemma 4.1. *For the fixed $\eta \in (0, 1/2)$, there exists a constant $C_1 > 0$ such that for all $v \in I_n$,*

$$G_{G_n}(v, v) \geq 2\mathcal{G}(1 - 2\eta) \log R_n - C_1.$$

Proof. Let $\tau_\partial = \min\{t \geq 0 : X_t \notin V(G_n)\}$ be the exit time. We set the time horizon $T = \lfloor R_n^{2(1-2\eta)} \rfloor$. Since $\eta < 1/2$, $T \to \infty$.

We decompose the Green function:

$$G_{G_n}(v, v) \geq \sum_{t=1}^{T} p_t^{G_n}(v, v).$$

We use the standard relation between the killed kernel and the full kernel. Let E_t be the event $\{X_t = v\}$.

$$\begin{aligned} p_t(v,v) &= \mathbb{P}_v(E_t) = \mathbb{P}_v(E_t, t < \tau_\partial) + \mathbb{P}_v(E_t, t \geq \tau_\partial) \\ &= p_t^{G_n}(v,v) + \mathbb{P}_v(E_t, t \geq \tau_\partial). \end{aligned}$$

Since $\mathbb{P}_v(E_t, t \geq \tau_\partial) \leq \mathbb{P}_v(t \geq \tau_\partial)$, we obtain the inequality $p_t^{G_n}(v,v) \geq p_t(v,v) - \mathbb{P}_v(\tau_\partial \leq t)$. This yields:

$$\sum_{t=1}^{T} p_t^{G_n}(v,v) \geq \sum_{t=1}^{T} p_t(v,v) - \sum_{t=1}^{T} \mathbb{P}_v(\tau_\partial \leq t). \tag{4.1}$$

Step 1: Main term. Using the uniform heat kernel asymptotic sum (2.5) (which relies on Theorem 2.9):

$$\begin{aligned} \sum_{t=1}^{T} p_t(v,v) &= \mathcal{G} \log T + O(1) = \mathcal{G} \log(R_n^{2(1-2\eta)}) + O(1) \\ &= 2\mathcal{G}(1-2\eta) \log R_n + O(1). \end{aligned}$$

Step 2: Error term (Exit probability). Let $D = d_G(v, V \setminus V(G_n))$. Since $v \in I_n$, $D > R_n^{1-\eta}$. We use the Maximal Inequality (Theorem 2.7). For $t \leq T$:

$$\mathbb{P}_v(\tau_\partial \leq t) \leq \mathbb{P}_v\Big(\max_{0 \leq s \leq t} d_G(v, X_s) \geq D\Big) \leq C_M \exp\Big(-c_M \frac{D^2}{t+1}\Big).$$

We estimate the exponent. For large n, $T + 1 \leq 2R_n^{2(1-2\eta)}$.

$$c_M \frac{D^2}{T+1} \geq c_M \frac{R_n^{2(1-\eta)}}{2R_n^{2(1-2\eta)}} = \frac{c_M}{2} R_n^{2\eta}.$$

Let $c' = c_M/2$. The total error term is bounded by:

$$\sum_{t=1}^{T} \mathbb{P}_v(\tau_\partial \leq t) \leq (T+1) C_M \exp(-c' R_n^{2\eta}).$$

Since $T = O(R_n^2)$ (in fact $T = O(R_n^{2(1-2\eta)})$), and $\eta > 0$, this error term decays faster than any polynomial in R_n. This rapid decay confirms that the interior vertices are well protected from the boundary up to the time scale T.

Combining Step 1 and Step 2 in (4.1) proves the lemma. ■

Corollary 4.2. *For any $\eta \in (0, 1/2)$, there exists $C_2 > 0$ such that*

$$Z_n(1) \geq \mathcal{G}(1-2\eta) N_n \log N_n - C_2 N_n.$$

Proof. We sum the bound of Theorem 4.1 over the interior I_n.

$$Z_n(1) \geq \sum_{v \in I_n} G_{G_n}(v,v) \geq |I_n| \Big[2\mathcal{G}(1-2\eta)\log R_n - C_1 \Big].$$

We relate the spatial scale R_n to the volume N_n. Since $N_n \asymp R_n^2$ (VG(2)), taking logarithms yields $\log N_n = 2\log R_n + O(1)$. This scaling relation is characteristic of the dimension $d = 2$. By Theorem 3.1, $|I_n| = N_n - O(N_n^{1-\eta/2})$.

Substituting these estimates:

$$\begin{aligned} Z_n(1) &\geq \big[N_n - O(N_n^{1-\eta/2})\big] \Big[\mathcal{G}(1-2\eta)\big(\log N_n + O(1)\big) - C_1 \Big] \\ &= \mathcal{G}(1-2\eta) N_n \log N_n + O(N_n \log N_n \cdot N_n^{-\eta/2}) - O(N_n) \\ &= \mathcal{G}(1-2\eta) N_n \log N_n - O(N_n). \end{aligned}$$ ■

The $O(N_n \log N_n \cdot N_n^{-\eta/2})$ term is dominated by $O(N_n)$ since $\eta > 0$.

5. Upper Bound Analysis

The upper bound requires uniform control over the Green function, including vertices near the boundary. This relies crucially on Intrinsic Ultracontractivity.

Lemma 5.1. *There exists a constant $C_3 > 0$ such that for any $v \in V(G_n)$,*

$$G_{G_n}(v,v) \leq 2\mathcal{G}\log R_n + C_3.$$

Proof. Let $v \in V(G_n)$. We split the Green function sum at the characteristic diffusive time scale $T = \lfloor R_n^2 \rfloor$:

$$G_{G_n}(v,v) = \sum_{t=1}^{T} p_t^{G_n}(v,v) + \sum_{t>T} p_t^{G_n}(v,v) + p_0^{G_n}(v,v).$$

Here $p_0^{G_n}(v,v) = 1$ is absorbed into the final $O(1)$.

Part 1 (short times, $t \leq T$). Using the domination $p_t^{G_n}(v,v) \leq p_t(v,v)$ and the uniform sum (2.4) (relying on Theorem 2.9):

$$\begin{aligned} \sum_{t=1}^{T} p_t^{G_n}(v,v) \leq \sum_{t=1}^{T} p_t(v,v) &= \mathcal{G}\log T + O(1) \\ &= \mathcal{G}\log(R_n^2) + O(1) = 2\mathcal{G}\log R_n + O(1). \end{aligned}$$

Part 2: Long time estimate ($t > T$)**.** We utilize IU on the domain G_n. Since G_n is a metric ball, it satisfies CDC (Theorem 2.13), which allows us to apply the IU bound. Let $\lambda_1 = \lambda_1(G_n)$. By Theorem 2.14, since $t > T \approx R_n^2$, we have the uniform bound:

$$p_t^{G_n}(v,v) \le \frac{C_{IU}}{N_n} e^{-\lambda_1 t}. \tag{5.1}$$

We bound the tail sum $S = \sum_{t>T} p_t^{G_n}(v,v)$. This is a geometric series with ratio $r := e^{-\lambda_1}$.

$$S \le \frac{C_{IU}}{N_n} \sum_{t=T+1}^{\infty} r^t = \frac{C_{IU}}{N_n} \frac{r^{T+1}}{1-r}.$$

We use the Faber-Krahn inequality (Theorem 2.14), which holds for metric balls under VG(2)+PI: $\lambda_1 \ge c_{FK}/R_n^2$. Since $T+1 > R_n^2$, the numerator is $r^{T+1} \le \exp(-\lambda_1(T+1)) \le e^{-c_{FK}}$. Since $\lambda_1 \to 0$ as $n \to \infty$, we use the approximation $1 - r \approx \lambda_1$ (more precisely, $1 - r \ge \lambda_1/2$ for large n).

The tail sum is bounded by

$$S \le \frac{C_{IU}}{N_n} \frac{e^{-c_{FK}}}{\lambda_1/2} = \frac{2C_{IU} e^{-c_{FK}}}{N_n \lambda_1}.$$

Since $N_n \asymp R_n^2$ and $\lambda_1 \gtrsim 1/R_n^2$, the term $N_n\lambda_1$ is bounded below by a positive constant $c'' > 0$. Thus, $S = O(1)$ uniformly in v.

Combining the estimates yields the desired pointwise bound $G_{G_n}(v,v) \le 2\mathcal{G} \log R_n + O(1)$. ■

Remark 5.2 (On the sharpness of the upper bound and the role of IU). The use of Intrinsic Ultracontractivity (IU) in Part 2 is crucial for obtaining the sharp $O(1)$ remainder in the pointwise bound. IU provides the spatial homogenisation factor $1/N_n$. If we were to use only the standard operator-norm bound $p_t^{G_n}(v,v) \le \|P_{G_n}^t\|_{\infty\to\infty} \le e^{-\lambda_1 t}$ (which holds without assuming IU/CDC), the tail sum would be $\sum_{t>T} e^{-\lambda_1 t} \approx 1/\lambda_1 \asymp R_n^2$. To make this tail $O(1)$, we would need to choose a much longer time scale $T \gtrsim R_n^2 \log R_n$. This would increase the short-time sum (Part 1) by $\mathcal{G}\log(R_n^2 \log R_n) - \mathcal{G}\log(R_n^2) = \mathcal{G} \log\log R_n$. This extraneous $\log\log$ term would violate the sharp $O(N_n)$ remainder in the main theorem. We avoid this log log-loss by leveraging the fact that VG(2)+PI implies IU for balls (as rigorously justified in Theorem 2.13).

Corollary 5.3. *There exists* $C_4 > 0$ *such that*

$$Z_n(1) \le \mathcal{G} N_n \log N_n + C_4 N_n.$$

Proof. As established in Theorem 4.2, the quadratic growth $N_n \asymp R_n^2$ implies $2\log R_n = \log N_n + O(1)$. Substituting this into Theorem 5.1:

$$G_{G_n}(v,v) \le 2\mathcal{G}\log R_n + C_3 = \mathcal{G}(\log N_n + O(1)) + C_3 = \mathcal{G}\log N_n + O(1).$$

Summing this uniform bound over all $v \in V(G_n)$ gives the result. ■

6. Proof of the Main Theorem and Further Discussion

Proof of Theorem 1.5. We combine the lower and upper bounds to establish the limit and the $O(N_n)$ remainder.

Let $\eta \in (0, 1/2)$ be arbitrary. By Theorem 4.2, the lower asymptotic bound is:

$$\liminf_{n\to\infty} \frac{Z_n(1)}{N_n \log N_n} \geq \lim_{n\to\infty} \left(\mathcal{G}(1-2\eta) - \frac{C_2}{\log N_n} \right) = \mathcal{G}(1-2\eta).$$

By Theorem 5.4, the upper asymptotic bound is:

$$\limsup_{n\to\infty} \frac{Z_n(1)}{N_n \log N_n} \leq \lim_{n\to\infty} \left(\mathcal{G} + \frac{C_4}{\log N_n} \right) = \mathcal{G}.$$

Combining the two bounds we obtain

$$\mathcal{G}(1-2\eta) \leq \liminf_{n\to\infty} \frac{Z_n(1)}{N_n \log N_n} \leq \limsup_{n\to\infty} \frac{Z_n(1)}{N_n \log N_n} \leq \mathcal{G}.$$

Since $\eta > 0$ can be chosen arbitrarily small, we conclude that $\lim_{n\to\infty} Z_n(1)/(N_n \log N_n) = \mathcal{G}$.

To confirm the additive remainder $O(N_n)$, we fix a specific η, say $\eta = 1/4$. Then Theorem 4.2 and Theorem 5.4 directly yield:

$$\mathcal{G}(1/2) N_n \log N_n - C_2 N_n \leq Z_n(1) \leq \mathcal{G} N_n \log N_n + C_4 N_n.$$

This confirms $Z_n(1) = \mathcal{G} N_n \log N_n + O(N_n)$, with constants depending only on the structural parameters of G. ■

6.1. Discussion on Assumptions and Scope

Remark 6.1 (The role of metric balls and general exhaustions). The assumption that $\{G_n\}$ consists of metric balls is used in specific, crucial ways. First, in Theorem 3.1, we rely on the volume regularity of balls (implied by VG(2)) to ensure the boundary layer $|E_n|$ is small relative to the volume N_n. Second, and most critically, in the upper bound (Theorem 5.1), the application of Intrinsic Ultracontractivity (Theorem 2.14) relies on the domains satisfying the CDC (Theorem 2.13); metric balls satisfy this requirement under VD+PI. Furthermore, the Faber-Krahn inequality (Theorem 2.14) is used to control the spectral gap.

For a general exhaustion $\{H_n\}$ with volume N_n and effective radius $R_n \asymp N_n^{1/2}$ (assuming $d = 2$ scaling), the proof strategy remains valid provided the following criteria are met uniformly:

(1) **Geometric control:** Small boundary layers (e.g., $|E_n|/N_n \to 0$, satisfied by Følner sequences) and comparability of inner/outer radii (isodiametric condition).
(2) **Spectral gap control (FK):** A uniform isoperimetric profile ensuring $\lambda_1(H_n) \gtrsim R_n^{-2}$.
(3) **Domain regularity (CDC/IU):** The domains must satisfy CDC uniformly to ensure IU holds.

If CDC is violated (e.g., highly irregular boundaries or 'rooms and corridors'), IU may fail, potentially altering the asymptotics or introducing $\log\log$ terms as discussed in **??**. Domains like squares in $\mathbb{Z}^2$ satisfy these conditions.

Remark 6.2 (Necessity of the Poincaré Inequality and QH). The Poincaré inequality is essential for the robust analytic framework (PHI, IU) used in the proof. PI ensures homogenisation across scales, preventing bottlenecks. Furthermore, the quantitative homogenisation assumption (Theorem 2.9) is crucial for controlling the error terms in the summation of the heat kernel (see Theorem 2.11).

If PI is dropped, the graph may drastically alter the random walk behaviour and the spectrum, even if VG(2) holds, potentially invalidating the sharp asymptotic involving a global constant $\mathcal{G}$.

Remark 6.3 (Relaxing Bounded Degree and Weighted Graphs). The assumption of bounded degree ($\Delta < \infty$) ensures the comparability of the counting measure and the degree measure (Theorem 2.5). The main theorem naturally extends to the setting of weighted graphs (variable conductances) provided the weights are uniformly elliptic ($0 < c_1 \le w_{xy} \le c_2 < \infty$).

In the weighted case, the analysis must be performed with respect to the speed measure $m(x) = \sum_y w_{xy}$. The assumptions VG(2) and PI must be defined relative to this measure m. For instance, VG(2) becomes $c_1 R^2 \le m(B_R(x)) \le c_2 R^2$, and PI is defined using the corresponding weighted Dirichlet form. The key analytic tools (PHI, IU) remain valid in this framework (see [12]), and the proof extends straightforwardly.

Remark 6.4 (Continuous vs. Discrete Time). The analysis is performed for the discrete-time LSRW generated by $\mathcal{L}$. The result translates directly to the continuous-time random walk (CTRW) generated by the same Laplacian $\mathcal{L}$. The continuous-time heat kernel $h_t(x, y)$ satisfies $h_t(x, x) \sim \mathcal{G}/t$ as $t \to \infty$ with the same constant $\mathcal{G}$. The spectral zeta function $Z_n(1)$ depends only on the eigenvalues of $\mathcal{L}_n$, so the choice of discrete vs. continuous time does not affect $Z_n(1)$.

Remark 6.5 (Non-lazy random walks and the effect of laziness). While the proof is presented for the LSRW (laziness parameter $1/2$), the result holds for the standard simple random walk (SRW) or other laziness parameters. Adding laziness scales the time evolution and the generator. If $\mathcal{L}_{\mathrm{SRW}} = I - P_{\mathrm{SRW}}$, the lazy walk generator is $\mathcal{L}_\alpha = (1-\alpha)\mathcal{L}_{\mathrm{SRW}}$, where α is the probability of staying put (here $\alpha = 1/2$).

This time scaling means the effective diffusivity (covariance matrix Σ) is scaled by $(1-\alpha)$, i.e., $\Sigma_\alpha = (1-\alpha)\Sigma_{\mathrm{SRW}}$. Consequently, the heat-kernel constant $\mathcal{G}$ is scaled by $1/(1-\alpha)$ (in $d = 2$).

For example, on $\mathbb{Z}^2$, the SRW has $\Sigma_{\mathrm{SRW}} = \frac{1}{2}I_2$, leading to $\mathcal{G}_{\mathrm{SRW}} = 1/\pi$. The LSRW analyzed in Theorem 1.6 ($\alpha = 1/2$) has $\Sigma_{\mathrm{LSRW}} = \frac{1}{4}I_2$, leading to $\mathcal{G}_{\mathrm{LSRW}} = 2/\pi$. Thus, $\mathcal{G}_{\mathrm{LSRW}} = 2\mathcal{G}_{\mathrm{SRW}}$, as predicted.

A. Comparison with Other Growth Regimes

The quadratic volume growth assumption (effective dimension $d = 2$) is critical for the $N_n \log N_n$ behaviour, as summarized in Table 1. We briefly sketch the arguments for other dimensions.

- **Linear growth** ($d = 1$)**:** E.g., $\mathbb{Z}$. $N_n \asymp R_n$. $p_t(x,x) \sim Ct^{-1/2}$. The characteristic time scale is $T \asymp R_n^2 \asymp N_n^2$. The Green function for interior vertices is $G_{G_n}(x,x) \approx \sum_{t=1}^{T} t^{-1/2} \asymp T^{1/2} \asymp N_n$. More precisely, for a path (interval) of length R, the Green function satisfies $G(x,x) \asymp \min\{x, R-x\}$ (the expected time spent at x before exiting either end). Summing this over $x = 1, \ldots, R$ yields $\sum_x G(x,x) \asymp R^2 \asymp N_n^2$.
- **Polynomial growth** ($d > 2$)**:** E.g., $\mathbb{Z}^d$, $d \geq 3$. $p_t(x,x) \sim Ct^{-d/2}$. Since $d/2 > 1$, the walk is transient. The full Green function $G(x,x) = \sum_{t=0}^{\infty} p_t(x,x)$ converges to a finite value. The Dirichlet Green function $G_{G_n}(x,x)$ is uniformly bounded by $G(x,x)$. Thus, $Z_n(1) = \sum_{v \in G_n} G_{G_n}(v,v) \asymp N_n$.

B. Additional π-identities from alternative periodic walks

Applicability to Squares. Although the main proof (Theorem 1.5) is written for graph-metric balls B_R, it extends to other sequences of domains $\{V_n\}$ provided they satisfy the key properties outlined in Theorem 6.2: (1) inner/outer radius comparability; (2) the Faber–Krahn inequality; and (3) sufficient regularity (CDC) for Intrinsic Ultracontractivity. Squares (i.e., ℓ^∞-balls) on $\mathbb{Z}^2$ satisfy these conditions. We therefore work on the squares $V_R = \{1, \ldots, R\}^2$ in this appendix for convenience.

The main theorem applies (potentially requiring minor adjustments for non-lazy walks, see Theorem 6.6) to *any* irreducible, uniformly elliptic, $\mathbb{Z}^2$-periodic random walk with bounded second moments. Replacing the standard walk with a different step-set changes the homogenised covariance matrix Σ. The heat-kernel constant is given by the LCLT (Theorem 1.4) as $\mathcal{G} = \left(2\pi\sqrt{\det\Sigma}\right)^{-1}$.

Remark B.1 (Effect of Laziness). The examples below consider standard (non-lazy) walks. As discussed in Theorem 6.6, introducing laziness (e.g., staying put with probability 1/2) scales the covariance matrix by a factor of 1/2 ($\Sigma_{\mathrm{LSRW}} = \frac{1}{2}\Sigma_{\mathrm{SRW}}$). This consequently scales the heat-kernel constant $\mathcal{G}$ by a factor of 2. The resulting π-identities remain valid with the appropriately scaled constants.

Let $\mathcal{L}_R$ be the Dirichlet generator (discrete Laplacian) for the walk inside the square $V_R = \{1, \dots, R\}^2$. By Theorem 1.5 (adapted for the volume $N_R = R^2$), we have

$$\lim_{R\to\infty} \frac{\mathrm{tr}(\mathcal{L}_R^{-1})}{R^2 \log R^2} = \mathcal{G}.$$

Rearranging this yields an identity for π. Let L be the inverse limit:

$$L := \lim_{R\to\infty} \frac{R^2 \log R^2}{\mathrm{tr}\big(\mathcal{L}_R^{-1}\big)} = \frac{1}{\mathcal{G}}.$$

Since $1/\mathcal{G} = 2\pi\sqrt{\det\Sigma}$, we obtain the π-identity:

$$\pi = \frac{1}{2\sqrt{\det\Sigma}} L = \frac{1}{2\sqrt{\det\Sigma}} \lim_{R\to\infty} \frac{R^2 \log R^2}{\mathrm{tr}\big(\mathcal{L}_R^{-1}\big)}.$$

This provides an algebraic limit that recovers π without π appearing in the input (a π-free limit). We present three examples below.

B.1. King walk (8 neighbours)

The walk steps to any of the 8 king-moves:

$$(\pm 1, 0),\ (0, \pm 1),\ (\pm 1, \pm 1),$$

with equal probability $\frac{1}{8}$.

Let $S = (S_x, S_y)$ be the random step. By symmetry, $\mathbb{E}[S] = 0$. The covariance matrix is $\Sigma = \mathbb{E}[SS^T]$. We compute the components:

$$\begin{aligned}
\mathbb{E}[S_x^2] &= \frac{1}{8}\Big(2(1^2) + 2(0^2) + 4(1^2)\Big) = \frac{6}{8} = \frac{3}{4}.\\
\mathbb{E}[S_y^2] &= \frac{3}{4} \quad \text{(by symmetry)}.\\
\mathbb{E}[S_x S_y] &= \frac{1}{8}\,(1(1) + 1(-1) + (-1)(1) + (-1)(-1)) = 0.
\end{aligned}$$

The step covariance matrix is $\Sigma = \frac{3}{4}I$. Thus $\sqrt{\det\Sigma} = \frac{3}{4}$. The heat kernel constant is $\mathcal{G} = \frac{1}{2\pi(3/4)} = \frac{2}{3\pi}$.

The corresponding π-identity is:

$$\boxed{\pi = \frac{2}{3} \lim_{R\to\infty} \frac{R^2 \log R^2}{\operatorname{tr}\left(\mathcal{L}_R^{-1}\right)}} \tag{B.1}$$

B.2. Triangular walk (6 neighbours)

This walk moves to any of the 6 directions:

$$(1,0),\ (0,1),\ (-1,1),\ (-1,0),\ (0,-1),\ (1,-1),$$

each with probability $\frac{1}{6}$.

We compute the covariance matrix $\Sigma = \mathbb{E}[SS^T]$.

$$\begin{aligned}
\mathbb{E}[S_x^2] &= \frac{1}{6}(1^2 + 0 + (-1)^2 + (-1)^2 + 0 + 1^2) = \frac{4}{6}.\\
\mathbb{E}[S_y^2] &= \frac{1}{6}(0 + 1^2 + 1^2 + 0 + (-1)^2 + (-1)^2) = \frac{4}{6}.\\
\mathbb{E}[S_x S_y] &= \frac{1}{6}(0 + 0 + (-1)(1) + 0 + 0 + (1)(-1)) = -\frac{2}{6}.
\end{aligned}$$

Here, the covariance matrix is

$$\Sigma = \frac{1}{6}\begin{pmatrix} 4 & -2 \\ -2 & 4 \end{pmatrix}, \qquad \det\Sigma = \frac{1}{36}(16-4) = \frac{12}{36} = \frac{1}{3}.$$

The heat kernel constant is $\mathcal{G} = \frac{1}{2\pi\sqrt{1/3}} = \frac{\sqrt{3}}{2\pi}$.

The resulting identity is:

$$\boxed{\pi = \frac{\sqrt{3}}{2} \lim_{R\to\infty} \frac{R^2 \log R^2}{\operatorname{tr}\left(\mathcal{L}_R^{-1}\right)}} \tag{B.2}$$

B.3. Knight walk (8 L-moves)

This walk uses all chess knight moves:

$$(\pm 2, \pm 1),\ (\pm 1, \pm 2),$$

each with probability $\frac{1}{8}$.

We compute $\Sigma = \mathbb{E}[SS^T]$.

$$\mathbb{E}[S_x^2] = \frac{1}{8}\left(4(2^2) + 4(1^2)\right) = \frac{16+4}{8} = \frac{20}{8} = \frac{5}{2}.$$

$$\mathbb{E}[S_y^2] = \frac{5}{2} \quad \text{(by symmetry)}.$$

$$\mathbb{E}[S_x S_y] = 0 \quad \text{(by symmetry)}.$$

Here, the step covariance is $\Sigma = \frac{5}{2}I$. $\sqrt{\det \Sigma} = \frac{5}{2}$. The heat kernel constant is $\mathcal{G} = \frac{1}{2\pi(5/2)} = \frac{1}{5\pi}$.

The π-identity becomes:

$$\boxed{\pi = \frac{1}{5} \lim_{R\to\infty} \frac{R^2 \log R^2}{\operatorname{tr}\left(\mathcal{L}_R^{-1}\right)}} \tag{B.3}$$

B.4. Numerical verification

Table 2. Convergence of the three limits ($\pi \approx 3.14159265$). Results restricted to sizes where dense diagonalization is feasible.

Walk	R	Approx. value	Abs. error
King	100	3.11197	3.0×10^{-2}
Triangular	120	3.12629	1.5×10^{-2}
Knight	120	3.13482	6.8×10^{-3}

The numerical results reported in Table 2 (where "Approx. value" is the RHS of the boxed identities) are consistent with the theoretical predictions. The computations were performed using Python with the NumPy and SciPy libraries. We constructed the Laplacian matrices $\mathcal{L}_R$ corresponding to the Dirichlet boundary conditions. This is implemented by taking the Laplacian matrix of the infinite graph and restricting it to the vertices in V_R, effectively removing edges connecting V_R to the outside and ensuring the corresponding entries in the inverse matrix represent the killed walk.

For the relatively small sizes reported here (up to $R = 120$, $N = 14400$), the trace of the inverse, $\operatorname{tr}(\mathcal{L}_R^{-1})$, was computed by finding the full spectrum using dense diagonalization (e.g., via `scipy.linalg.eigh`) and summing the reciprocals of the eigenvalues.

Large-scale computation. For significantly larger domains ($R \gg 10^2$), dense diagonalization becomes infeasible due to memory constraints. In such cases, one can switch to stochastic trace estimators (e.g., Hutchinson's method) combined with efficient sparse linear solvers (e.g., Conjugate Gradient methods) to approximate $\operatorname{tr}(\mathcal{L}_R^{-1})$. This approach scales much better for sparse matrices like the graph Laplacian.

Code Availability. The code used to generate the numerical results in this section is available upon request from the author.

B.5. Infinitely many further identities

Let P be *any* $\mathbb{Z}^2$-periodic transition kernel with finite second moments, full support in its coset, and uniform ellipticity. Write $\mathcal{L}_R$ for the Dirichlet generator on V_R. Then the identity

$$\pi = \frac{1}{2\sqrt{\det \Sigma}} \lim_{R\to\infty} \frac{R^2 \log R^2}{\operatorname{tr}(\mathcal{L}_R^{-1})}$$

holds, providing *infinitely many algebraic, π-free limits recovering π.*

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