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Fluctuation results for size of the vacant set for random walks on discrete torus

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Abstract. We consider one or more independent random walks on the $d \geqslant 3$ dimensional discrete torus. The walks start from vertices chosen independently and uniformly at random. We analyze the fluctuation behavior of the size of some random sets arising from the trajectories of the random walks at a time proportional to the size of the torus. Examples include vacant sets and the intersection of ranges. Interestingly, unlike the random interlacement model, the fluctuation order has no phase transition. The proof relies on a refined analysis of tail estimates for hitting time and can be applied to other vertex-transitive graphs.

1. Introduction

Consider finitely many independent random walks on the $d \geqslant 3$ dimensional discrete torus with large side length, each starting from vertices chosen independently and uniformly at random. We are interested in the mean and fluctuation behavior of the size of some random sets arising from the trajectories of the random walks at a time proportional to the size of the torus. Examples include the vacant set or the set of vertices not visited by any of the walks and the size of the intersection of ranges, among others.

In particular, we fix a positive integer $\ell \geqslant 1$, where ℓ denotes the number of independent random walks. The discrete torus is denoted by $\mathbb{Z}_n^d = (\mathbb{Z}/n\mathbb{Z})^d$, with side length n. Note that n controls the size of the graph, and we are interested in the large n limit with a fixed d. We consider ℓ many independent $\frac{1}{2}$–lazy random walks $(X_{t,i})_{t\geqslant 0}, i \in [\ell] := \{1, 2, \dots, \ell\}$ starting from $X_{0,i} = \xi_i, i \in [\ell]$, respectively, where ξ_i's are i.i.d. uniformly distributed over $\mathbb{Z}_n^d$. We will use $\pi = \pi_n$ to denote the uniform distribution over $\mathbb{Z}_n^d$.

We define the range of the i-th random walk at time t as

$$\mathcal{R}_i(t) := \{X_{s,i} \mid s = 0, 1, \dots, t\} \quad \text{for } i = 1, 2, \dots, \ell; \tag{1.1}$$

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the size of vacant set, *i.e.*, the number of vertices not visited by any of the ℓ walks at time t as

$$V_n^{(\ell)}(t) := \left|\mathbb{Z}_n^d \setminus \cup_{i=1}^{\ell} \mathcal{R}_i(t)\right|, \tag{1.2}$$

and the size of the intersection of ranges at time t as

$$R_n^{(\ell)}(t) := \left|\cap_{i=1}^{\ell} \mathcal{R}_i(t)\right|. \tag{1.3}$$

If we define $\tau_i(v)$ as the hitting time at the vertex v for the i-th random walk, *i.e.*,

$$\tau_i(v) := \min\{t \geqslant 0 \mid X_{t,i} = v\},$$

then we have for all $t \geqslant 0$

$$V_n^{(\ell)}(t) = \sum_{v\in\mathbb{Z}_n^d}\prod_{i=1}^{\ell} \mathbf{1}_{\{\tau_i(v)>t\}} \text{ and } R_n^{(\ell)}(t) = \sum_{v\in\mathbb{Z}_n^d}\prod_{i=1}^{\ell} \mathbf{1}_{\{\tau_i(v)\leqslant t\}}.$$

One can easily check that

$$\mathbb{E}\, V_n^{(\ell)}(t) = n^d\, \mathbb{P}_\pi(\tau_1(0) > t)^\ell \text{ and } \mathbb{E}\, R_n^{(\ell)}(t) = n^d\, \mathbb{P}_\pi(\tau_1(0) \leqslant t)^\ell.$$

In particular when $t/n^d \to u$ we have $n^{-d}\,\mathbb{E}\, V_n^{(\ell)}(t) \to e^{-\ell u/G(0)}$ and $n^{-d}\,\mathbb{E}\, R_n^{(\ell)}(t) \to (1 - e^{-u/G(0)})^\ell$ as $n \to \infty$ where

$$G(\xi) = G_{1/2}(\xi) = \text{ expected number of visits to } \xi$$
$$\text{for a } 1/2\text{–lazy random walk on } \mathbb{Z}^d \text{ starting from } 0.$$

The above result follows from standard literature, for instance see Brummelhuis and Hilhorst (1991, Equation (2.26)), Aldous and Brown (1992, Theorem 1) or Teixeira and Windisch (2011, Proposition 3.7). Moreover, for an ε–lazy random walk, one can easily check that $G_\varepsilon(\cdot) = (1-\varepsilon)^{-1}G_*(\cdot)$, where G_* is the classical Green's function for the simple random walk on $\mathbb{Z}^d$. If needed, we will use $G(0;\mathbb{Z}^d)$ instead of $G(0)$ to emphasize the dependence on the dimension d.

For $\xi \in \mathbb{Z}_n^d$, we define

$$g_n(\xi) := \sum_{t=0}^{\infty}(\mathbb{P}_0(X_t = \xi) - \mathbb{P}_\pi(X_t = \xi))$$
$$\text{and } g_n'(\xi) := \sum_{t=1}^{\infty} t(\mathbb{P}_0(X_t = \xi) - \mathbb{P}_\pi(X_t = \xi)).$$

Note that, heuristically $g_n(0)$ is the difference between the expected number of visits to 0 by two $\frac{1}{2}$–lazy random walks on $\mathbb{Z}_n^d$ starting from the origin and the uniform distribution, respectively, up to a large multiple of the mixing time. Moreover, for fixed $\xi \in \mathbb{Z}^d$, we have $g_n(\xi) \to G(\xi)$ as $n \to \infty$. One can easily check that

$$g_n'(0) = \sum_{\xi\in\mathbb{Z}_n^d} g_n(\xi)^2 - g_n(0) > 0.$$

We remark that $g_n'(0)$ stays bounded in $d \geqslant 5$ and $g_n'(0)$ grows at rate $\log n$ when $d = 4$, and at rate n when $d = 3$. See Lemma 2.1 for an upper bound on the growth rate of $g_n(\xi)$ and $g_n'(\xi)$. We write down the mean behavior with first-order correction in the following Lemma.

Lemma 1.1. *Let $d \geqslant 3$ and $\ell \geqslant 1$ be fixed. Define $u := (t+1)/n^d \in (0,\infty)$, then*

$$\mathbb{E}(V_n^{(\ell)}(t)) = n^d e^{-\frac{\ell u}{g_n(0)}} + \ell\left(\frac{u g_n'(0)}{g_n(0)^3} + \frac{u}{2g_n(0)^2} - \frac{g_n'(0)}{g_n(0)^2}\right) + O(n^{-d+3}).$$

Our first main result is the following explicit variance for $V_n^{(\ell)}(t)$. Define

$$\sigma_{n,\ell}^2(t) := \operatorname{Var}(V_n^{(\ell)}(t)). \tag{1.4}$$

Theorem 1.2. *Let $d \geqslant 5$ and $\ell \geqslant 1$ be fixed. Assume that $t/n^d \to u \in (0,\infty)$. There exists a function $\nu_d : (0,\infty) \to (0,\infty)$ such that*

$$\lim_{n\to\infty} \frac{1}{n^d}\sigma^2_{n,\ell}(t) = \nu_d(2\ell u/G(0)).$$

Moreover, we have an explicit formula for $\nu_d(u)$ given by

$$\nu_d(u) = e^{-u} \sum_{\xi\in\mathbb{Z}^d} \left(\exp\left(\frac{uG(\xi)}{G(0)+G(\xi)}\right) - 1 - \frac{uG(\xi)}{G(0)+G(\xi)} + \frac{uG(\xi)^2(G(\xi)-\mathbb{1}_{\{\xi=0\}})}{G(0)^2(G(0)+G(\xi))} \right). \tag{1.5}$$

Note that the limiting variance in (1.5) is strictly positive as $e^x - 1 - x \geqslant x^2/2 > 0$ for $x > 0$ and $G(0) > 1$. Also, it is finite as $\sum_{\xi\in\mathbb{Z}^d} G(\xi)^2 < \infty$ for $d \geqslant 5$.

One can see from the proof of Theorem 1.2 that $n^{-d}\sigma^2_{n,\ell}(t)$ is governed by $\sum_{\xi\in\mathbb{Z}^d_n} g_n(\xi)^2$. This sum can be written as $g_n'(0) + g_n(0)$, whose growth rate is

$$h_d(n) := \begin{cases} n & \text{when } d = 3, \\ \log n & \text{when } d = 4 \text{ and,} \\ 1 & \text{when } d \geqslant 5. \end{cases}$$

Thus, it is expected that the correct scaling order for the variance is n^4 when $d = 3$ and $n^4 \log n$ when $d = 4$, and heuristically the variance with right scaling converges to the sum of the second order term of the exponential in (1.5). The following theorem affirms that this is indeed the case.

Theorem 1.3. *Let $d \in \{3,4\}$ and $\ell \geqslant 1$ be fixed. Assume that $t/n^d \to u \in (0,\infty)$. Then we have*

$$\lim_{n\to\infty} \frac{1}{n^d h_d(n)}\sigma^2_{n,\ell}(t) = \nu_d(2\ell u/G(0)).$$

where $h_3(n) = n$, $h_4(n) = \log n$,

$$\nu_d(u) = \frac{1}{2}\alpha_d u^2 e^{-u}, \tag{1.6}$$

and

$$\alpha_3 := \frac{9}{\pi^4 \cdot G(0;\mathbb{Z}^3)^2} \sum_{v\in\mathbb{Z}^3} \|v\|^{-4}, \quad \alpha_4 := \frac{16}{\pi^4 \cdot G(0;\mathbb{Z}^4)^2} \lim_{n\to\infty} \frac{1}{\log n} \sum_{\|v\|\leqslant n} \|v\|^{-4}.$$

One can quickly check that the limit in α_4 exists and is finite. Note that this constant also appears in the fluctuation behavior for competing random walks in Miller (2013).

Remark 1.4. *One can extend the fluctuation behavior of the vacant set from discrete-time random walks to continuous-time random walks. Let $(T(s))_{s\geqslant 0}$ be a Poisson process with intensity 1, independent of X_t. Let $Y_s = X_{T(s)}$ and $\widetilde{V}_n^{(\ell)}(t)$ be the vacant set of Y_s up to time t. Then, the variance of $\widetilde{V}_n^{(\ell)}(t)$ can be computed via conditioning with Lemma 1.1 and Theorems 1.2, 1.3. Indeed, it follows that*

$$\mathrm{Var}(\widetilde{V}_n^{(\ell)}(t)) = \mathbb{E}(\mathrm{Var}(\widetilde{V}_n^{(\ell)}(t) \mid T(t) = s)) + \mathrm{Var}(\mathbb{E}(\widetilde{V}_n^{(\ell)}(t) \mid T(t) = s)),$$

for $t \approx un^d$. Then, we apply the fluctuation results for $V_n^{(\ell)}(s)$.

Remark 1.5. *We remark that the order of the variance $\sigma^2_{n,\ell}(t)$ at $t \approx un^d$ is the same as that of the variance for competing random walks in Miller (2013). Unlike our proof, which relies on an elementary and analytic approach using the generating function of hitting probabilities, Miller (2013) made use of the conditioning argument at the mixing time to obtain the cancellation in the expansion of the variance, which leads to the precise asymptotic for the variance. It would be interesting to get a probabilistic proof and interpretation of our results on the asymptotic of the variance $\sigma^2_{n,\ell}(t)$.*

We can generalize the above result to the size of the intersection of ranges and similar sets in the following way. For any subset $I \subseteq [\ell]$, we define

$$R^I_{n,\ell}(t) := \sum_{v\in\mathbb{Z}^d_n} \prod_{i\in I} \mathbf{1}_{\{\tau_i(v)\leqslant t\}} \prod_{j\in I^c} \mathbf{1}_{\{\tau_j(v)>t\}}$$

as the number of vertices in $\mathbb{Z}^d_n$ that are visited by walks indexed by I but not by walks indexed by $[\ell]\setminus I$ at time t. We define the random vector indexed by $I \subseteq [\ell]$

$$\boldsymbol{R}_{n,\ell}(t) := (R^I_{n,\ell}(t))_{I\subseteq[\ell]}.$$

Note that $R^{\emptyset}_{n,\ell}(t) = V^{(\ell)}_n(t)$ and $R^{[\ell]}_n(t) = R^{(\ell)}_n(t)$ as defined in (1.2) and (1.3). We can compute the variance-covariance structure for the random vector $\boldsymbol{R}_{n,\ell}(t)$ when $t \approx un^d$.

Theorem 1.6. *For $I, J \subseteq [\ell]$ and $t/n^d \to u \in (0,\infty)$, we have*

$$\begin{aligned}\lim_{n\to\infty} &\frac{1}{n^d h_d(n)} \operatorname{Cov}(R^I_{n,\ell}(t), R^J_{n,\ell}(t)) \\ &= \sum_{m=0}^{|I\cup J|} \theta_{k,r,m}(\exp(-u/G(0)))\cdot \nu_d(2(\ell-m)u/G(0))\end{aligned}$$

where $k = |I\cap J|, r = |I\Delta J|$, $\nu_d(\cdot)$ is as given by (1.5)–(1.6), and

$$\theta_{k,r,m}(a) := \sum_{j=(m-k)_+}^{r\wedge m} \binom{k}{m-j}\binom{r}{j}(1-2a)^{m-j}(-1)^{r-j}a^j.$$

Remark 1.7. *Under suitable assumptions, our analysis could be applied to general vertex-transitive graphs with $g_n(0)$ bounded above. In particular, we consider the vacant set of an ε–lazy random walk on the hyper-cube $\mathbb{Z}^n_2$. Since we have explicit formulas for the Green's function, the eigenvalues, and the eigenfunctions as in Chung and Yau (2000, Section 7), we can apply our method to obtain the fluctuation behavior of the vacant set as $n\to\infty$. Suppose $\xi \in \mathbb{Z}^n_2$ belongs to the k-th level for $0 \leqslant k \leqslant n$, then the Green's function is given by*

$$\begin{aligned}g_n(\xi) &= \frac{1}{(1-\varepsilon)2^n} \sum_{v\in\mathbb{Z}^n_2, v\neq 0} \frac{n}{\|v\|_1}\cdot(-1)^{\langle v,\xi\rangle} \\ &= \frac{1}{(1-\varepsilon)2^n}\left(\sum_{i=1}^n \frac{n}{i}\binom{n}{i} - 2\sum_{i=1}^k \frac{1}{\binom{n-1}{i-1}}\sum_{j=i}^n \binom{n}{j}\right),\end{aligned}$$

see Beveridge (2016, Section 4) and Chung and Yau (2000, Example 4). In particular, $g_n(0) \to 2/(1-\varepsilon)$ as $n\to\infty$. Similarly, using the spectral representation, one can compute that $g'_n(0) \to 4/(1-\varepsilon)^2 - 2/(1-\varepsilon)$. Thus, $\sum_{\xi\in\mathbb{Z}^n_2} g_n(\xi)^2 - g_n(0)^2 \to 0$. Then, when $t/2^n \to u$, the variance of the size of the vacant set $V^{(\ell)}_n(t)$ is of order 2^n and

$$2^{-n}\operatorname{Var}(V^{(\ell)}_n(t)) \to \nu((1-\varepsilon)\ell u) \text{ with } \nu(x) = e^{-x}(e^{x/2} - 1 - (1-\varepsilon)x/4).$$

One might need to verify the detail somewhere else for other vertex-transitive graphs such as the Cayley graph of the symmetric group S_n.

The first step in the proof of Theorems 1.2 and 1.3 is the following simplification, which follows from the transitivity of the graph and independence of the random walks:

$$\operatorname{Var}(V^{(\ell)}_n(t)) = n^d \sum_{\xi\in\mathbb{Z}^d_n}\Big(\mathbb{P}(\tau(0,\xi)>t)^\ell - \mathbb{P}(\tau(0)>t)^{2\ell}\Big), \tag{1.7}$$

where

$$\tau(0,\xi) := \inf\{t \geqslant 0 : X_t \in \{0,\xi\}\}$$

is the hitting time of the set $\{0,\xi\}$ for the random walk X_t. In particular, we need a precise estimate of the tail behavior for the hitting time.

Lemma 1.8. *For $d \geqslant 3$, $\xi \in \mathbb{Z}_n^d$, and $u = (t+1)/n^d \in (0,\infty)$, we have*

$$\mathbb{P}_\pi(\tau(0,\xi) > t) = e^{-\frac{u}{f_n(\xi)}}\left(1 + \frac{u}{n^d}\left(\frac{f_n'(\xi)}{f_n(\xi)^3} + \frac{1}{2f_n(\xi)^2}\right) - \frac{f_n'(\xi)}{n^d f_n(\xi)^2}\right) + O(n^{-2d+3})$$

where

$$f_n(\xi) := \frac{1}{2}(g_n(0) + g_n(\xi)), \quad f_n'(\xi) := \frac{1}{2}(g_n'(0) + g_n'(\xi)). \tag{1.8}$$

Remark 1.9. *It is easy to check that $0 \leqslant f_n'(\xi) \leqslant f_n'(0)$ for all ξ using the spectral representation (2.4). Moreover, $n^{-d}\sum_\xi f_n'(\xi) = \frac{1}{2}f_n'(0)$.*

1.1. *Related Literature.* We first review the relevant literature on the range of simple random walks on the square lattice $\mathbb{Z}^d$. Dvoretzky and Erdös (1951) proved the strong law of large numbers for the range on $\mathbb{Z}^d$ for $d \geqslant 2$. A central limit theorem was obtained by Jain and Orey (1968). They showed that for strongly transient random walks, the variance of the range up to time t is of order t, and the range with a suitable normalization converges to normal distribution. Note that a simple random walk on $\mathbb{Z}^d$ is strongly transient if and only if $d \geqslant 5$. Later, Jain and Pruitt (1970) considered the general transient case. It was shown in Jain and Pruitt (1970) that the variance of the range up to time t is of order t if $d = 4$, and $t \log t$ if $d = 3$, and that the central limit theorem holds for $d = 3, 4$. The recurrent case ($d = 2$) was studied by Le Gall (1986), who proved that if $\mathcal{R}_t$ is the range up to time t, then $(\mathcal{R}_t - \mathbb{E}(\mathcal{R}_t))/(t(\log t)^{-2})$ converges to the intersection local time of a planar Brownian motion, which is a non-Gaussian distribution.

There have been efforts to study the capacity of the range of random walks on $\mathbb{Z}^d$. For a finite set $A \subset \mathbb{Z}^d$ in $d \geqslant 3$, the capacity of A is defined by the probability that a simple random walk starting from A never returns to A. Jain and Orey (1968) showed the law of large numbers for the capacity of the range of a simple random walk when $d \geqslant 5$. Later, Chang (2017) extended the result for $d = 3, 4$. Furthermore, it was shown in Chang (2017) that when $d = 3$, the capacity of the range converges to that of Brownian motion. Recently, Asselah et al. (2018, 2019) derived the central limit theorems for the capacity of the range when $d \geqslant 6$ and $d = 4$.

Sznitman (2010) introduced the random interlacement model to study the trace left by a simple random walk in a discrete torus $\mathbb{Z}_n^d$ for a time n^d. The random interlacement at level u, denoted by $\mathcal{I}^u$, can be constructed via a Poisson point process on the set of doubly infinite nearest neighbor paths on $\mathbb{Z}^d$ with intensity measure given in terms of the Newtonian capacity. The model provides the local picture of the trace left by a simple random walk in a discrete torus. The vacant set $\mathcal{V}_n(t)$ at a time of order $n^d \log n^d$ was studied in Aldous (1991); Belius (2013); Miller and Sousi (2017). The cover time τ_{cov} is the maximum of the hitting times $\tau(\xi)$ over $\xi \in \mathbb{Z}_n^d$. Let $t_{\text{cov}} = \max_x \mathbb{E}_x[\tau_{\text{cov}}]$. It is well-known that $t_{\text{cov}} = C_d n^d \log n^d(1 + o(1))$ as $n \to \infty$. Belius (2013) proved that the fluctuations of τ_{cov} are governed by the Gumbel distribution, in a sense that $\tau_{\text{cov}}/(C_d n^d) - \log n^d$ converges to Gumbel in law as $n \to \infty$ for $d \geqslant 3$. He also showed that the scaling limit of the vacant set up to time $C_d n^d \log n^d$ as a set-valued process in $(\mathbb{R}/\mathbb{Z})^d$ is indeed a Poisson point process. Heuristically, the Gumbel fluctuation of the cover time implies that, at a time of order $n^d \log n^d$, the hitting times $\tau(\xi)$, $\xi \in \mathbb{Z}_n^d$, are approximately almost exponential and independent. A natural question is the limiting behavior of the vacant set $\mathcal{V}_n(t)$ at a time $t = \alpha t_{\text{cov}}(1 + o(1))$ for $\alpha > 0$. Miller and Sousi (2017) showed that there are two thresholds $\alpha_0(d) < \alpha_1(d)$ such that $\mathcal{V}_n(t)$ is approximately Bernoulli random variable indexed by $\mathbb{Z}_n^d$ if $\alpha > \alpha_1(d)$, and the total variation distance between $\mathcal{V}_n(t)$ and Bernoulli random variable is 1 if $\alpha < \alpha_0(d)$.

Miller (2013) investigated the fluctuation behavior of the trace by competing random walks. Consider ℓ independent simple random walks $(X_{t,i})$, $i \in [\ell]$, on $\mathbb{Z}_n^d$. We assume that each site ξ is painted by i irreversibly at time t if $X_{t,i} = \xi$. Let $\mathcal{A}_i(t)$ be the set of sites painted by i up to time t. Miller (2013) computed the limiting behavior of the variance of $|\mathcal{A}_i(\infty)|$ for $d \geqslant 3$ and $\ell = 2$. Indeed, it was shown that the order of the variance of $|\mathcal{A}_i(\infty)|$ has the same order as the sum of squares of the $\mathbb{Z}^d$ Green's function, which coincides with our fluctuation behavior. He also extended the result to vertex-transitive graphs with some assumptions on the mixing time and provided precise limits of the variances for the hypercube and the Cayley graph of S_n as a corollary.

1.2. *Contributions.* One of the motivations for the random interlacement model is to investigate the percolative properties of the vacant set on $\mathbb{Z}_n^d$ up to time proportional to the size of the discrete torus. It was shown in Sznitman (2010) that there exists a critical u_* such that the vacant set does not percolate for large $u > u_*$ when $d \geqslant 3$, and percolates for small $u < u_*$ when $d \geqslant 7$. Later, Teixeira and Windisch (2011) showed that if $u > 0$ is large enough, then the volumes of all the components of the vacant set are of order $(\log n)^{\lambda(u)}$ and if $u > 0$ is small enough then there exists a macroscopic component. They also proved that if $d \geqslant 5$, the macroscopic component is unique in the small u regime. The proofs of these results are based on couplings of a simple random walk on $\mathbb{Z}^d$ with the random interlacement. Procaccia and Shellef (2014) examined certain geometric properties, including internal distance and mixing bounds, of the range of a random walk on the $d \geqslant 3$ dimensional torus at n^d time scale. Černý and Popov (2012) improved the internal distance bound to prove that distance-wise, the range of the random walk on the torus resembles the torus at a poly-logarithmic or higher scale.

Unlike the vacant set's percolative properties, the fluctuation of its size does not have any threshold at the time level u. This is because the local behavior of the random walk is crucial in studying the percolative property, whereas the variance of its size depends on both global and local properties.

The random interlacement captures the local behavior of a simple random walk on the discrete torus, in a sense that one can be approximated by the other as $n \to \infty$ in a box of size smaller order than the size of the torus. Consider the vacant set left by the random interlacement $\mathcal{I}^u$ in a box $[-n/2, n/2)^d$, say $W_n^u := [-n/2, n/2)^d \setminus \mathcal{I}^u$. Since $\mathbb{P}(\{x, y\} \subset W_n^u) = \exp(-2u/(G_*(0)+G_*(x-y)))$ where $G_*(x)$ is the Green's function for $\mathbb{Z}^d$, the variance of the vacant set W_n^u can be computed as

$$\mathrm{Var}(W_n^u) = n^d \sum_{\xi \in [-\frac{n}{2}, \frac{n}{2})^d} \left(\exp\left(-\frac{2u}{G_*(0) + G_*(\xi)} \right) - \exp\left(-\frac{2u}{G_*(0)} \right) \right) + o(1).$$

Note that the sum in the right-hand side does not converge as $n \to \infty$ for $d \geqslant 3$, while the sum in (1.5) does. Compared to Theorem 1.2, one can see that the contribution from the global fluctuation matters in the variance computation of the vacant set $V_n^{(l)}(t)$. Thus, the coupling with the random interlacement seems not suitable for the variance analysis.

To capture the global fluctuation, we employ a detailed analysis of the Green function. Higher-order estimates for the tail behavior of the hitting time via the Green function enable us to deal with both the global and local behaviors of the range of random walks, which leads to the limiting variance with the correct orders.

The analytic approaches using the Green function also allow us to more general settings. Our method holds for the intersection of ranges and vacant sets by multiple random walks and similar results for other graphs where Green's functions behave in a similar way.

1.3. *Roadmap.* The article is structured as follows.Section 2 contains notations, background details, and preliminary results for later analysis. We provide proofs of the main theorems in Section 3 and proofs of auxiliary results in Section 5. Section 4 contains the proof for accurately computing coefficients from specific functions of a power series, which will play a crucial role in estimating the upper tail behavior for the hitting time of two-point sets. Finally, we conclude with a discussion and the list of open problems in Section 6.

2. Preliminaries

2.1. *Notations and Conventions.* For the rest of the article, we use X_t and S_t for $\frac{1}{2}$–lazy random walks on $\mathbb{Z}_n^d$ and $\mathbb{Z}^d$, respectively. We explicitly write the dependence on n, d when needed. For a set $A \subseteq \mathbb{Z}_n^d$, the hitting time for A is denoted by

$$\tau(A) := \inf\{t \geqslant 0 : X_t \in A\}.$$

We will add extra subscript i when working with the i–th lazy random walk. If $A = \{x\}$ or $A = \{x, y\}$, we simply write $\tau(x)$ and $\tau(x, y)$, instead of $\tau(A)$. Let $\mathbb{P}$ and $\mathbb{E}$ be the probability and the expectation of X_t starting from the uniform distribution π_n on $\mathbb{Z}_n^d$. We will use $\mathbb{P}_\xi$ and $\mathbb{E}_\xi$ to denote the probability and the expectation of X_t starting from $X_0 = \xi$. For $v = (v_1, v_2, \cdots, v_d)$ in $\mathbb{Z}_n^d$ and $p \in [1, \infty)$, we use the notation

$$\|v\|_p := \big(|v_1|^p \wedge (n - |v_1|)^p + |v_2|^p \wedge (n - |v_2|)^p + \cdots + |v_d|^p \wedge (n - |v_d|)^p\big)^{1/p}.$$

For simplicity, we drop the subscript p when $p = 2$, that is, $\|v\| = \|v\|_2$.

We will write $a_n \lesssim b_n$, when there exists a finite positive constant c such that $a_n \leqslant cb_n$ for all n. Similarly, we will use $a_n \simeq b_n$, when $a_n \lesssim b_n$ and $b_n \lesssim a_n$. We will also use $a_n = O(b_n)$ or $b_n = \Omega(a_n)$ for $a_n \lesssim b_n$ and $a_n = \Theta(b_n)$ for $a_n \simeq b_n$.

2.2. *Green's Function.* We recall the Green's functions and their basic properties on $\mathbb{Z}^d$ and $\mathbb{Z}_n^d$. For further detail, we refer Chung and Yau (2000, Section 7) for the discrete torus and Lawler (2013); Lawler and Limic (2010) for the lattice. The Green's function on $\mathbb{Z}_n^d$ for a $\frac{1}{2}$–lazy simple random walk is defined by

$$g_n(\xi, \eta) = \sum_{t=0}^{\infty} (\mathbb{P}_\xi(X_t = \eta) - \pi(\eta)). \tag{2.1}$$

For simplicity, we use the notation $g_n(\xi) := g_n(0, \xi)$ and drop the subscript n when there is no ambiguity. For a $\frac{1}{2}$–lazy simple random walk S_t on $\mathbb{Z}^d$, the Green's function $G(\xi, \eta)$ is the expected number of visit to η from ξ,

$$G(\xi, \eta) = \mathbb{E}_\xi \left(\sum_{t=0}^{\infty} \mathbf{1}_{\{X_t = \eta\}} \right) = \sum_{t=0}^{\infty} \mathbb{P}_\xi(X_t = \eta).$$

Let $G(\xi) := G(0, \xi)$.

The Green's function has the following spectral representation. The Laplacian matrix for the random walk is given by $\Delta_n = I - P_n = \frac{1}{2}(I - \frac{1}{2d}A_n)$ where A_n is the adjacency matrix of $\mathbb{Z}_n^d$, that is, $A_n(\xi, \eta) = 1$ if ξ is a neighbor of η for $\xi, \eta \in \mathbb{Z}_n^d$, and otherwise 0. Let $e_n(x) := \exp(2\pi i x/n)$, for $x \in \mathbb{R}$. It is well known that

$$\varphi_v(\xi) = n^{-\frac{d}{2}} e_n(\langle v, \xi \rangle), \quad \xi \in \mathbb{Z}_n^d \tag{2.2}$$

for $v \in \mathbb{Z}_n^d$ gives a complete set of orthonormal eigenfunctions for Δ_n with the corresponding eigenvalues

$$\lambda_v := \frac{1}{2}\left(1 - \frac{1}{d} \sum_{j=1}^{d} \cos\big(2\pi v_j/n\big)\right) = \frac{1}{d} \sum_{j=1}^{d} \sin^2(\pi v_j/n) \in [0, 1]. \tag{2.3}$$

In particular, Δ_n is diagonalizable and

$$\Delta_n(\xi,\eta) = \sum_{v\in\mathbb{Z}_n^d} \lambda_v \varphi_v(\xi)\overline{\varphi_v(\eta)} \quad \text{for } \xi,\eta\in\mathbb{Z}_n^d$$

where $\bar{z}$ denotes the complex conjugate of $z\in\mathbb{C}$. Then, the Green's function can be written as

$$g_n(\xi,\eta) = \sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \frac{1}{\lambda_v}\varphi_v(\xi)\overline{\varphi_v(\eta)} = n^{-d}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \frac{1}{\lambda_v} e_n(\langle \xi-\eta, v\rangle). \tag{2.4}$$

Using the spectral representation, one can see that the Green's function $G(\xi)$ for $\mathbb{Z}^d$ $(d\geqslant 3)$ is the limit of $g_n(\xi)$ as $n\to\infty$. Indeed, we have

$$G(\xi) = \lim_{n\to\infty} g_n(\xi) = \int_{[0,1]^d} \frac{d}{\sum_{j=1}^d \sin^2(\pi x_j)} e^{2\pi i\xi\cdot x}\, dx \text{ for all } \xi\in\mathbb{Z}^d.$$

Let $\varphi_d(x) := \frac{d}{\sum_{j=1}^d \sin^2(\pi x_j)}$ for $x\in[0,1]^d$, then $G(\xi)$ is the Fourier transform of φ. By Plancherel's identity (Grafakos, 2008, Proposition 3.1.16), if $d\geqslant 5$ then

$$\int_{[0,1]^d} \varphi_d(x)^2\, dx = \sum_{\xi\in\mathbb{Z}^d} G(\xi)^2.$$

This fact will be used in the proof of the main results (see (3.1)).

2.3. *Generating Function.* The Green's generating function for the torus is defined by

$$g_n(\xi,\eta;z) := \sum_{t=0}^{\infty} \left(\mathbb{P}_\xi(X_t=\eta) - \pi(\eta)\right) z^t \text{ for } z\in\mathbb{C}, |z|<1. \tag{2.5}$$

For simplicity, we use $g_n(\xi;z) = g_n(0,\xi;z)$ and drop the subscript n if there is no ambiguity. Note that the spectral representation provides

$$g_n(\xi,\eta;z) = \sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \frac{1}{1-z\widehat{\lambda}_v}\varphi_v(\xi)\overline{\varphi_v(\eta)} = n^{-d}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \frac{e_n(\langle\xi-\eta,v\rangle)}{1-z\widehat{\lambda}_v} \tag{2.6}$$

where $\widehat{\lambda}_v := 1-\lambda_v$. Also note that $g_n(\xi;z)$ is defined for $z\notin\{\widehat{\lambda}_v^{-1} \mid v\in\mathbb{Z}_n^d\setminus\{0\}\}$ and $g_n(\xi) = g_n(\xi;1)$. Moreover, the Green's generating function defined in (2.5) satisfies

$$\sum_{\xi\in\mathbb{Z}_n^d} g_n(\xi;z) = 0 \text{ for all } z.$$

Let

$$\begin{aligned} g_n'(\xi;1) := \frac{d}{dz} g_n(\xi;z)\Big|_{z=1} &= \sum_{t=0}^{\infty} t\left(\mathbb{P}_0(X_t=\xi) - \pi(\xi)\right) \\ &= n^{-d}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} (1-\lambda_v)\lambda_v^{-2} e_n(\langle\xi,v\rangle). \end{aligned}$$

We simply denote by $g_n'(\xi) = g_n'(\xi;1)$. One can easily check that

$$\sum_{\xi\in\mathbb{Z}_n^d} g_n(\xi)^2 = n^{-d}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \lambda_v^{-2} = g_n(0) + g_n'(0).$$

For $\xi\in\mathbb{Z}^d$ and $z\in\mathbb{C}$ with $|z|<1$, we define $G(\xi;z) = \sum_{t=0}^{\infty} z^t\,\mathbb{P}_0(S_t=\xi)$ and

$$G'(\xi) = \frac{d}{dz}G(\xi;z)|_{z=1} = \sum_{t=0}^{\infty} t\,\mathbb{P}_0(S_t=\xi) > 0,$$

where S_t is a $\frac{1}{2}$–lazy simple random walk on $\mathbb{Z}^d$. Note that $\lim_{n\to\infty} g_n'(\xi) = G'(\xi)$ for each $\xi \in \mathbb{Z}^d$ when $d \geqslant 5$. The Green's generating function has a probabilistic interpretation. Consider two independence $\frac{1}{2}$–lazy simple random walks on $\mathbb{Z}^d$, $S_{t,1}$ and $S_{t,2}$ starting at 0 and ξ respectively. Then, $\mathbb{E}\,|\{(s,t) \mid S_{s,1} = S_{t,2}\}|$, the expected size of the intersection of two random walk trajectories (counted with multiplicities), can be written as

$$\begin{aligned}\sum_{v\in\mathbb{Z}^d} G(v)G(v-\xi) &= \sum_{t,s=0}^{\infty} \mathbb{P}_{0,\xi}(S_{t,1} = S_{s,2}) \\ &= \sum_{t,s=0}^{\infty}\sum_{v\in\mathbb{Z}^d} \mathbb{P}_0(S_{t,1} = v)\,\mathbb{P}_\xi(S_{s,2} = v) \\ &= \sum_{t,s=0}^{\infty} \mathbb{P}_0(S_{t+s} = \xi) = \sum_{t=0}^{\infty}(t+1)\,\mathbb{P}_0(S_t = \xi) = G(\xi) + G'(\xi). \qquad (2.7)\end{aligned}$$

In this paper, the main results are given in terms of the Green's function G for a $\frac{1}{2}$–lazy random walk on $\mathbb{Z}^d$. One can replace G with the standard Green's function G_* with minor modification if needed. If $G_\varepsilon(\xi)$ is the Green's function for the ε–lazy random walk on $\mathbb{Z}^d$, $\varepsilon \in (0,1)$, then one can see that

$$G_\varepsilon(\xi) = \frac{1}{1-\varepsilon}G_*(\xi), \qquad G_\varepsilon'(\xi) = \frac{\varepsilon}{(1-\varepsilon)^2}G_*(\xi) + \frac{1}{(1-\varepsilon)^2}G_*'(\xi).$$

In particular, we have $G(\xi) = 2G_*(\xi)$ and $G'(\xi) = 2G_*(\xi) + 4G_*'(\xi)$.

The following Lemma 2.1 will be used to compute the growth rate of $g_n'(0)$ depending on n and the dimension d by taking $k = 2$.

Lemma 2.1. *For $k \geqslant 1$, we have*

$$\frac{1}{n^d}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \lambda_v^{-k} \simeq \begin{cases} 1 & \text{if } d > 2k \\ \log n & \text{if } d = 2k \\ n^{2k-d} & \text{otherwise.}\end{cases}$$

As a direct consequence, we have

$$\left.\frac{d^k}{dz^k} g_n(0;z)\right|_{z=1} \simeq \begin{cases} 1 & \text{if } d > 2k+2 \\ \log n & \text{if } d = 2k+2 \\ n^{2k+2-d} & \text{otherwise.}\end{cases}$$

Proof: Recall that we say $a_n \simeq b_n$ if there are constants $c_1, c_2 > 0$ such that $a_n \leqslant c_1 b_n$ and $b_n \leqslant c_2 a_n$. From (2.3), it is easy to see that $\lambda_v \simeq \|v\|^2/(dn^2)$. Thus, we have

$$\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \lambda_v^{-k} \simeq n^{2k}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \|v\|^{-2k} \simeq n^{2k}\sum_{r=1}^{n} r^{-2k}r^{d-1} \simeq \begin{cases} n^d & \text{if } d > 2k \\ n^d\log n & \text{if } d = 2k \\ n^{2k} & \text{otherwise.}\end{cases}$$

The second assertion follows from the fact that

$$\left.\frac{d^k}{dz^k} g_n(0;z)\right|_{z=1} = \frac{k!}{n^d}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} \lambda_v^{-(k+1)}(1-\lambda_v)^k$$

and this completes the proof. ∎

The next Lemma 2.2 tells us that $g_n(\xi)$ and $g_n'(\xi)$ converge to 0 as $\|\xi\|$ becomes large, uniformly in n, which will be frequently used in the proofs of the main results. The proof is given in Section 5.

Lemma 2.2. *We have*

$$g_n(\xi) = O(n^{-\min\{d-2,2\}} + (1+\|\xi\|)^{-\min\{d-2,(d+2)/2\}}) \qquad \text{for } d \geqslant 3,$$
$$g'_n(\xi) = O(n^{-\min\{d-4,(d-2)/2\}} + (1+\|\xi\|)^{-\min\{d-4,d/2\}}) \qquad \text{for } d \geqslant 5$$

uniformly in $n, \xi \in \mathbb{Z}_n^d$.

Let

$$f_n(\xi; z) := \frac{1}{2}(g_n(0; z) + g_n(\xi; z)) \qquad \text{and} \qquad f_n(\xi) := f_n(\xi; 1). \tag{2.8}$$

The generating function for $\mathbb{P}(\tau(0,\xi) > t)$ can be expressed in terms of the function $f_n(\xi; z)$ as follows (see Brummelhuis and Hilhorst, 1991).

Lemma 2.3. *For* $|z| < 1$ *and* $\xi \in \mathbb{Z}_n^d$, *we have*

$$\sum_{t=0}^{\infty} z^t\, \mathbb{P}(\tau(0,\xi) > t) = \frac{f_n(\xi; z)}{n^{-d} + (1-z) f_n(\xi; z)}. \tag{2.9}$$

From Lemma 2.3, finding a precise estimate on the hitting probability $\mathbb{P}(\tau(0,\xi) > t)$ boils down to a refined analysis on the coefficients of the series expansion of the function on the right-hand side in (2.9). We investigate the series expansion of such functions in Section 4. We give a proof of Lemma 2.3 for completeness.

Proof of Lemma 2.3: Suppose $\xi \in \mathbb{Z}_n^d \setminus \{0\}$ and $|z| < 1$. Let

$$g_n^+(\xi; z) := \sum_{t=0}^{\infty} z^t\, \mathbb{P}_0(X_t = \xi).$$

Note that $g_n^+(\xi; z) = g_n(\xi; z) + n^{-d}(1-z)^{-1}$ and $\sum_{\xi \in \mathbb{Z}_n^d} g_n^+(\xi; z) = (1-z)^{-1}$. For $x \in \mathbb{Z}_n^d$, we have

$$\begin{aligned} g_n^+(x; z) + g_n^+(x+\xi; z) &= \sum_{t=0}^{\infty} z^t\, \mathbb{P}_0(X_t \in \{x, x+\xi\}) \\ &= \sum_{t=0}^{\infty} \sum_{s=0}^{t} z^t\, \mathbb{P}_0(X_t \in \{x, x+\xi\}, \tau(x, x+\xi) = s) \\ &= \sum_{s=0}^{\infty} \sum_{t=0}^{\infty} z^{t+s}\, \mathbb{P}_0(X_{t+s} \in \{x, x+\xi\}, \tau(x, x+\xi) = s). \end{aligned}$$

Applying the strong Markov property at τ_x and $\tau_{x+\xi}$, we have

$$\begin{aligned} &\mathbb{P}_0(X_{t+s} = x, \tau(x, x+\xi) = s) \\ &\quad = \mathbb{P}_0(X_{t+s} = x, \tau(x, x+\xi) = s = \tau(x)) + \mathbb{P}_0(X_{t+s} = x, \tau(x, x+\xi) = s = \tau(x+\xi)) \\ &\quad = \mathbb{P}_0(X_t = 0)\, \mathbb{P}_0(\tau(x, x+\xi) = s = \tau(x)) + \mathbb{P}_0(X_t = \xi)\, \mathbb{P}_0(\tau(x, x+\xi) = s = \tau(x+\xi)). \end{aligned}$$

Similarly, we have

$$\begin{aligned} &\mathbb{P}_0(X_{t+s} = x+\xi, \tau(x, x+\xi) = s) \\ &\quad = \mathbb{P}_0(X_{t+s} = x+\xi, \tau(x, x+\xi) = s = \tau(x)) + \mathbb{P}_0(X_{t+s} = x+\xi, \tau(x, x+\xi) = s = \tau(x+\xi)) \\ &\quad = \mathbb{P}_0(X_t = \xi)\, \mathbb{P}_0(\tau(x, x+\xi) = s = \tau(x)) + \mathbb{P}_0(X_t = 0)\, \mathbb{P}_0(\tau(x, x+\xi) = s = \tau(x+\xi)) \end{aligned}$$

and so

$$\mathbb{P}_0(X_{t+s} \in \{x, x+\xi\}, \tau(x, x+\xi) = s) = (\mathbb{P}_0(X_t = 0) + \mathbb{P}_0(X_t = \xi))\, \mathbb{P}_0(\tau(x, x+\xi) = s).$$

Thus, we get

$$g_n^+(x;z) + g_n^+(x+\xi;z) = (g_n^+(0;z) + g_n^+(\xi;z)) \sum_{s=0}^{\infty} z^s \,\mathbb{P}_0(\tau(x, x+\xi) = s).$$

Averaging over x, we have

$$2n^{-d}(1-z)^{-1} = (2n^{-d}(1-z)^{-1} + 2f_n(\xi;z)) \sum_{s=0}^{\infty} z^s \,\mathbb{P}(\tau(0,\xi) = s)$$

$$\text{or} \quad \sum_{s=0}^{\infty} z^s \,\mathbb{P}(\tau(0,\xi) = s) = \frac{n^{-d}}{n^{-d} + (1-z) f_n(\xi;z)}.$$

Therefore,

$$\begin{aligned}
\sum_{t=0}^{\infty} z^t \,\mathbb{P}(\tau(0,\xi) > t) &= \sum_{t=0}^{\infty} \sum_{s=t+1}^{\infty} z^t \,\mathbb{P}(\tau(0,\xi) = s) \\
&= \sum_{s=1}^{\infty} \sum_{t=0}^{s-1} z^t \,\mathbb{P}(\tau(0,\xi) = s) \\
&= \sum_{s=0}^{\infty} (1-z^s)(1-z)^{-1} \,\mathbb{P}(\tau(0,\xi) = s) \\
&= \frac{1}{1-z}\left(1 - \frac{n^{-d}}{n^{-d} + (1-z) f_n(\xi;z)}\right) = \frac{f_n(\xi;z)}{n^{-d} + (1-z) f_n(\xi;z)}.
\end{aligned}$$

The same argument holds for the case $\xi = 0$. ■

From the uniform convergence of $g_n(\xi)$ and $|g_n(\xi)| \leqslant g_n(0)$, one can guess that $f_n(\xi)$ is uniformly away from 0 in n. The next lemma asserts that this is the case. The proof is given in Section 5.

Lemma 2.4. *There exists $C > 0$ independent of n, such that $f_n(\xi) \geqslant C$ for all $\xi \in \mathbb{Z}_n^d$.*

3. Proofs of Main Results

3.1. *Proof of Theorem 1.2.* We will omit the subscript n in f_n, g_n for simplicity. By Lemma 1.8 and (1.7), we have

$$\begin{aligned}
n^{-d}\,\mathrm{Var}(V_n^{(\ell)}(t)) &= \sum_{\xi \in \mathbb{Z}_n^d} (\mathbb{P}(\tau(0,\xi) > t)^{\ell} - \mathbb{P}(\tau(0) > t)^{2\ell}) \\
&= \sum_{\xi \in \mathbb{Z}_n^d} (e^{-\frac{\ell u}{f(\xi)}} - e^{-\frac{2\ell u}{f(0)}}) + \frac{\ell}{n^d} \sum_{\xi \in \mathbb{Z}_n^d} e^{-\frac{\ell u}{f(\xi)}} \left(u\left(\frac{f'(\xi)}{f(\xi)^3} + \frac{1}{2f(\xi)^2}\right) - \frac{f'(\xi)}{f(\xi)^2}\right) \\
&\quad - 2\ell e^{-\frac{2\ell u}{f(0)}} \left(u\left(\frac{f'(0)}{f(0)^3} + \frac{1}{2f(0)^2}\right) - \frac{f'(0)}{f(0)^2}\right) + o(1).
\end{aligned}$$

It follows from $\sum_{\xi \in \mathbb{Z}_n^d} g(\xi) = 0$ that

$$\begin{aligned}
&\sum_{\xi \in \mathbb{Z}_n^d} (e^{-\frac{\ell u}{f(\xi)}} - e^{-\frac{2\ell u}{f(0)}}) \\
&\quad = e^{-\frac{2\ell u}{f(0)}} \left(\sum_{\xi \in \mathbb{Z}_n^d} \left(e^{\frac{\ell u g(\xi)}{f(0) f(\xi)}} - 1 - \frac{\ell u g(\xi)}{f(0) f(\xi)}\right) - \frac{\ell u}{f(0)^2} \sum_{\xi \in \mathbb{Z}_n^d} \frac{g(\xi)^2}{f(\xi)}\right).
\end{aligned}$$

Recall that $f_n(\xi) \geqslant C > 0$ for all n and ξ by Lemma 2.4. Since $e^t - 1 - t \leqslant \frac{1}{2}t^2 \max\{e^t, 1\}$ and $g(\xi) \leqslant g(0) = f(0)$, we have

$$e^{\frac{\ell u g(\xi)}{f(0)f(\xi)}} - 1 - \frac{\ell u g(\xi)}{f(0)f(\xi)} \leqslant \frac{1}{2}\left(\frac{\ell u g(\xi)}{f(0)f(\xi)}\right)^2 \max\{e^{\frac{\ell u g(\xi)}{f(0)f(\xi)}}, 1\}$$
$$\leqslant \frac{\ell^2 u^2}{2C^2} \max\{e^{\frac{\ell u}{C}}, 1\} g(\xi)^2.$$

Since $\lim_{n\to\infty} g_n(\xi) = G(\xi)$ for each ξ and

$$\lim_{n\to\infty} \sum_{\xi\in\mathbb{Z}_n^d} g(\xi)^2 = \lim_{n\to\infty} \frac{1}{n^d} \sum_{v\in\mathbb{Z}_n^d} \frac{1}{\lambda_v^2} = \int_{[0,1]^d} \varphi_d(x)^2\, dx = \sum_{\xi\in\mathbb{Z}^d} G(\xi)^2 < \infty \tag{3.1}$$

for $d \geqslant 5$ where $\varphi_d(x) = d(\sum_{j=1}^d \sin^2(\pi x_j))^{-1}$, the dominated convergence theorem implies that

$$\lim_{n\to\infty} \sum_{\xi\in\mathbb{Z}_n^d} (e^{-\frac{\ell u}{f(\xi)}} - e^{-\frac{2\ell u}{f(0)}}) = \sum_{\xi\in\mathbb{Z}^d} \left(e^{-\frac{2\ell u}{(G(0)+G(\xi))}} - e^{-\frac{2\ell u}{G(0)}} - 2\ell u e^{-\frac{2\ell u}{G(0)}} \frac{G(\xi)}{G(0)^2}\right).$$

By Lemma 2.2, for any $\varepsilon > 0$, there exist N and K such that

$$\left|f_n(\xi) - \frac{1}{2}G(0)\right| < \varepsilon \text{ and } \left|f_n'(\xi) - \frac{1}{2}G'(0)\right| < \varepsilon,$$

for all $n \geqslant N$ and $\|\xi\| \geqslant K$. Thus, one can see that

$$\frac{1}{n^d} \sum_{\xi\in\mathbb{Z}_n^d} e^{-\frac{\ell u}{f(\xi)}} \left(u\left(\frac{f'(\xi)}{f(\xi)^3} + \frac{1}{2f(\xi)^2}\right) - \frac{f'(\xi)}{f(\xi)^2}\right)$$
$$\to 2e^{-\frac{2\ell u}{G(0)}} \left(\frac{2uG'(0)}{G(0)^3} + \frac{u}{G(0)^2} - \frac{G'(0)}{G(0)^2}\right)$$

as $n \to \infty$. Therefore, it follows from (2.7) that

$$\begin{aligned}\lim_{n\to\infty} n^{-d} \operatorname{Var}(V_n^{(\ell)}(t)) &= \sum_{\xi\in\mathbb{Z}^d} \left(e^{-\frac{2\ell u}{(G(0)+G(\xi))}} - e^{-\frac{2\ell u}{G(0)}} - 2\ell u e^{-\frac{2\ell u}{G(0)}} \frac{G(\xi)}{G(0)^2}\right) \\ &\quad + 2\ell u e^{-\frac{2\ell u}{G(0)}} \left(\frac{G'(0)}{G(0)^3} + \frac{1}{2G(0)^2}\right) \\ &= \nu_d(2\ell u/G(0))\end{aligned}$$

where

$$\nu_d(u) := e^{-u} \sum_{\xi\in\mathbb{Z}^d} \left(\exp\left(\frac{uG(\xi)}{G(0)+G(\xi)}\right) - 1 - \frac{uG(\xi)}{G(0)}\right) + ue^{-u}\left(\frac{G'(0)}{G(0)^2} + \frac{1}{2G(0)}\right).$$

Using $G(0) + G'(0) = \sum_{\xi\in\mathbb{Z}^d} G(\xi)^2$, we conclude

$$\begin{aligned}e^u \nu_d(u) &= \sum_{\xi\in\mathbb{Z}^d} \left(\exp\left(\frac{uG(\xi)}{G(0)+G(\xi)}\right) - 1 - \frac{uG(\xi)}{G(0)} + \frac{uG(\xi)^2}{G(0)^2}\right) - \frac{1}{2G(0)} \\ &= \sum_{\xi\in\mathbb{Z}^d} \left(\exp\left(\frac{uG(\xi)}{G(0)+G(\xi)}\right) - 1 - \frac{uG(\xi)}{G(0)+G(\xi)} + \frac{uG(\xi)^3}{G(0)^2(G(0)+G(\xi))}\right) - \frac{1}{2G(0)} \\ &= \sum_{\xi\in\mathbb{Z}^d} \left(\exp\left(\frac{uG(\xi)}{G(0)+G(\xi)}\right) - 1 - \frac{uG(\xi)}{G(0)+G(\xi)} + \frac{uG(\xi)^2(G(\xi) - \mathbb{1}_{\{\xi=0\}})}{G(0)^2(G(0)+G(\xi))}\right).\end{aligned}$$

3.2. *Proof of Theorem 1.3*. Note that $g_n'(0) \to \infty$ as $n \to \infty$ for $d = 3, 4$. Again, we will omit the subscript n in f_n, g_n for simplicity. We have

$$\begin{aligned}\frac{1}{n^d g'(0)} \mathrm{Var}(V_n^{(\ell)}(t)) &= \frac{1}{g'(0)} \sum_{\xi \in \mathbb{Z}_n^d} (\mathbb{P}(\tau(0,\xi) > t)^\ell - \mathbb{P}(\tau(0) > t)^{2\ell}) \\ &= \frac{1}{g'(0)} \sum_{\xi \in \mathbb{Z}_n^d} (e^{-\frac{\ell u}{f(\xi)}} - e^{-\frac{2\ell u}{f(0)}}) + \frac{\ell}{n^d} \sum_{\xi \in \mathbb{Z}_n^d} \left(\frac{u e^{-\frac{\ell u}{f(\xi)}}}{f(\xi)^3} - \frac{e^{-\frac{\ell u}{f(\xi)}}}{f(\xi)^2} \right) \frac{f'(\xi)}{g'(0)} \\ &\quad - 2\ell \left(\frac{u e^{-\frac{2\ell u}{g(0)}}}{g(0)^3} - \frac{e^{-\frac{2\ell u}{g(0)}}}{g(0)^2} \right) + o(1).\end{aligned}$$

Here the $o(1)$ is $O(n^{3-d}/g'(0))$. Let $\varepsilon > 0$. By Lemma 2.2, there exist N and K such that for all $n \geqslant N$ and $\|\xi\| \geqslant K$, $|g(\xi)| < \varepsilon$. Note that there exist C_1, C_2 independent of n and ξ such that $0 < C_1 \leqslant f(\xi) \leqslant C_2 < \infty$ by Lemma 2.4 and $|g(\xi)| \leqslant g(0)$. Consider

$$\psi(x) := u x^{-3} e^{-\ell u/x} - x^{-2} e^{-\ell u/x}$$

for $x \in [C_1, C_2]$. One can easily see that ψ is bounded and Lipschitz on $[C_1, C_2]$. Indeed, there exists C_3 such that $|\psi(x) - \psi(y)| \leqslant C_3(|x-y| \wedge 1)$ and for $x, y \in [C_1, C_2]$ and for $i = 1, 2$. Thus,

$$\begin{aligned}|\psi(f(\xi)) - \psi(g(0)/2)| &= \left| \left(\frac{u e^{-\frac{\ell u}{f(\xi)}}}{f(\xi)^3} - \frac{e^{-\frac{\ell u}{f(\xi)}}}{f(\xi)^2} \right) - \left(\frac{8u e^{-\frac{2\ell u}{g(0)}}}{g(0)^3} - \frac{4 e^{-\frac{2\ell u}{g(0)}}}{g(0)^2} \right) \right| \\ &\leqslant C_3 \left| f(\xi) - \frac{1}{2} g(0) \right|.\end{aligned}$$

Note that

$$\frac{1}{n^d} \sum_{\xi \in \mathbb{Z}_n^d} \psi(g(0)/2) \frac{f'(\xi)}{g'(0)} = \frac{1}{2} \psi(g(0)/2) = \frac{4u e^{-\frac{2\ell u}{G(0)}}}{G(0)^3} - \frac{2 e^{-\frac{2\ell u}{G(0)}}}{G(0)^2}$$

because $\sum_{\xi \in \mathbb{Z}_n^d} g'(\xi) = 0$, and that $0 \leqslant f'(\xi) \leqslant g'(0)$ for all n, ξ. Since $\left| f(\xi) - \frac{1}{2} g(0) \right| < \varepsilon/2$ for all $n \geqslant N$, we get

$$\begin{aligned}\left| \frac{1}{n^d} \sum_{\xi \in \mathbb{Z}_n^d} (\psi(f(\xi)) - \psi(g(0)/2)) \frac{f'(\xi)}{g'(0)} \right| &\leqslant \frac{\varepsilon C_3}{2n^d} \sum_{\xi \in \mathbb{Z}_n^d, \|\xi\| \geqslant K} \frac{f'(\xi)}{g'(0)} + \frac{C_3}{n^d} \sum_{\xi \in \mathbb{Z}_n^d, \|\xi\| < K} \frac{f'(\xi)}{g'(0)} \\ &\leqslant \frac{\varepsilon C_3}{2} + \frac{C_4 K^d}{n^d},\end{aligned}$$

which yields in turn that

$$\lim_{n \to \infty} \frac{\ell}{n^d} \sum_{\xi \in \mathbb{Z}_n^d} \left(\frac{u e^{-\frac{\ell u}{f(\xi)}}}{f(\xi)^3} - \frac{e^{-\frac{\ell u}{f(\xi)}}}{f(\xi)^2} \right) \frac{f'(\xi)}{g'(0)} = 2\ell e^{-\frac{2\ell u}{G(0)}} \left(\frac{2u}{G(0)^3} - \frac{1}{G(0)^2} \right).$$

On the other hand, if

$$w_n = w = 2\ell u / g_n(0), \tag{3.2}$$

then

$$\sum_{\xi \in \mathbb{Z}_n^d} (e^{-\frac{\ell u}{f(\xi)}} - e^{-\frac{2\ell u}{f(0)}}) = e^{-w} \sum_{\xi \in \mathbb{Z}_n^d} (e^{-\frac{w g(\xi)}{g(0) + g(\xi)}} - 1).$$

It follows from Lemma 2.4 and $\left|e^s - 1 - s - s^2/2\right| \leqslant C(a)|s|^3$ for $|s| \leqslant a$, that

$$\left|e^{-\frac{wg(\xi)}{g(0)+g(\xi)}} - 1 - \frac{wg(\xi)}{g(0)+g(\xi)} - \frac{w^2 g(\xi)^2}{2(g(0)+g(\xi))^2}\right| \leqslant \frac{w^3 |g(\xi)|^3}{6(g(0)+g(\xi))^3} \leqslant \frac{w^3}{C} |g(\xi)|^3 .$$

We claim that

$$\lim_{n\to\infty} \frac{1}{g'(0)} \sum_{\xi\in\mathbb{Z}_n^d} |g(\xi)|^3 = 0. \tag{3.3}$$

Indeed, this follows from

$$\frac{\sum_{\xi\in\mathbb{Z}_n^d} |g(\xi)|^3}{\sum_{\xi\in\mathbb{Z}_n^d} g(\xi)^2} \leqslant \frac{\sum_{\xi\in\mathbb{Z}_n^d, \|\xi\|<K} |g(\xi)|^3}{\sum_{\xi\in\mathbb{Z}_n^d} g(\xi)^2} + \varepsilon \frac{\sum_{\xi\in\mathbb{Z}_n^d, \|\xi\|\geqslant K} g(\xi)^2}{\sum_{\xi\in\mathbb{Z}_n^d} g(\xi)^2} \leqslant \frac{CK^d}{\sum_{\xi\in\mathbb{Z}_n^d} g(\xi)^2} + \varepsilon < 2\varepsilon$$

for large n, and $g'(0) = \sum_{\xi\in\mathbb{Z}_n^d} g(\xi)^2 - g(0) \to \infty$ as $n\to\infty$. Thus, we obtain

$$\lim_{n\to\infty} \frac{1}{g'(0)} \sum_{\xi\in\mathbb{Z}_n^d} \left(e^{-\frac{wg(\xi)}{g(0)+g(\xi)}} - 1 - \frac{wg(\xi)}{g(0)+g(\xi)} - \frac{w^2 g(\xi)^2}{2(g(0)+g(\xi))^2}\right) = 0.$$

Using $\sum_{\xi\in\mathbb{Z}_n^d} g(\xi) = 0$, one can write

$$\begin{aligned}\sum_{\xi\in\mathbb{Z}_n^d} \frac{g(\xi)}{g(0)+g(\xi)} &= -\sum_{\xi\in\mathbb{Z}_n^d} \frac{g(\xi)^2}{g(0)(g(0)+g(\xi))} \\ &= \sum_{\xi\in\mathbb{Z}_n^d} \frac{g(\xi)^3}{g(0)^2(g(0)+g(\xi))} - \sum_{\xi\in\mathbb{Z}_n^d} \frac{g(\xi)^2}{g(0)^2}.\end{aligned}$$

By Lemma 2.4 and the claim (3.3), we conclude that

$$\lim_{n\to\infty} \frac{1}{g'(0)} \sum_{\xi\in\mathbb{Z}_n^d} \frac{g(\xi)}{g(0)+g(\xi)} = -\frac{1}{G(0)^2}.$$

Here, we used the fact that $\frac{1}{g'(0)} \sum_{\xi\in\mathbb{Z}_n^d} g(\xi)^2 \to 1$ as $n\to\infty$. Similarly,

$$\lim_{n\to\infty} \frac{1}{g'(0)} \sum_{\xi\in\mathbb{Z}_n^d} \frac{g(\xi)^2}{(g(0)+g(\xi))^2} = \frac{1}{G(0)^2}.$$

Thus, for w as defined in (3.2) we have

$$\lim_{n\to\infty} \frac{e^{-w}}{g'(0)} \sum_{\xi\in\mathbb{Z}_n^d} (e^{-\frac{wg(\xi)}{g(0)+g(\xi)}} - 1) = 2\ell e^{-\frac{2\ell u}{G(0)}} \left(\frac{\ell u^2}{G(0)^4} - \frac{u}{G(0)^3}\right).$$

Therefore,

$$\begin{aligned}\lim_{n\to\infty} \frac{\mathrm{Var}(V_n^{(\ell)}(t))}{n^d g_n'(0)} &= 2\ell e^{-\frac{2\ell u}{G(0)}} \left(\frac{\ell u^2}{G(0)^4} - \frac{u}{G(0)^3}\right) + 2\ell e^{-\frac{2\ell u}{G(0)}} \left(\frac{2u}{G(0)^3} - \frac{1}{G(0)^2}\right) \\ &\quad - 2\ell e^{-\frac{2\ell u}{G(0)}} \left(\frac{u}{G(0)^3} - \frac{1}{G(0)^2}\right) \\ &= 2\ell^2 u^2 e^{-\frac{2\ell u}{G(0)}} G(0)^{-4}.\end{aligned}$$

Let $\alpha_d := \lim_{n\to\infty} \frac{g'(0)}{h_d(n)G(0)^2}$, then it follows from $\sum_{\xi\in\mathbb{Z}_n^d} g_n(\xi)^2 = g_n(0) + g_n'(0)$, $g_n'(0) \to \infty$, and $g_n(0) < \infty$ for $d = 3, 4$ that

$$\alpha_d = \lim_{n\to\infty} \frac{1}{h_d(n)G(0;\mathbb{Z}^d)^2} \sum_{\xi\in\mathbb{Z}_n^d} g_n(\xi)^2.$$

It follows from Lemma 2.1 that α_d is finite for $d = 3, 4$. To simplify α_d further, first, we consider the case $d = 3$.

Using the spectral representation of $g_n(\xi)$ and (2.3), we see

$$\frac{1}{n} \sum_{\xi\in\mathbb{Z}_n^3} g_n(\xi)^2 = \frac{1}{n^4} \sum_{v\in\mathbb{Z}_n^3\setminus\{0\}} \lambda_v^{-2} = \frac{9}{\pi^4} \sum_{v\in\mathbb{Z}_n^3\setminus\{0\}} \left(\frac{n^2}{\pi^2} \sum_{j=1}^{3} \sin^2(\pi v_j/n) \right)^{-2}.$$

We split the summation over v on the right-hand side into two parts $\|v\| \geqslant K_0$ and $\|v\| < K_0$, where $K_0 > 0$ will be determined later. Then, we have

$$\sum_{v\in\mathbb{Z}_n^3, \|v\|\geqslant K_0} \left(\frac{n^2}{\pi^2} \sum_{j=1}^{3} \sin^2(\pi v_j/n) \right)^{-2} \leqslant C \sum_{v\in\mathbb{Z}_n^3, \|v\|\geqslant K_0} \|v\|^{-4} \leqslant \frac{C}{K_0}.$$

On the other hand, we choose n large enough that

$$\sum_{v\in\mathbb{Z}_n^3, 0<\|v\|<K_0} \left(\frac{n^2}{\pi^2} \sum_{j=1}^{3} \sin^2(\pi v_j/n) \right)^{-2} = \sum_{v\in\mathbb{Z}_n^3, 0<\|v\|<K_0} \|v\|^{-4} + o(1).$$

By taking large enough K_0, we conclude

$$\alpha_3 = \lim_{n\to\infty} \frac{g_n'(0)}{nG(0)^2} = \lim_{n\to\infty} \frac{1}{nG(0)^2} \sum_{\xi\in\mathbb{Z}_n^3} g_n(\xi)^2 = \frac{9}{\pi^4 G(0)^2} \sum_{v\in\mathbb{Z}^3} \|v\|^{-4}.$$

Similarly, for $d = 4$, we have

$$\alpha_4 = \lim_{n\to\infty} \frac{1}{n^4 \log n \cdot G(0)^2} \sum_{\xi\in\mathbb{Z}_n^4} \lambda_v^{-2} = \frac{16}{\pi^4 G(0)^2} \lim_{n\to\infty} \frac{1}{\log n} \sum_{v\in\mathbb{Z}_n^4} \left(\frac{n^2}{\pi^2} \sum_{j=1}^{4} \sin^2(\pi v_j/n) \right)^{-2}.$$

Let $\varepsilon \in (0, 1)$. Using $|\sin t| \leqslant Ct$ for all t and $\sin t = t + O(t^3)$ as $t \to 0$, we obtain

$$\begin{aligned} \frac{1}{\log n} \sum_{\|v\|\geqslant n^\varepsilon} \left(\frac{n^2}{\pi^2} \sum_{j=1}^{4} \sin^2(\pi v_j/n) \right)^{-2} &\leqslant \frac{C}{\log n} \sum_{\|v\|\geqslant n^\varepsilon} \|v\|^{-4} \\ &\lesssim \frac{1}{\log n} \int_{n^\varepsilon}^{n} r^{-1}\, dr \lesssim \frac{|\log \varepsilon|}{\log n} \end{aligned}$$

and

$$\lim_{n\to\infty} \frac{1}{\log n} \sum_{\|v\|\leqslant n^\varepsilon} \left(\frac{n^2}{\pi^2} \sum_{j=1}^{4} \sin^2(\pi v_j/n) \right)^{-2} = \lim_{n\to\infty} \frac{1}{\log n} \sum_{\|v\|\leqslant n^\varepsilon} \|v\|^{-4}.$$

Since this holds for any $\varepsilon \in (0, 1)$, we get

$$\alpha_4 = \frac{16}{\pi^4 G(0)^2} \lim_{n\to\infty} \frac{1}{\log n} \sum_{\|v\|\leqslant n} \|v\|^{-4}.$$

3.3. *Proof of Theorem 1.6.* A direct computation yields

$$n^{-d}\,\mathbb{E}(R^I_{n,\ell}(t)R^J_{n,\ell}(t)) = \sum_{\xi\in\mathbb{Z}^d_n} \mathbb{P}(\tau(0,\xi)\leqslant t)^{|I\cap J|}\,\mathbb{P}(\tau(0,\xi)>t)^{|I^c\cap J^c|}\,\mathbb{P}(\tau(0)\leqslant t<\tau(\xi))^{|I\Delta J|}.$$

Let

$$|I\cap J|=k,\ |I^c\cap J^c|=k',\ |I\Delta J|=r,\ \mathbb{P}(\tau(0)>t)=a \text{ and } \mathbb{P}(\tau(0,\xi)>t)=b.$$

Then $k+k'+r=\ell$ and

$$\begin{aligned}
n^{-d}\,\mathbb{E}(R^I_{n,\ell}(t)R^J_{n,\ell}(t)) &= \sum_{\xi\in\mathbb{Z}^d_n}(1-2a+b)^k b^{k'}(a-b)^r\\
&= \sum_{\xi\in\mathbb{Z}^d_n}\sum_{i=0}^{k}\sum_{j=1}^{r}\binom{k}{i}\binom{r}{j}(1-2a)^i(-1)^{r-j}a^j b^{k-i+k'+r-j}\\
&= \sum_{\xi\in\mathbb{Z}^d_n}\sum_{m=0}^{k+r} b^{\ell-m}\left(\sum_{j=(m-k)_+}^{r\wedge m}\binom{k}{m-j}\binom{r}{j}(1-2a)^{m-j}(-1)^{r-j}a^j\right)\\
&= \sum_{m=0}^{k+r}\theta_{k,r,m}(a)\sum_{\xi\in\mathbb{Z}^d_n} b^{\ell-m}.
\end{aligned}$$

Similarly, we have

$$\mathbb{E}(R^I_{n,\ell}(t))\,\mathbb{E}(R^J_{n,\ell}(t)) = n^{2d}\sum_{m=0}^{k+r} a^{2(\ell-m)}\theta_{k,r,m}(a)$$

and so

$$\begin{aligned}
\mathrm{Cov}(R^I_{n,\ell}(t),R^J_{n,\ell}(t)) &= \sum_{m=0}^{k+r}\theta_{k,r,m}(a)\cdot n^d\sum_{\xi\in\mathbb{Z}^d_n}(b^{\ell-m}-a^{2(\ell-m)})\\
&= \sum_{m=0}^{k+r}\theta_{k,r,m}(a)\cdot\sigma^2_{n,\ell-m}(t).
\end{aligned}$$

By Theorem 1.2, we conclude

$$\lim_{n\to\infty}\frac{1}{n^d h_d(n)}\mathrm{Cov}(R^I_{n,\ell}(t),R^J_{n,\ell}(t)) = \sum_{m=0}^{|I|+|J|}\theta_{k,r,m}(e^{-\frac{u}{G(0)}})\nu_d((\ell-m)u).$$

4. Series expansion

Fix an integer $k\geqslant 1$. Let $\alpha_0,\alpha_i, i\in[k]$ be a sequence of positive real numbers and $\zeta_0:=1<\zeta_1<\zeta_2<\cdots<\zeta_k$ be an increasing sequence of real numbers. Define the function

$$f(z)=\sum_{i=1}^{k}\alpha_i(\zeta_i-z)^{-1} \text{ for } z\notin\{\zeta_i, i\in[k]\}.$$

We notice that f is denoted by a generic function of such form only in this section and different from the one in (2.8).

Lemma 4.1. *The degree k polynomial given by*

$$P_k(z):=\sum_{i=0}^{k}\alpha_i\prod_{0\leqslant j\leqslant k, j\neq i}(\zeta_j-z)=(\alpha_0+(1-z)f(z))\prod_{1\leqslant j\leqslant k}(\zeta_j-z)$$

has k distinct real roots $\gamma_1 < \gamma_2 < \cdots < \gamma_k$. Moreover, we have $1 < \gamma_1 < \zeta_1 < \gamma_2 < \zeta_2 < \cdots < \gamma_k < \zeta_k$ and if $\gamma := 1 + \alpha_0/f(1) < \zeta_1$, then

$$1 + \frac{\alpha_0}{f(\gamma)} \leqslant \gamma_1 \leqslant 1 + \frac{\alpha_0}{f(1)}.$$

Proof of Lemma 4.1: We note that the function $\phi(z) := \alpha_0(1-z)^{-1} + f(z)$ is continuous and strictly increasing in each of the interval (ζ_{i-1}, ζ_i) for $i \in [k]$. Moreover, $\phi(\zeta_i-) = \infty, \phi(\zeta_i+) = -\infty$ for each $i = 0, 1, \ldots, k$. Thus there is a root of ϕ in the interval (ζ_{i-1}, ζ_i), say γ_i, for $i \in [k]$. Now, any root of ϕ is also a root of $P_k(z) := \phi(z)(1-z)\prod_{1\leqslant j\leqslant k}(\zeta_j - z)$. Since P_k is a degree k polynomial, it has exactly k roots and thus $\gamma_i, i \in [k]$ are all the roots of P_k.

Note that f is strictly increasing in the interval $(1, \zeta_1)$. Assume that, $\gamma := 1 + \alpha_0/f(1) < \zeta_1$. It is easy to check that $\hat{\phi}(z) := \alpha_0 + (1-z)f(z)$ satisfies $\hat{\phi}(1) = \alpha_0 > 0$ and $\hat{\phi}(\gamma) = \alpha_0 - \alpha_0 f(\gamma)/f(1) < \alpha_0 - \alpha_0 = 0$. Thus $\gamma_1 < \gamma$.

Moreover, $\alpha_0 + (1-\gamma_1)f(\gamma_1) = 0$ implies that $\gamma_1 = 1 + \alpha_0/f(\gamma_1) > 1 + \alpha_0/f(\gamma)$ as f is increasing and we are done. ■

Note that we have

$$f(\gamma_i) = \frac{\alpha_0}{\gamma_i - 1} > 0, f'(\gamma_i) = \sum_{j=1}^{k} \alpha_j(\zeta_j - \gamma_i)^{-2} > 0 \text{ for } i \in [k].$$

In applications, we have $\alpha_0/f(1) \approx n^{-d} \ll \zeta_1 - 1 \approx n^{-2}$ for $d \geqslant 3$ and thus we have good control on the first root $\gamma_1 \approx 1 + \alpha_0/f(1)$.

Let $\hat{\alpha}_i, i \in [k]$ be another sequence of positive real numbers. Define the function

$$\hat{f}(z) = \sum_{i=1}^{k} \hat{\alpha}_i(\zeta_i - z)^{-1} \text{ for } z \notin \{\zeta_i, i \in [k]\}$$

and

$$g(z) := \frac{\hat{f}(z)}{\alpha_0 + (1-z)f(z)} \text{ for } z \notin \{\gamma_i, i \in [k]\}.$$

Here we define $g(\zeta_i) := \frac{\hat{\alpha}_i}{(1-\zeta_i)\alpha_i}$ so that g is continuously differentiable everywhere except at $\gamma_1, \gamma_2, \ldots, \gamma_k$.

Lemma 4.2. *We have*

$$g(z) = \sum_{i=1}^{k} \frac{1}{\gamma_i - z} \cdot \frac{\hat{f}(\gamma_i)/f(\gamma_i)}{1 + \alpha_0 f'(\gamma_i)f(\gamma_i)^{-2}} \text{ for } z \notin \{\gamma_i, i \in [k]\}.$$

In particular, the coefficient of $z^t, t \geqslant 0$ in the series expansion of g around 0 is given by

$$\sum_{i=1}^{k} \frac{\hat{f}(\gamma_i)}{f(\gamma_i)} \cdot \frac{\gamma_i^{-t-1}}{1 + \alpha_0 f'(\gamma_i)f(\gamma_i)^{-2}} = \frac{\hat{f}(\gamma_1)}{f(\gamma_1)} \cdot \frac{\gamma_1^{-t-1}}{1 + \alpha_0 f'(\gamma_1)f(\gamma_1)^{-2}} + e(t)$$

where

$$|e(t)| \leqslant \max_{i\in[k]} \left|\frac{\hat{f}(\gamma_i)}{f(\gamma_i)}\right| \cdot \zeta_1^{-t}.$$

Proof of Lemma 4.2: We can write g as a ratio of a degree $(k-1)$ and a degree k-polynomial, as

$$g(z) = \frac{\hat{f}(z)\prod_{i=1}^{k}(\zeta_i - z)}{(\alpha_0 + (1-z)f(z))\prod_{i=1}^{k}(\zeta_i - z)} = \frac{\sum_{i=1}^{k} \hat{\alpha}_i \prod_{1\leqslant j\leqslant k, j\neq i}(\zeta_j - z)}{\sum_{i=0}^{k} \alpha_i \prod_{0\leqslant j\leqslant k, j\neq i}(\zeta_j - z)}.$$

The denominator has k distinct real roots given by $\gamma_i, i \in [k]$. Thus, we can write

$$g(z) = \sum_{i=1}^{k} a_i(\gamma_i - z)^{-1}$$

for some real numbers $a_i, i \in [k]$. Moreover, we have

$$a_i = \lim_{z \to \gamma_i} (\gamma_i - z)g(z) = \frac{-\hat{f}(\gamma_i)}{(\alpha_0 + (1-z)f(z))'|_{z=\gamma_i}} = \frac{\hat{f}(\gamma_i)}{f(\gamma_i) + (\gamma_i - 1)f'(\gamma_i)}.$$

Finally we used the fact that $f(\gamma_i) = \frac{\alpha_0}{\gamma_i - 1} > 0$.

The coefficient result follows since $(\gamma_i - z)^{-1} = \sum_{t=0}^{\infty} \gamma_i^{-t-1} z^t$ for $|z| < 1$. Since $\gamma_i > \zeta_1 > 1$ for $i > 1$,

$$|e(t)| \leqslant \sum_{i=2}^{k} |a_i| \cdot \gamma_i^{-t-1} \leqslant \zeta_1^{-t} \cdot \max_{i \in [k]} \left| \frac{\hat{f}(\gamma_i)}{f(\gamma_i)} \right| \cdot \sum_{i=1}^{k} \frac{\gamma_i^{-1}}{1 + \alpha_0 f'(\gamma_1)/f(\gamma_1)^2}$$

and the last sum is $f(0)/(\alpha_0 + f(0)) < 1$, we obtain the bound of $e(t)$ as desired. ■

In our case, we have $\gamma_1 \approx 1 + \Theta(\alpha_0), \alpha_0 = \Theta(n^{-d}), t = \Theta(n^d), \zeta_1 = 1 + \Theta(n^{-2})$, thus the error term is $\exp(-\Theta(n^{d-2}))$ whereas the first term is $\Theta(1)$.

5. Proofs of Auxiliary Results

5.1. *Proof of Lemma 2.2.* By symmetry and translation invariance, it suffices to assume that $0 \leqslant \xi_j \leqslant \frac{n}{2}$ for all $j = 1, 2, \ldots, d$. Recall that $\pi(\xi) = n^{-d}$ is the uniform distribution. Let T_{mix} be the mixing time. It is well known (see Levin et al., 2009, Chapter 4) that $T_{\text{mix}} = O(n^2)$ and there exist $\bar{\gamma} > 0, c > 0$ such that

$$\sup_{\xi \in \mathbb{Z}_n^d} |\mathbb{P}_0(X_t = \xi) - \pi(\xi)| = O(n^{-d} e^{-\bar{\gamma} t/n^2})$$

for $t \geqslant cn^2$. In particular,

$$\sum_{t=cn^2}^{\infty} |\mathbb{P}_0(X_t = \xi) - \pi(\xi)| = O(n^{-d+2})$$

$$\text{and} \sum_{t=cn^2}^{\infty} t\,|\mathbb{P}_0(X_t = \xi) - \pi(\xi)| = O(n^{-d+4}).$$

Clearly, $\mathbb{P}_0(X_t = \xi) = 0$ for $t < \|\xi\|_1$. Thus, what is left is to control the contribution for $\|\xi\|_1 \leqslant t \leqslant cn^2$.

Let S_t be a $\frac{1}{2}$–lazy random walk on $\mathbb{Z}^d$. We can couple the two random walks (S_t, X_t) on $\mathbb{Z}^d, \mathbb{Z}_n^d$, respectively, by defining $X_t = S_t \mod n$, coordinate-wise. Then

$$\mathbb{P}_0(X_t = \xi) = \sum_{k \in \mathbb{Z}^d, \|\xi + nk\|_1 \leqslant t} \mathbb{P}_0(S_t = \xi + nk).$$

In time $t = O(n^2)$, the random walk S_t can visit up to distance of order n with high probability and $\|\xi + nk\|_1 = \Omega(\max\{n, \|\xi\|_1\})$ for $k \neq 0$. In fact, from the local limit theorem (see Lawler, 2013, Theorem 1.2.1), it follows that there exists $K > 0$ such that

$$\mathbb{P}_0(S_t = \xi + nk) \lesssim \left(\frac{d}{2\pi t}\right)^{\frac{d}{2}} e^{-\frac{d\|\xi + nk\|^2}{2t}} + \|\xi + nk\|^{-2} t^{-\frac{d}{2}}$$

for $t \geqslant K$. Assume that $\|\xi\|_1 \geqslant K$. We have

$$I_1 := \sum_{t=\|\xi\|_1}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|\xi+nk\|_1\leqslant t, \|k\|\leqslant\sqrt{d}}} \|\xi + nk\|^{-2} t^{-\frac{d}{2}} \lesssim \|\xi\|^{-2} \sum_{t=\|\xi\|_1}^{cn^2} t^{-\frac{d}{2}} \simeq \|\xi\|^{-\frac{d+2}{2}} .$$

If $\|k\| > \sqrt{d}$, using $\|\xi/n\| \leqslant \sqrt{d}/2$, we have $\frac{1}{2}\|k\| < \|k + \xi/n\| < 2\|k\|$ and

$$\sum_{\substack{k\in\mathbb{Z}^d \\ \|\xi+nk\|_1\leqslant t, \|k\|>\sqrt{d}}} \|\xi + nk\|^{-2} \lesssim n^{-2} \sum_{k\in\mathbb{Z}^d, \|k\|<Ct/n} \|k\|^{-2} \simeq n^{-d} t^{d-2}.$$

Thus

$$I_2 := \sum_{t=\|\xi\|_1}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|\xi+nk\|_1\leqslant t, \|k\|>\sqrt{d}}} \|\xi + nk\|^{-2} t^{-\frac{d}{2}} \simeq n^{-d} \sum_{t=\|\xi\|_1}^{cn^2} t^{\frac{d}{2}-2} \simeq n^{-2}.$$

On the other hand,

$$\begin{aligned} I_3 := \sum_{t=\|\xi\|_1}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|\xi+nk\|_1< t, \|k\|\leqslant\sqrt{d}}} t^{-\frac{d}{2}} e^{-\frac{d\|\xi+nk\|^2}{2t}} &\lesssim \sum_{t=\|\xi\|_1}^{cn^2} t^{-\frac{d}{2}} e^{-\frac{d\|\xi\|^2}{2t}} \\ &\simeq \int_0^\infty t^{-\frac{d}{2}} e^{-\frac{d\|\xi\|^2}{2t}} \simeq \|\xi\|^{2-d} \end{aligned}$$

and

$$I_4 := \sum_{t=\|\xi\|_1}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|\xi+nk\|_1< t, \|k\|>\sqrt{d}}} t^{-\frac{d}{2}} e^{-\frac{d\|\xi+nk\|^2}{2t}} \lesssim \sum_{t=\|\xi\|_1}^{cn^2} \sum_{k\in\mathbb{Z}^d, \|k\|<Ct/n} t^{-\frac{d}{2}} e^{-\frac{dn^2\|k\|^2}{8t}} \lesssim n^{2-d}.$$

In the last inequality, we used the fact that $\sum_{k\in\mathbb{Z}^d} s^{-\frac{d}{2}} e^{-C\|k\|^2/s} \lesssim 1$. Therefore,

$$\begin{aligned} |g_n(\xi)| &\leqslant \sum_{t=cn^2}^{\infty} |\mathbb{P}_0(X_t = \xi) - \pi(\xi)| + \sum_{t=0}^{cn^2} \pi(\xi) + \sum_{t=\|\xi\|_1}^{cn^2} \mathbb{P}_0(X_t = \xi) \\ &\lesssim n^{2-d} + I_1 + I_2 + I_3 + I_4 \\ &\lesssim n^{2-d} + \|\xi\|^{-\frac{d+2}{2}} + \|\xi\|^{2-d} + n^{2-d} + n^{-2}. \end{aligned}$$

We now prove the second assertion. Since $g_n(\xi; z) = \sum_{t=0}^{\infty} z^t(\mathbb{P}_0(X_t = \xi) - \pi(\xi))$, $g_n'(\xi)$ can be written as

$$g_n'(\xi) = \frac{d}{dz} g_n'(\xi; z)\Big|_{z=1} = \sum_{t=0}^{\infty} t(\mathbb{P}_0(X_t = \xi) - \pi(\xi)).$$

As before, it suffices to estimate the summation over $\|\xi\|_1 \leqslant t \leqslant cn^2$. Let $\beta \in (1,2)$. Then

$$\begin{aligned} J_1 &:= \sum_{t=\|\xi\|_1}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|\xi+nk\|_1<n^\beta}} \|\xi+nk\|^{-2} t^{-\frac{d}{2}+1} \\ &\lesssim \|\xi\|^{-2} \sum_{t=\|\xi\|_1}^{cn^2} t^{-\frac{d}{2}+1} + n^{-2} \sum_{t=0}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|k\|<Cn^{\beta-1}}} \|k\|^{-2} t^{-\frac{d}{2}+1} \\ &\lesssim \|\xi\|^{-\frac{d}{2}} + n^{(2-d)(2-\beta)} \end{aligned}$$

and

$$\begin{aligned} J_2 &:= \sum_{t=\|\xi\|_1}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|\xi+nk\|_1<n^\beta}} t^{-\frac{d}{2}+1} e^{-\frac{\|\xi+nk\|^2}{t}} \\ &\lesssim \sum_{t=\|\xi\|_1}^{cn^2} t^{-\frac{d}{2}+1} e^{-\frac{d\|\xi\|^2}{2t}} + \sum_{t=\|\xi\|_1}^{cn^2} \sum_{\substack{k\in\mathbb{Z}^d \\ \|k\|<Cn^{\beta-1}}} t^{-\frac{d}{2}+1} e^{-\frac{dn^2\|k\|^2}{8t}} \lesssim \|\xi\|^{4-d} + n^{4-d}. \end{aligned}$$

By Lawler (2013, Lemma 1.5.1), we get

$$\begin{aligned} J_3 := \sum_{t=\|\xi\|_1}^{cn^2} \sum_{n^\beta\leqslant\|\xi+nk\|_1<t} t\,\mathbb{P}_0(S_t=\xi+nk) &\lesssim \sum_{t=\|\xi\|_1}^{cn^2} \sum_{n^\beta\leqslant\|\xi+nk\|_1<t} t\,\mathbb{P}_0(\|S_t\|\geqslant cn^{\beta+1}) \\ &\lesssim \sum_{t=\|\xi\|_1}^{cn^2} \sum_{n^\beta\leqslant\|\xi+nk\|_1<t} te^{-\frac{cn^{\beta+1}}{t}} \\ &\lesssim n^{d+4} e^{-cn^{\beta-1}}. \end{aligned}$$

Thus, the local central limit theorem yields that for large $\|\xi\|$,

$$\begin{aligned} |g_n'(\xi)| &\leqslant \sum_{t=cn^2}^{\infty} t\,|\mathbb{P}_0(X_t=\xi)-\pi(\xi)| + \sum_{t=0}^{cn^2} t\pi(\xi) + \sum_{t=\|\xi\|_1}^{cn^2} t\,\mathbb{P}_0(X_t=\xi) \\ &\lesssim n^{4-d} + J_1 + J_2 + J_3 \\ &\lesssim n^{4-d} + n^{(2-d)(2-\beta)} + n^{d+4}e^{-cn^{\beta-1}} + \|\xi\|^{-\frac{d}{2}} + \|\xi\|^{4-d} \end{aligned}$$

as desired.

5.2. *Proof of Lemma 2.4*. Take $\varepsilon = G(0)/4 > 0$. By Lemma 2.2, there exist positive integers N_1 and K such that

$$|g_n(0) - G(0)| \leqslant \varepsilon, |g_n(\xi)| \leqslant \varepsilon \text{ for all } \|\xi\| \geqslant K, \xi \in \mathbb{Z}_n^d, n \geqslant N_1.$$

Moreover, we can choose $N \geqslant N_1$, such that

$$\sup_{\|\xi\|\leqslant K} |g_n(\xi) - G(\xi)| \leqslant \varepsilon \text{ for all } n \geqslant N.$$

Fix $n \geqslant N$. Recall that $f_n(\xi) = (g_n(0) + g_n(\xi))/2$. For $\xi \in \mathbb{Z}_n^d$ with $\|\xi\| \geqslant K$ we have

$$f_n(\xi) \geqslant \frac{1}{2}G(0) - \frac{1}{2}|g_n(0) - G(0)| - \frac{1}{2}|g_n(\xi)| \geqslant \varepsilon.$$

For $\xi \in \mathbb{Z}_n^d$ with $\|\xi\| \leqslant K$ we have

$$f_n(\xi) \geqslant \frac{1}{2}(G(0)+G(\xi)) - \frac{1}{2}|g_n(0)-G(0)| - \frac{1}{2}|g_n(\xi)-G(\xi)| \geqslant \varepsilon.$$

5.3. *Proof of Lemma 1.8.* Let $k := \left|\{\lambda_v \mid v \in \mathbb{Z}_n^d\}\right| - 1$. We order the elements of the set $\{1/\widehat{\lambda}_v \mid v \in \mathbb{Z}_n^d \setminus \{0\}\}$ as $\zeta_1 < \zeta_2 < \cdots < \zeta_k$. Clearly, we have,

$$\zeta_1 = \frac{1}{1-\min_{v\in\mathbb{Z}_n^d\setminus\{0\}}\lambda_v} = \frac{1}{1-d^{-1}\sin^2(\pi/n)} = 1 + \frac{\pi^2}{dn^2}(1+o(1))$$

where the minimum is achieved at $\pm e_i, i \in [d]$. One can also see that

$$f_n(\xi;z) = \sum_{i=1}^{k} \alpha_i(\xi)(\zeta_i - z)^{-1}$$

where $\alpha_i(\xi) \geqslant 0$ and $\alpha_1(\xi) \neq 0$. We fix $\xi \in \mathbb{Z}_n^d$ and simply write $\alpha_i(\xi) = \alpha_i$. Let $\alpha_0 = \frac{1}{n^d}$ and $\zeta_0 = 1$. By Lemma 4.1, there exist the distinct roots $\gamma_1(\xi) < \gamma_2(\xi) < \cdots < \gamma_k(\xi)$ for the equation

$$P_k(z) := \sum_{i=0}^{k} \alpha_i \prod_{0\leqslant j\leqslant k, j\neq i} (\zeta_j - z) = (\alpha_0 + (1-z)f_n(\xi;z)) \prod_{1\leqslant j\leqslant k} (\zeta_j - z) = 0.$$

It then follows from Lemma 2.3 and Lemma 4.2, for $t = \Theta(n^d)$ and $f = \widehat{f}$, that

$$\begin{aligned}\mathbb{P}(\tau(0,\xi) > t) &= \sum_{i=1}^{k} \frac{\gamma_i(\xi)^{-t-1}}{1+n^{-d}f_n'(\xi;\gamma_i(\xi))f_n(\xi;\gamma_i(\xi))^{-2}} \\ &= \frac{\gamma_1(\xi)^{-t-1}}{1+n^{-d}f_n'(\xi;\gamma_1(\xi))f_n(\xi;\gamma_1(\xi))^{-2}} + e(t) \qquad (5.1)\end{aligned}$$

where $|e(t)| \leqslant \zeta_1^{-t} \leqslant e^{-\Theta(n^{d-2})}$ and $\gamma_1(\xi) = 1 + \frac{n^{-d}}{f_n(\xi;\gamma_1(\xi))}$. From now on, we use $r_n(\xi) = \gamma_1(\xi)$ to emphasize its dependence on n.

Let $z = r_n(\xi)$, then $z - 1 = \frac{1}{n^d f_n(\xi;z)}$. We use the notations $f_n(\xi) = f_n(\xi;1)$ and $f_n'(\xi) = f_n'(\xi;1)$. There exist $\widetilde{z}$ and $\overline{z}$ between 1 and γ_1 such that

$$\begin{aligned}f_n(\xi;z) &= f_n(\xi) + f_n'(\xi)(z-1) + \frac{1}{2}f_n''(\xi;\widetilde{z})(z-1)^2 \\ &= f_n(\xi) + \frac{f_n'(\xi)}{n^d f_n(\xi)}\left(1 + \frac{f_n'(\xi;\overline{z})}{n^d f_n(\xi) f_n(\xi;z)}\right)^{-1} + \frac{f_n''(\xi;\widetilde{z})}{2n^{2d} f_n(\xi;z)^2}.\end{aligned}$$

Note that, $|f''(\xi;z)| \leqslant |f_n''(0)| \leqslant n^{-d}\sum_{v\in\mathbb{Z}_n^d\setminus\{0\}} |\lambda_v|^{-3}$ for $|z| \leqslant 1$. By Lemma 2.1 with $k = 3$, we have $f_n''(\xi;\widetilde{z}) = O(n^3)$. It then follows from Lemma 2.4 that

$$f_n(\xi;r_n(\xi)) = f_n(\xi)\left(1 + \frac{f_n'(\xi)}{n^d f_n(\xi)^2} + O(n^{3-2d})\right). \qquad (5.2)$$

Applying (5.2) to $r_n(\xi)$, we get

$$\begin{aligned}\log(r_n(\xi)) &= \log\left(1 + \frac{1}{n^d f_n(\xi;r_n(\xi))}\right) \\ &= \log\left(1 + \frac{1}{n^d f_n(\xi)}\left(1 - \frac{f_n'(\xi)}{n^d f_n(\xi)^2} + O(n^{3-2d})\right)\right) \\ &= \frac{1}{n^d f_n(\xi)} - \frac{1}{n^{2d}}\left(\frac{f_n'(\xi)}{f_n(\xi)^3} + \frac{1}{2f_n(\xi)^2}\right) + O(n^{3-3d}),\end{aligned}$$

which yields

$$r_n(\xi)^{-(t+1)} = e^{-\frac{u}{f_n(\xi)}} \left(1 + \frac{u}{n^d}\left(\frac{f_n'(\xi)}{f_n(\xi)^3} + \frac{1}{2f_n(\xi)^2}\right) + O(n^{3-2d})\right).$$

By (5.2) and (5.1), we conclude

$$\begin{aligned}\mathbb{P}(\tau(0,\xi) > t) &= \frac{r_n(\xi)^{-t-1}}{1 + n^{-d} f_n'(\xi; r_n(\xi)) f_n(\xi; r_n(\xi))^{-2}} + e(t) \\ &= e^{-\frac{u}{f_n(\xi)}} \left(1 + \frac{u}{n^d}\left(\frac{f_n'(\xi)}{f_n(\xi)^3} + \frac{1}{2f_n(\xi)^2}\right) - \frac{f_n'(\xi)}{n^d f_n(\xi)^2}\right) + O(n^{3-2d}).\end{aligned}$$

6. Discussion and Further Questions

(1) As we have seen, our proofs are based on a precise tail probability of the hitting time at two points, which follows from an analytic observation of the generation function of hitting probabilities. A natural question is whether one can obtain an accurate tail behavior on the hitting time based on a probabilistic argument such as conditioning or constructing an appropriate coupling. Such an approach might give us an intuitive explanation of the asymptotic behavior and enable us to understand how the variance is created and grows.

(2) Once the limiting behavior of the mean and the variance of the size of the vacant set are known, it is natural to ask if the size of the vacant set with an appropriate normalization converges to a limiting distribution. Simulation results for $d = 3, 4, 5$ (see Figure 6.1) suggest that a Gaussian central limit theorem holds for all $d \geqslant 3$ and $u > 0$. It would also be interesting to figure out the covariance structure of the vacant sets at different times and see if the vacant set's size as a stochastic process indexed by u converges to a Gaussian process.

(3) Instead of the size, one can consider the vacant set $\mathcal{V}_n^{(\ell)}(un^d)$ or its complement as a set-valued process indexed by u. Then, it would be interesting to see the scaling limit of the random set up to a time proportional to the size of $\mathbb{Z}_n^d$ as a subset of the continuum torus $[0,1]^d$. Results about internal distance for the range of a random walk up to time un^d are studied in Procaccia and Shellef (2014); Černý and Popov (2012) for $d \geqslant 3$. Note that up to the cover time of order $n^d \log n$, the scaling limit of the vacant set is studied by Belius (2013); Miller and Sousi (2017).

(4) Miller (2013) studied the trace by two competing random walks on the discrete torus $\mathbb{Z}_n^d$ until the torus is fully covered. It is natural to consider the trace at a time scale proportional to n^d. In particular, one can ask how the variance behaves as the time level grows and see if there is a time threshold for the limiting variance.

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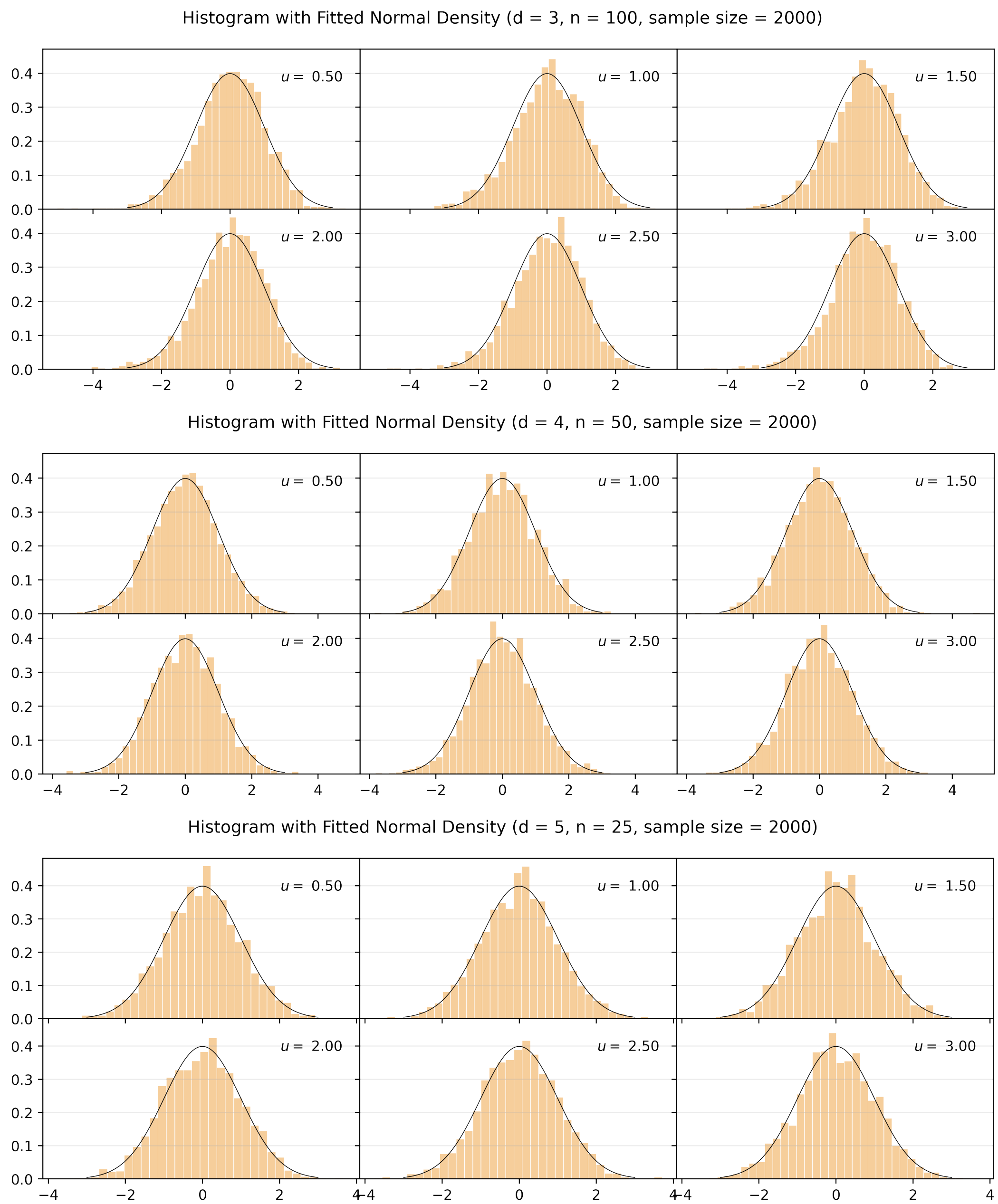

FIGURE 6.1. Histograms with fitted Gaussian density based on 2000 samples in dimension $d = 3, 4$ and 5, respectively.

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