Homogenization of a Random Walk with Irreversible Rates on a Graph in d Dimensions

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Preston Donovan and Muruhan Rathinam

Department of Mathematics and Statistics, University of Maryland, Baltimore County
1000 Hilltop Circle
Baltimore, MD 21250, USA

Abstract

We study a periodic, directed graph and the continuous time random walk $Z(t)$ on the graph's nodes (assumed to be isolated points in $\mathbb{R}^d$), which jumps along the graph's edges with jump rates given by the edge weights. We do not assume that the edge weights are reversible. The main result is that, under certain conditions on the graph, the scaled process $\varepsilon Z(t/\varepsilon^2)$ converges weakly in the Skorokhod space to a Brownian motion. The diffusivity of the limiting Brownian motion can be computed by solving a set of linear algebra problems. An intuitive derivation via formal asymptotic expansion and a rigorous proof of convergence are provided. We show that reversible rates, detailed balance, and certain symmetries of the graph are each alone sufficient for the convergence. For the case of reversible jump rates, an equivalent variational formulation is derived. This derivation involves developing notions of gradient for functions on the graph's nodes, divergence for $\mathbb{R}^d$-valued functions on the graph's edges, and a divergence theorem. This work is partially motivated by the modeling of a particle's random motion in an obstructed environment where the particle may interact with the obstructions.

1 Introduction

We consider a periodic, weighted, directed graph embedded in the Euclidean space $\mathbb{R}^d$ and the associated random walk $Z(t)$ in continuous time $t \geq 0$. The random walk takes place on the nodes (vertices) of the graph and jumps along the edges with jump rates given by the edge weights. The main result is that, under certain conditions on the graph, the scaled process $\varepsilon Z(t/\varepsilon^2)$ converges weakly to a Brownian motion. The diffusivity of the limiting Brownian motion can be computed by solving a set of linear algebra problems.

The motivation for our problem arises, in part, from modeling the random motion of a particle in an environment with obstructions. The particle may have some form of interaction (attraction, repulsion, or bonding) with the obstructions and the mean path length of the random motion of the particle may be nonnegligible compared to the characteristic fine-scale length of the environment. Such a situation arises for a solute in an aqueous polymer gel or polymer solution where the solute may have interactions with the polymer molecules forming the obstruction. Moreover, since the

"pore sizes" in the gels can be as small as 10 nanometers or less, the mean path length in water of a solute may be nonnegligible. This leads one to consider, as a starting point, a fine-scale model involving a random walk with nonzero path length or jump sizes.

To the best of our knowledge, current literature on scaling limits of random walks on graphs is limited to the special case of lattices $\mathbb{Z}^d$ where edges connect the lattice's nodes with their $2d$ nearest neighbors. Additionally, current literature assumes the jump rates are assumed to be reversible, meaning that the rate of jumping from x to y is equal to that of jumping from y to x. We refer the reader to [17, 13, 15] for the earliest results on this topic where the scaling limit of a random walk on a lattice with random conductances (assumed to be reversible) is considered. We note that the terminology "conductance" was used for jump rates. These works assumed nonzero conductances with a uniform lower bound. Later work [2, 9, 18, 4] studied the scaling limit of a random walk on a percolation lattice, where the conductances were allowed to be zero with a probability that ensures the existence of a unique infinite cluster. Additional related results can be found in [19, 11, 7, 10].

The reversible jump rates assumption does not allow one to capture interactions such as attraction, repulsion, and bond formation mentioned above. Our work does not assume reversible jump rates. Moreover, the graph structure considered is very general in that the set of nodes (vertices) is not confined to the lattice $\mathbb{Z}^d$ (or a subset of it) and the edges can be very general. On the other hand, while most of the aforementioned works consider either i.i.d. or stationary and ergodic jump rates, our work is restricted to the simpler periodic case. We believe that, by exploiting the ideas that connect the periodic case with the stationary and ergodic case [19, 10], the results of this manuscript can be extended to the stationary and ergodic case.

From an application point of view, our previous work [6] demonstrated the feasibility of applying homogenization theory to predict solute motion in aqueous polymer solutions via comparison with experimental data. This work considered the simplest possible geometry of periodically placed spherical obstacles with the diffusion equation. To properly model polymer gels, more complex geometries and interactions with the solute are needed. We believe that the discrete graph approach provides a simple way to deal with complex obstruction geometries as well as interactions.

The paper is organized as follows. Details of the graph structure and its induced random walk are outlined in Section 2. Section 3 provides an intuitive derivation of the effective diffusivity via a formal asymptotic expansion. This yields a set of so-called "unit-cell" problems to be solved. For non-reversible jump rates, the unit-cell problem may not be solvable. We provide the necessary and sufficient condition for the solvability of the unit-cell problem. Usually, the verification of these conditions involves computing the stationary distribution of a process Y that is related to Z. In Section 4 we provide some sufficient conditions for the solvability of the unit-cell problems that can be verified without computing the stationary distribution. Section 5 derives an equivalent variational formulation that holds when the jump rates are reversible. This result generalizes the existing results in the literature to graphs with nodes that are not necessarilly subsets of the integer lattice $\mathbb{Z}^d$. Section 6 proves the rigorous convergence result for the scaled random walk. In Section 7 we provide some numerical results that illustrate how the path length variation and interactions of the random walker with obstructions (attraction, repulsion or bonding) affect the effective diffusivity. Appendix A confirms that the effective diffusivities predicted by the rigorous result and the formal asymptotics agree.

2 Mathematical preliminaries

2.1 Directed graph

Define a *weighted, directed graph* to be a triple $(\mathcal{S}, \mathcal{E}, \lambda)$, where $\mathcal{S} \subset \mathbb{R}^d$ is a countable set of *nodes*, $\mathcal{E} \subset \mathcal{S} \times \mathcal{S}$ is the *directed edge set*, and $\lambda : \mathcal{E} \to (0, \infty)$ is a positive edge function. We will use the term *graph* and *weighted, directed graph* interchangeably. A directed graph is *strongly connected* if each node can reach every other node via traversing edges in the direction they point.

   Assumption 1: The graph $(\mathcal{S}, \mathcal{E}, \lambda)$ is strongly connected and invariant under integer translations and the node set $\mathcal{S} \subset \mathbb{R}^d$ is countable.

   Invariance under integer vector translations means for all $n \in \mathbb{Z}^d$,

1. If $x \in \mathcal{S}$ then $x + n \in \mathcal{S}$.

2. If $(x, y) \in \mathcal{E}$ then $(x + n, y + n) \in \mathcal{E}$.

3. If $(x, y) \in \mathcal{E}$ then $\lambda(x + n, y + n) = \lambda(x, y)$.

We sometimes write $\lambda(e)$ as λ_e. For an edge $e = (x, y) \in \mathcal{E}$, denote the *originating node* $\partial_- e := x$ and the *terminal node* $\partial_+ e := y$. Given a node $y \in \mathcal{S}$, let $\mathcal{E}_y$ denote the subset of edges that originate in y and conversely let $\mathcal{E}'_y$ denote the subset of edges that terminate in y. That is,

$$\mathcal{E}_y := \{e \in \mathcal{E} : \partial_- e = y\} \text{ and } \mathcal{E}'_y := \{e \in \mathcal{E} : \partial_+ e = y\}.$$

2.2 Random walk on graph

A graph $(\mathcal{S}, \mathcal{E}, \lambda)$ satisfying Assumption 1 induces a Markov process $Z(t)$ in continuous time taking values in $\mathcal{S}$ with *intensity* or *jump rate* from $x \in \mathcal{S}$ to $y \in \mathcal{S}$ given by $\lambda(x, y)$. The *generator* of Z is given by

$$\sum_{(y,z) \in \mathcal{E}_y} (f(z) - f(y))\lambda(y, z),$$

where $f \in \mathbb{R}^{\mathcal{S}}$ is bounded. If $\mathcal{E}_y$ is finite for all y, this is defined for all $f \in \mathbb{R}^{\mathcal{S}}$.

   Introduce the following equivalence relation on $\mathcal{S}$: two nodes $x, y \in \mathcal{S}$ are equivalent if and only if $x - y \in \mathbb{Z}^d$. Let $\bar{\mathcal{S}}$ denote the set of equivalent classes of $\mathcal{S}$. We shall identify $\bar{\mathcal{S}} = \mathcal{S} \cap [0, 1)^d$. By Assumption 1, $\bar{\mathcal{S}}$ is strongly connected. Let $\Pi : \mathcal{S} \to \bar{\mathcal{S}}$ be the natural projection that maps an element to its equivalent class.

   Introduce the following equivalence relation on $\mathcal{E}$: two edges $(x, x'), (y, y') \in \mathcal{E}$ are equivalent if and only if there exists $n \in \mathbb{Z}^d$ such that $x - y = x' - y' = n$. Let $\bar{\mathcal{E}}$ denote the set of equivalence classes of $\mathcal{E}$. Note that $\bar{\mathcal{E}}$ may not be a subset of $\bar{\mathcal{S}} \times \bar{\mathcal{S}}$ and that we may identify $\bar{\mathcal{E}} = \cup_{y \in \bar{\mathcal{S}}} \mathcal{E}_y$. By Assumption 1, if $e_1, e_2 \in \mathcal{E}$ belong to the same equivalence class then $\lambda(e_1) = \lambda(e_2)$.

   Assumption 2: The node set $\bar{\mathcal{S}}$ and edge set $\bar{\mathcal{E}}$ contain finitely many elements.

   Thus, $\mathcal{S}$ and $\mathcal{E}$ are countable. For any edge function $g \in (\mathbb{R}^d)^{\mathcal{E}}$, we have the following trivial but useful identities:

$$\sum_{e \in \bar{\mathcal{E}}} g(e) = \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} g(e) = \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}'_y} g(e). \tag{1}$$

By Assumption 2, these summations are well defined.

By Assumptions 1 and 2, the projected process

$$Y(t) := \Pi Z(t)$$

is a Markov process with the finite state space $\bar{\mathcal{S}}$ that jumps along edges in $\mathcal{E}_\Pi = (\Pi \times \Pi)(\mathcal{E})$. The jump rate is given by $\bar{\lambda} : \mathcal{E}_\Pi \to (0, \infty)$ where

$$\bar{\lambda}(x, y) = \sum_{\substack{(x,z) \in \mathcal{E}_x \\ \pi(z) = y}} \lambda(x, z)$$

for $(x, y) \in \mathcal{E}_\Pi$. Note the following properties of $\mathcal{E}_\Pi$:

1. $\mathcal{E}_\Pi \subset \bar{\mathcal{S}} \times \bar{\mathcal{S}}$.

2. For every $e \in \mathcal{E}_\Pi$ there exists at least one edge $e' \in \bar{\mathcal{E}}$ such that $\Pi(e') = e$.

3. For every $e \in \mathcal{E}_\Pi$, $\bar{\lambda}(e) > 0$.

The third property follows because $\lambda > 0$. Clearly the graph $(\bar{\mathcal{S}}, \mathcal{E}_\Pi)$ is strongly connected. This implies that Y is an ergodic Markov process, which will be useful.

For each edge $e = (x, y) \in \mathcal{E}$, we denote the *jump size* by $\nu_e := y - x$. Hence, using the random time change representation [8] we can write

$$Z(t) = z_0 + \sum_{e \in \bar{\mathcal{E}}} \nu_e R_e \left(\lambda_e \int_0^t 1_{\{\partial_- e\}}(Y(s)) ds \right), \tag{2}$$

where $\{R_e\}_{e \in \bar{\mathcal{E}}}$ is a collection of independent unit-rate Poisson processes.

Define the *rate matrix* $L : \bar{\mathcal{S}} \times \bar{\mathcal{S}} \to \mathbb{R}$ of $(\mathcal{S}, \mathcal{E}, \lambda)$ by

$$L(x, y) := \begin{cases} \bar{\lambda}(x, y) & x \neq y \\ -\sum_{y \in \bar{\mathcal{S}} \setminus \{x\}} L(x, y) & x = y \\ 0 & \text{otherwise.} \end{cases} \tag{3}$$

We may regard L as a linear map $\mathbb{R}^{\bar{\mathcal{S}}} \to \mathbb{R}^{\bar{\mathcal{S}}}$ where

$$(Lf)(y) = \sum_{e \in \mathcal{E}_y} (f(y + \nu_e) - f(y)) \lambda_e, \tag{4}$$

for $f \in \mathbb{R}^{\bar{\mathcal{S}}}$. In this view, L is the generator of the process Y and we note that arithmetic involving ν_e is calculated modulo 1.

For $y \in \bar{\mathcal{S}}$ define

$$\lambda^0(y) := \sum_{e \in \mathcal{E}_y} \bar{\lambda}(e). \tag{5}$$

The transpose of L, given by $L^T(y, z) = L(z, y)$, can also be regarded as a linear operator on $\mathbb{R}^{\bar{\mathcal{S}}}$ where

$$(L^T f)(y) = \sum_{e \in \mathcal{E}'_y} f(y - \nu_e) \lambda_e - f(y) \lambda^0(y), \tag{6}$$

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for $f \in \mathbb{R}^{\bar{S}}$. Throughout this discussion we typically regard L and L^T as linear operators rather than functions on $\bar{S} \times \bar{S}$. The appropriate interpretation will be obvious.

Standard Markov process theory shows that Y is an ergodic process because $\bar{S}$ is finite and $(\bar{S}, \mathcal{E}_\Pi)$ is strongly connected. Hence, L^T has a one-dimensional null space that contains a function $\pi \in \mathbb{R}^{\bar{S}}$ such that $\pi(y) > 0$ for all $y \in \bar{S}$ and $\sum_{y \in \bar{S}} \pi(y) = 1$. In other words, π is the unique stationary probability measure of process Y. In the following discussion, π will play a central role.

For any $\varepsilon > 0$, define the scaled process

$$Z_\varepsilon(t) := \varepsilon Z(t/\varepsilon^2). \tag{7}$$

Our main result is that, under certain assumptions, Z_ε converges weakly to a Brownian motion as $\varepsilon \to 0$. We first demonstrate the result in Section 3 via an asymptotic expansion, in an intuitive but formal approach. The result is confirmed rigorously in Section 6, which makes use of the random time change representation, martingale functional central limit theorem, and ergodicity of Y.

3 Formal asymptotics

The homogenization result for PDEs is often motivated by a formal asymptotic expansion, which leads to the so-called unit-cell problems [12, 1]. We shall derive an analogous asymptotic expansion leading to unit-cell problems and a formula for the effective diffusivity. This result will be proven rigorously in Section 6.

3.1 Anzats

Denote the probability mass function of $Z_\varepsilon(t)$ by $p_\varepsilon(t, z)$, where $z \in \varepsilon S$. The Kolmogorov forward equations are:

$$\frac{\partial p_\varepsilon}{\partial t}(t, z) = \frac{1}{\varepsilon^2} \sum_{e \in \mathcal{E}'_y} p_\varepsilon(t, z - \varepsilon \nu_e) \lambda_e - \frac{1}{\varepsilon^2} \lambda^0(y) p_\varepsilon(t, z), \tag{8}$$

for all $z \in \varepsilon S$. We shall seek an asymptotic expansion of the form

$$p_\varepsilon(t, z) = p_0(t, z, y) + \varepsilon p_1(t, z, y) + \varepsilon^2 p_2(t, z, y) + \dots, \tag{9}$$

where $p_j : [0, \infty) \times \mathbb{R}^d \times \bar{S} \to [0, \infty)$ and $y = \Pi(z/\varepsilon) \in \bar{S}$. We assume that p_j is sufficiently differentiable in z for $j = 0, 1, 2$. The machinery behind this asymptotic analysis involves substitution of the expansion (9) into the forward equations (8) and Taylor expansion about z, which yields:

$$
\begin{aligned}
\frac{\partial p_0}{\partial t}(t, z) = {} & \frac{1}{\varepsilon^2} \sum_{e \in \mathcal{E}'_y} \Big(p_0(t, z, y - \nu_e) \lambda_e + \varepsilon p_1(t, z, y - \nu_e) \lambda_e + \varepsilon^2 p_2(t, z, y - \nu_e) \Big) \lambda_e \\
& - \frac{1}{\varepsilon} \sum_{e \in \mathcal{E}'_y} \Big(\nu_e^T \nabla_z p_0(t, z, y - \nu_e) \lambda_e + \varepsilon \nu_e^T \nabla_z p_1(t, z, y - \nu_e) \Big) \lambda_e \\
& + \frac{1}{2} \sum_{e \in \mathcal{E}'_y} \nu_e^T D_{zz} p_0(t, z, y - \nu_e) \nu_e \lambda_e \\
& - \frac{1}{\varepsilon^2} \lambda^0(y) \Big(p_0(t, z, y) + \varepsilon p_1(t, z, y) + \varepsilon^2 p_2(t, z, y) \Big) + O(\varepsilon).
\end{aligned} \tag{10}
$$

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We note that we use ∇_z for the first derivative and D_{zz} for the second derivative so that $D_{zz}p_0$ is the Hessian. Equating like powers of $\varepsilon^{-2}, \varepsilon^{-1}$, and ε^0 in (10) yields a hierarchy of problems. Solving these problems yields the homogenized equation governing p_0, which is (formally) the probability density function describing the limiting motion of Z_ε as $\varepsilon \to 0$.

3.2 Stationary distribution

Equating like powers of ε^{-2} in (10), we have:

$$0 = -\lambda^0(y)p_0(t, z, y) + \sum_{e \in \mathcal{E}'_y} p_0(t, z, y - \nu_e)\lambda_e,$$

for all $z \in \varepsilon\mathcal{S}$ and $y = \Pi(z/\varepsilon) \in \bar{\mathcal{S}}$. This can be written as $L^T p_0(t, z, .) = 0$. Since $(\bar{\mathcal{S}}, \mathcal{E}_\Pi, \lambda)$ is a strongly connected graph, Y is an ergodic Markov process and L^T has a one dimensional null space spanned by the stationary distribution $\pi \in \mathbb{R}^{\bar{\mathcal{S}}}$. Thus for any fixed t, z, there exists a constant $\bar{p}(t, z)$ such that

$$p_0(t, z, y) = \bar{p}(t, z)\pi(y), \tag{11}$$

where

$$(L^T \pi)(y) = 0, \quad \sum_{y \in \bar{\mathcal{S}}} \pi(y) = 1. \tag{12}$$

3.3 Unit-cell problem

Equating like powers of ε^{-1} in (10), we have:

$$0 = \sum_{e \in \mathcal{E}'_y} p_1(t, z, y - \nu_e)\lambda_e - \sum_{e \in \mathcal{E}'_y} \nu_e^T \nabla_z \bar{p}(t, z)\lambda_e \pi(y - \nu_e) - \lambda^0(y)p_1(t, z, y),$$

for all $z \in \varepsilon\mathcal{S}$ and $y = \Pi(z/\varepsilon) \in \bar{\mathcal{S}}$. Defining $\sigma \in (\mathbb{R}^d)^{\bar{\mathcal{S}}}$ by

$$\sigma(y) := \sum_{e \in \mathcal{E}'_y} \nu_e \lambda_e \pi(y - \nu_e), \tag{13}$$

this can be written as

$$(L^T p_1(t, z, \cdot))(y) = \nabla_z \bar{p}(t, z)^T \sigma(y).$$

Hence the relationship between p_1 and $\bar{p}$:

$$p_1(t, z, y) = \nabla_z \bar{p}(t, z)^T \omega(y), \tag{14}$$

where $\omega \in (\mathbb{R}^d)^{\bar{\mathcal{S}}}$ is a solution to the *unit-cell problem*:

$$(L^T \omega)(y) = \sigma(y) \quad \text{for all } y \in \bar{\mathcal{S}}. \tag{15}$$

The unit-cell problem and its solvability will play a crucial role throughout this discussion.

Lemma 3.1. *The unit-cell problem (15) is solvable if and only if*

$$\sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e \lambda_e \pi(y) = 0. \tag{16}$$

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Proof. In order for the unit-cell problem to be solvable, it is necessary and sufficient that σ be orthogonal to the null space of L. Because the null space of L consists of constant functions, this is equivalent to $\sum_{y \in \bar{S}} \sigma(y) = 0$. That is,

$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}'_y} \nu_e \lambda_e \pi(y - \nu_e) = 0.$$

Using (1) and noting $y - \nu_e = \partial_- e$ for all $e \in \mathcal{E}'_y$, this is equivalent to

$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \nu_e \lambda_e \pi(y) = 0.$$

$\square$

3.4 Effective diffusivity

We now show $\bar{p}$ is governed by the diffusion equation with effective diffusivity matrix, $K \in \mathbb{R}^{d \times d}$:

$$\frac{\partial \bar{p}}{\partial t}(t, z) = \text{div}_z \cdot (K \nabla_z \bar{p}(t, z)). \tag{17}$$

This suggests that Z_ε tends to a Brownian motion whose covariance matrix is given by $2Kt$. Before proceeding, we introduce an easily verifiable lemma.

Lemma 3.2. *For any symmetric $A \in \mathbb{R}^{d \times d}$ and $x, y \in \mathbb{R}^d$,*

$$\text{trace}(A D_{zz} \bar{p}(t, z)) = \text{div}_z(A \nabla_z \bar{p}(t, z))$$

and

$$\text{trace}(A x y^T) = x^T A y.$$

Balancing the ε^0 terms in (10) yields

$$\frac{\partial \bar{p}}{\partial t}(t, z) \pi(y) = (L^T p_2(t, z, .))(y) - \sum_{e \in \mathcal{E}'_y} \nu_e^T \nabla_z p_1(t, z, y - \nu_e) \lambda_e$$

$$+ \frac{1}{2} \sum_{e \in \mathcal{E}'_y} \nu_e^T D_{zz} \bar{p}(t, z) \nu_e \lambda_e \pi(y - \nu_e)$$

for all $z \in \varepsilon S$ and $y = \Pi(z/\varepsilon) \in \bar{S}$. Since the range of L^T consists of functions that sum to zero, summing the above over $y \in \bar{S}$ eliminates p_2 terms and yields

$$\frac{\partial \bar{p}}{\partial t}(t, z) = \frac{1}{2} \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}'_y} \nu_e^T D_{zz} \bar{p}(t, z) \nu_e \lambda_e \pi(y - \nu_e) - \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}'_y} \nu_e^T D_{zz} \bar{p}(t, z) \omega(y - \nu_e) \lambda_e,$$

where we have used (14). Use (1) to rewrite this as

$$\frac{\partial \bar{p}}{\partial t}(t, z) = \frac{1}{2} \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \nu_e^T D_{zz} \bar{p}(t, z) \nu_e \lambda_e \pi(y) - \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \nu_e^T D_{zz} \bar{p}(t, z) \omega(y) \lambda_e.$$

Then by symmetry of $D_{zz}\bar{p}(t,z)$ and Lemma 3.2,

$$\frac{\partial\bar{p}}{\partial t}(t,z) = \frac{1}{2}\text{trace}\left[D_{zz}\bar{p}(t,z)\sum_{y\in\bar{S}}\sum_{e\in\mathcal{E}_y}\left(\nu_e\nu_e^T\lambda_e\pi(y) - \nu_e\omega(y)^T\lambda_e - \omega(y)\nu_e^T\lambda_e\right)\right]$$

$$= \text{div}_z(K\nabla_z\bar{p}(t,z)),$$

where

$$K := \frac{1}{2}\sum_{y\in\bar{S}}\sum_{e\in\mathcal{E}_y}\left(\nu_e\nu_e^T\lambda_e\pi(y) - \nu_e\omega(y)^T\lambda_e - \omega(y)\nu_e^T\lambda_e\right). \tag{18}$$

4 Solvability conditions

Given the graph $(\mathcal{S},\mathcal{E},\lambda)$ define the *drift field* $\rho:\bar{S}\to\mathbb{R}^d$ by

$$\rho(y) = \sum_{e\in\mathcal{E}_y}\nu_e\lambda_e. \tag{19}$$

Then the Lemma 3.1 states that the unit-cell problem is solvable if and only if the expected value of the drift field with respect to the stationary distribution π is zero. We take a closer look at this condition in this section.

4.1 Detailed balance implies solvability

When the generator L is symmetric, that is when the jump rates are reversible, it is easy to verify that the unit-cell problem is always solvable by using the fact that π is the uniform distribution and the relation (1). Theorem 4.2 generalizes this observation to provide a sufficient condition.

Recall that $\bar{S}$ is a finite set of nodes. Define the inner product on $(\mathbb{R}^d)^{\bar{S}}$ with respect to a measure p by

$$(f,g)_p := \sum_{y\in\bar{S}}f(y)^Tg(y)p(y). \tag{20}$$

for $f,g\in(\mathbb{R}^d)^{\bar{S}}$. If no measure is specified, we assume $p\equiv 1$. A linear map $A:(\mathbb{R}^d)^{\bar{S}}\to(\mathbb{R}^d)^{\bar{S}}$ is said to be *symmetric with respect to p* if $(Af,g)_p = (f,Ag)_p$ for all $f,g\in\mathbb{R}^{\bar{S}}$. The projected process Y is said to satisfy *detailed balance* if

$$L(y,z)\pi(y) = L(z,y)\pi(z). \tag{21}$$

for all $y,z\in\bar{S}$.

Lemma 4.1. *The process Y satisfies the detailed balance condition if and only if L is symmetric with respect to the stationary distribution.*

Proof. Suppose L is symmetric with respect to the stationary distribution, π. Fix distinct $w,x\in\bar{S}$ and let $f(y) = 1_{\{w\}}(y)$ and $g(y) = 1_{\{x\}}(y)$. Then by symmetry of L with respect to π,

$$\sum_{y\in\bar{S}}(Lf)(y)g(y)\pi(y) = \sum_{y\in\bar{S}}f(y)(Lg)(y)\pi(y),$$

which is equivalent to
$$L(w,x)\pi(w) = L(x,w)\pi(x).$$
Now, suppose the detailed balance condition holds. Then for any $f, g \in \mathbb{R}^{\bar{S}}$,
$$(Lf, g)_\pi = \sum_{y \in \bar{S}} (Lf)(y)g(y)\pi(y) = \sum_{y \in \bar{S}} \sum_{z \in \bar{S}} L(y,z)f(z)g(y)\pi(y)$$
$$= \sum_{y \in \bar{S}} \sum_{z \in \bar{S}} L(y,z)f(z)g(y)\pi(y) = (f, Lg)_\pi.$$

Hence L is symmetric with respect to the stationary distribution and we have the desired result. $\square$

Theorem 4.2. *If Y satisfies the detailed balance condition (21) then the unit-cell problem (15) is solvable. As a special case, if L is symmetric (i.e., rates are reversible) then the unit-cell problem is solvable.*

Proof. From Lemma 4.1, detailed balance is equivalent to symmetry with respect to the stationary distribution. Substituting definitions and moving all terms to one side, it is simple to show that L being symmetric with respect to the stationary distribution is equivalent to: for all $f, g \in (\mathbb{R}^d)^{\bar{S}}$,
$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \left(g(\partial_+ e)^T f(\partial_- e) - f(\partial_+ e)^T g(\partial_- e) \right) \lambda_e \pi(y) = 0.$$

Substituting $g(y) = y$ and $f(y) = c$ for some nonzero constant c, we have
$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} (\partial_+ e - \partial_- e)\lambda_e \pi(y) = 0,$$

which is equivalent to solvability of the unit-cell problem. If L is symmetric, then π is a constant function and the solvability follows immediately. $\square$

Note that the reverse implication of Theorem 4.2 does not hold. As a counter example, consider the "whirlpool" graph depicted in Figure 1. Here,
$$\bar{S} = \{(0,0), (1/3,0), (2/3,0), (0,1/3), (2/3,1/3), (0,2/3), (1/3,2/3), (2/3,2/3)\}$$
$$=: \{y_1, y_2, y_3, y_4, y_5, y_6, y_7, y_8\}.$$

The edge set can easily be deduced from Figure 1. The edge set $\bar{\mathcal{E}}$ is depicted. Every edge has the same jump rate $\bar{\lambda} > 0$. We show that this graph has a solvable unit-cell problem, but L is not symmetric with respect to the stationary distribution.

Simple algebra shows that σ, the right-hand side of the unit-cell problem (13), is given by
$$\sigma_1(y_i) := \begin{cases} 1/8 & i = 1,2,3 \\ 0 & i = 4,5 \\ -1/8 & i = 6,7,8 \end{cases}$$
and
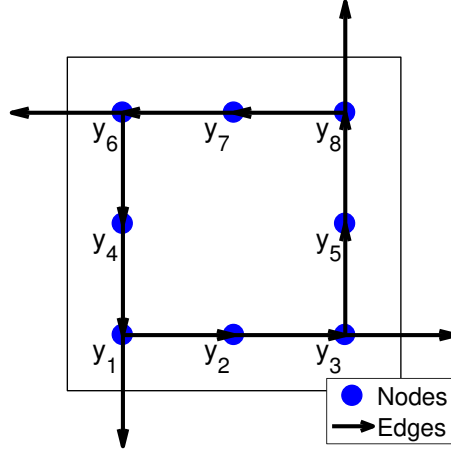$$\sigma_2(y_i) := \begin{cases} 1/8 & i = 3,5,8 \\ 0 & i = 2,7 \\ -1/8 & i = 1,4,6. \end{cases}$$

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Figure 1: The "whirlpool" example has a solvable unit-cell problem and a rate matrix L that is not symmetric with respect to π. All edges have the same jump rate $\bar{\lambda}$.

Clearly, $\sum_{y \in \bar{S}} \sigma(y) = 0$ and thus the unit-cell problem is solvable. Note that the stationary distribution is given by $\pi(y) = 1/8$ for all $y \in \bar{S}$. This can easily be seen by examining the rate matrix L. To see that L is not symmetric with respect to π, fix any $(p, q) \in \bar{\mathcal{E}}$ and let $f(y) = 1_{\{p\}}(y)$ and $g(y) = 1_{\{q\}}(y)$. Then $(Lf, g)_\pi \neq (f, Lg)_\pi$.

4.2 Sufficient symmetries of the graph imply solvability

Since the verification of the condition in Lemma 3.1 for the solvability of the unit-cell problem involves the knowledge of π, it may be useful to find conditions that guarantee the solvability without having to compute π. We shall provide some results in this subsection that show that if the graph has sufficient symmetries then the unit-cell problem is solvable.

Given any vector space V over $\mathbb{R}$, let $\mathcal{L}(V)$ denote the vector space (over $\mathbb{R}$) of all continuous linear maps from V into V. Let $\phi : \bar{S} \to \bar{S}$ be a bijection. We associate with it the *pull-back* $\phi^* \in \mathcal{L}(\mathbb{R}^{\bar{S}})$ defined by

$$\phi^* f = f \circ \phi \quad \forall f \in \mathbb{R}^{\bar{S}}.$$

We state some basic lemmas about ϕ^* and ultimately arrive at a sufficient condition for solvability of the unit-cell problem (15).

Lemma 4.3. *Let $\phi : \bar{S} \to \bar{S}$ be a bijection. Then $(\phi^*)^T = (\phi^{-1})^*$ and ϕ^* preserves the inner product: $(\phi^* f, \phi^* g) = (f, g)$ for all $f, g \in \mathbb{R}^{\bar{S}}$.*

Lemma 4.4. *Let $\phi : \bar{S} \to \bar{S}$ be a bijection and $A \in \mathcal{L}(\mathbb{R}^{\bar{S}})$. The following are equivalent:*

1. $A(\phi(x), \phi(y)) = A(x, y) \quad \forall x, y \in \bar{S}$.

2. $A \circ \phi^* = \phi^* \circ A$.

3. $A^T \circ (\phi^{-1})^* = (\phi^{-1})^* \circ A^T$.

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Proof. It is adequate to note that $\phi^* : \bar{\mathcal{S}} \times \bar{\mathcal{S}} \to \mathbb{R}$ is given by

$$\phi^*(x, y) = (\phi^* \delta_y)(x) = \begin{cases} 1 & \phi(x) = y \\ 0 & \text{otherwise.} \end{cases}$$

$\square$

If ϕ satisfies the conditions in the above lemma, then ϕ or the associated ϕ^* is called a *symmetry* of $A \in \mathcal{L}(\mathbb{R}^{\bar{\mathcal{S}}})$.

The previous lemmas apply to very general A. Now assume that A (and hence A^T) has a one dimensional null space, which is the case when A is the generator of an ergodic Markov process.

Lemma 4.5. *Let $A \in \mathcal{L}(\mathbb{R}^{\bar{\mathcal{S}}})$ and suppose A has a one dimensional null space. Suppose ϕ is a symmetry of A such that $\phi = \phi^{-1}$. Let $f \in \mathbb{R}^{\bar{\mathcal{S}}}$ span the null space of A^T. Then $\phi^* f = f$.*

Proof. Because ϕ is a symmetry of A, we have

$$A^T \circ (\phi^{-1})^* f = (\phi^{-1})^* \circ A^T f = 0.$$

That is, $(\phi^{-1})^* f$ is in the null space of A^T. Because A^T has a one dimensional null space and $\phi^{-1} = \phi$, we have $\phi^* f = \alpha f$ for some $\alpha \neq 0$. Since ϕ^* is a bijection on $\bar{\mathcal{S}}$, $\alpha = 1$. $\square$

Before we present the main result, we observe that we can write the unit-cell solvability condition (16) as

$$(\rho_i, \pi) = 0, \quad i = 1, \ldots, d,$$

where ρ is the drift field.

Theorem 4.6. *Consider a graph $(\mathcal{S}, \mathcal{E}, \lambda)$ with generator (rate matrix) $L \in \mathcal{L}(\mathbb{R}^{\bar{\mathcal{S}}})$ (3) and stationary distribution π (12). Suppose that for each $i = 1, \ldots, d$ there exists a symmetry ϕ_i of L such that $\phi_i^* \rho_i = -\rho_i$ and $\phi_i^{-1} = \phi_i$. Then the unit-cell problem (15) is solvable.*

Proof. For each $i = 1, \ldots, d$

$$(\rho_i, \pi) = (\phi_i^* \rho_i, \phi_i^* \pi) = (-\rho_i, \pi).$$

Thus $(\rho_i, \pi) = 0$. $\square$

Remark 1. Note that if we have a reflection symmetry about each direction i and denote the reflection map by ϕ_i, then the assumptions of Theorem 4.6 are satisfied.

5   Variational formulation for the reversible rates case $L = L^T$

When the rates are reversible, the generator L is symmetric. In the continuous (PDE) homogenization case, when the analogous differential operator L is symmetric, the effective diffusivity may be characterized by a variational formulation [16]. Likewise in the discrete lattice ($\mathbb{Z}^d$) setting with reversible rates a variational characterization may be found in [5].

We shall derive a variational characterization of the effective diffusivity in our graph setting for the symmetric (reversible rates) case. Thus we assume $L = L^T$ throughout this section. In the continuous case of the Laplace operator, the variational characterization involves the use of results from vector calculus such as the divergence theorem. In the lattice case [5] due to the Cartesian

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structure, the discrete analog of the gradient and divergence operators are relatively easier to define. In the general graph setting considered here, we develop the analogous operators of gradient and divergence and also the divergence theorem in order to provide the variational formulation. In our setting, the gradient operator ∇ applies to node functions while the divergence applies to $\mathbb{R}^d$-valued edge functions.

Note that symmetry of L implies reverse edges are present: if $(x,y) \in \bar{\mathcal{E}}$ then $(y,x) \in \bar{\mathcal{E}}$.

5.1   Gradient, divergence, etc.

We introduce some analogous versions of gradient and divergence as they apply to a graph. For $f \in \mathbb{R}^{\bar{\mathcal{S}}}$, let the *gradient* $\nabla : \mathbb{R}^{\bar{\mathcal{S}}} \to (\mathbb{R}^d)^{\mathcal{E}}$ be defined by

$$(\nabla f)(e) = (f(\partial_+ e) - f(\partial_- e))\frac{\nu_e}{|\nu_e|^2}. \tag{22}$$

For $f : \bar{\mathcal{E}} \to \mathbb{R}^d$, let the *divergence* div $: (\mathbb{R}^d)^{\bar{\mathcal{E}}} \to \mathbb{R}^{\bar{\mathcal{S}}}$ be defined by

$$(\text{div} f)(y) = \sum_{e \in \mathcal{E}_y} \frac{\nu_e^T f(e)}{|\nu_e|^2}. \tag{23}$$

Define the edge function $A : \bar{\mathcal{E}} \to \mathbb{R}^{d \times d}$ by

$$A(e) = \nu_e \nu_e^T \lambda_e, \tag{24}$$

which will be used throughout this section. Define the inner product on $(\mathbb{R}^d)^{\bar{\mathcal{E}}}$ by

$$(f, g) := \sum_{e \in \bar{\mathcal{E}}} f(e)^T g(e) \tag{25}$$

for $f, g \in (\mathbb{R}^d)^{\bar{\mathcal{E}}}$.

5.2   Some general lemmas

Lemma 5.1. *Let $f \in \mathbb{R}^{\bar{\mathcal{E}}}$ and $g \in \mathbb{R}^{\bar{\mathcal{S}}}$. Suppose $f(x,y) = -f(y,x)$ for all $(x,y) \in \bar{\mathcal{E}}$. Then*

$$\sum_{e \in \bar{\mathcal{E}}} f(e)(g(\partial_+ e) - g(\partial_- e)) = \sum_{e \in \bar{\mathcal{E}}} -2f(e)g(\partial_- e)$$

Proof.

$$\sum_{e \in \bar{\mathcal{E}}} f(e)(g(\partial_+ e) - g(\partial_- e)) = \sum_{e \in \bar{\mathcal{E}}} f(e)g(\partial_+ e) - \sum_{e \in \bar{\mathcal{E}}} f(e)g(\partial_- e)$$

$$= \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}'_y} f(e)g(\partial_+ e) - \sum_{e \in \bar{\mathcal{E}}} f(e)g(\partial_- e) = \sum_{e \in \bar{\mathcal{E}}} -2f(e)g(\partial_- e).$$

$\square$

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Lemma 5.2 (Divergence theorem)**.** *Let* $f \in (\mathbb{R}^d)^{\bar{\mathcal{E}}}$ *and* $g \in \mathbb{R}^{\bar{\mathcal{S}}}$. *Suppose at least one of the following hold:*

$$f(x, y) = f(y, x) \text{ for all } (x, y) \in \bar{\mathcal{E}}, \tag{26}$$

$$g(\partial_+ e) = -g(\partial_- e) \text{ for all } e \in \bar{\mathcal{E}}. \tag{27}$$

Then

$$(f, \nabla g) = -2 \sum_{y \in \bar{\mathcal{S}}} (\mathrm{div} f)(y) g(y).$$

Note that (26) will hold if f is the gradient of a function.

Proof. Suppose (26) holds. Notice that the function

$$e \mapsto \frac{f(e)^T \nu_e}{|\nu_e|^2}$$

satisfies the assumption of Lemma 5.1. Thus, applying Lemma 5.1 we get

$$(f, \nabla g) = \sum_{e \in \bar{\mathcal{E}}} f(e)^T (\nabla g)(e) = -2 \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \frac{f(e)^T \nu_e}{|\nu_e|^2} g(y) = -2 \sum_{y \in \bar{\mathcal{S}}} (\mathrm{div} f)(y) g(y).$$

Suppose (27) holds. Then

$$(f, \nabla g) = \sum_{e \in \bar{\mathcal{E}}} f(e)^T (g(\partial_+ e) - g(\partial_- e)) \frac{\nu_e}{|\nu_e|^2}$$

$$= \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \frac{\nu_e^T f(e)}{|\nu_e|^2} (-g(\partial_- e) - g(\partial_- e)) = -2 \sum_{y \in \bar{\mathcal{S}}} (\mathrm{div} f)(y) g(y).$$

$\square$

5.3 The unit-cell problem in terms of ∇ and div

The following theorem formulates the unit-cell problem in terms of ∇ and div.

Theorem 5.3 (Unit-cell)**.** *Let* $\xi \in \mathbb{R}^d$. *Then* $\Upsilon_\xi \in \mathbb{R}^{\bar{\mathcal{S}}}$ *solves the (modified) unit-cell problem:*

$$(L^T \Upsilon_\xi)(y) = \xi^T \sigma(y) \text{ for all } y \in \bar{\mathcal{S}}. \tag{28}$$

if and only if Υ_ξ *satisfies*

$$\mathrm{div}(A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|} \xi))(y) = 0 \text{ for all } y \in \bar{\mathcal{S}}. \tag{29}$$

By linearity of the unit-cell problem (15), $\Upsilon_\xi(y) = \xi^T \omega(y)$ *where* $\omega \in \mathbb{R}^{\bar{\mathcal{S}}}$ *is a solution to the unit-cell problem.*

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Proof. For any $f \in \mathbb{R}^{\bar{\mathcal{S}}}$,

$$\operatorname{div}(A(e)\nabla f(e))(y) = \sum_{e \in \mathcal{E}_y} \frac{\nu_e^T A(e)\nabla f(e)}{|\nu_e|^2} = \sum_{e \in \mathcal{E}_y} \frac{\nu_e^T \nu_e \nu_e^T \lambda_e (f(\partial_+ e) - f(\partial_- e))\nu_e}{|\nu_e|^4}$$

$$= \sum_{e \in \mathcal{E}_y} (f(\partial_+ e) - f(\partial_- e))\lambda_e = \sum_{e \in \mathcal{E}_y} (f(y + \nu_e) - f(y))\lambda_e = (Lf)(y).$$

Then given $\xi \in \mathbb{R}^d$ and setting $f = \Upsilon_\xi$, this allows us to rewrite the left-hand side of the unit-cell problem as (note that $L = L^T$)

$$(L\Upsilon_\xi)(y) = \operatorname{div}(A(e)\nabla\Upsilon_\xi(e))(y).$$

Noting that $\pi = 1/|\bar{\mathcal{S}}|$, the right-hand side of the unit-cell problem can be rewritten as

$$-\xi^T \sigma(y) = -\sum_{e \in \mathcal{E}'_y} \lambda_e \pi(y - \nu_e)\nu_e^T \xi = -\frac{1}{|\bar{\mathcal{S}}|}\sum_{e \in \mathcal{E}'_y} \lambda_e \nu_e^T \xi = \frac{1}{|\bar{\mathcal{S}}|}\sum_{e \in \mathcal{E}_y} \lambda_e \nu_e^T \xi$$

$$= \frac{1}{|\bar{\mathcal{S}}|}\sum_{e \in \mathcal{E}_y} \frac{\nu_e^T \nu_e \nu_e^T \lambda_e \xi}{|\nu_e|^2} = \frac{1}{|\bar{\mathcal{S}}|}\operatorname{div}(\nu_e \nu_e^T \lambda_e \xi)(y) = \frac{1}{|\bar{\mathcal{S}}|}\operatorname{div}(A(e)\xi)(y).$$

$\square$

5.4   Alternative formula for the effective diffusivity matrix K

We provide an equivalent representation of K that will be necessary for deriving the variational formulation.

Lemma 5.4. *Define K as in (18). Then*

$$K\xi = \frac{1}{2}\sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} A(e)(\nabla\Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi), \quad \forall \xi \in \mathbb{R}^d.$$

Proof. Note that from Lemma 5.1

$$\sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} -2\nu_e \lambda_e \Upsilon_\xi(y) = \sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} -2\nu_e \nu_e^T \lambda_e \Upsilon_\xi(y)\frac{\nu_e}{|\nu_e|^2}$$

$$= \sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} \nu_e \nu_e^T \lambda_e \big(\Upsilon_\xi(\partial_+ e) - \Upsilon_\xi(\partial_- e)\big)\frac{\nu_e}{|\nu_e|^2} = \sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} A(e)\nabla\Upsilon_\xi(e).$$

Also, $\pi(y) = 1/|\bar{\mathcal{S}}|$ for all $y \in \bar{\mathcal{S}}$ by symmetry of L. Then

$$K\xi = \frac{1}{2}\sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} \Big(\frac{\nu_e \nu_e^T}{|\bar{\mathcal{S}}|}\lambda_e - 2\nu_e \omega(y)^T \lambda_e\Big)\xi = \sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} \nu_e \lambda_e \Big(\frac{\nu_e^T \xi}{2|\bar{\mathcal{S}}|} - \omega(y)^T \xi\Big)$$

$$= \sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} \nu_e \lambda_e \Big(\frac{\nu_e^T \xi}{2|\bar{\mathcal{S}}|} - \Upsilon_\xi(y)\Big) = \frac{1}{2}\sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} -2\nu_e \lambda_e \Upsilon_\xi(y) + \frac{1}{|\bar{\mathcal{S}}|}\nu_e \nu_e^T \lambda_e \xi$$

$$= \frac{1}{2}\sum_{y \in \bar{\mathcal{S}}}\sum_{e \in \mathcal{E}_y} A(e)(\nabla\Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi).$$

$\square$

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5.5 Sign of the effective diffusivity

We now show that K is positive semi-definite and provide a necessary and sufficient condition for K to be positive definite.

Lemma 5.5. *For all* $\phi \in \mathbb{R}^{\bar{\mathcal{S}}}$,

$$\frac{1}{2} \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \left(A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)^T (\nabla \phi(e) + \frac{1}{|\bar{\mathcal{S}}|}\mu)$$

$$= \frac{1}{2} \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \left(A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)^T \frac{1}{|\bar{\mathcal{S}}|}\mu.$$

In particular, when $\phi(y) = \mu^T \omega(y)$,

$$\frac{1}{2} \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \left(A(e)(\nabla(\xi^T \omega)(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)^T (\nabla(\mu^T \omega)(e) + \frac{1}{|\bar{\mathcal{S}}|}\mu)$$

$$= \frac{1}{2} \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \left(A(e)(\nabla(\xi^T \omega)(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)^T \frac{1}{|\bar{\mathcal{S}}|}\mu. \tag{30}$$

Proof. It is easy to check that the edge function $e \mapsto A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi)$ satisfies the first assumption of Lemma 5.2 (the "divergence theorem"). Thus for any $\phi \in \mathbb{R}^{\bar{\mathcal{S}}}$,

$$\frac{1}{2} \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \left(A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)^T (\nabla \phi)(e)$$

$$= -\sum_{y \in \bar{\mathcal{S}}} \mathrm{div}\left(\left(A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right) \right)(y)\phi(y).$$

Multiply (29) in Theorem 5.3 by ϕ and sum over y to get

$$\sum_{y \in \bar{\mathcal{S}}} \mathrm{div}\left(A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)(y)\phi(y) = 0$$

Combine these two equalities to get

$$\frac{1}{2} \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \left(A(e)(\nabla \Upsilon_\xi(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)^T (\nabla \phi)(e) = 0,$$

which yields the desired result. $\qquad\square$

Lemma 5.6. *For all* $\xi \in \mathbb{R}^d$,

$$\xi^T K \xi = \frac{|\bar{\mathcal{S}}|}{2} \sum_{e \in \bar{\mathcal{E}}} \lambda_e (\nu_e^T \tilde{\xi}_e)^2,$$

where $\tilde{\xi}_e = \nabla(\xi^T \omega)(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi$. *Since* $\lambda_e > 0$, *this implies* K *is positive semi-definite.*

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Proof. By Lemmas 5.4 and 5.5,

$$\frac{\xi^T K \mu}{|\bar{\mathcal{S}}|} = \frac{1}{2} \sum_{e \in \bar{\mathcal{E}}} \left(A(e)(\nabla(\xi^T \omega)(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right)^T (\nabla(\mu^T \omega) + \frac{1}{|\bar{\mathcal{S}}|}\mu).$$

That is,

$$\xi^T K \mu = \frac{|\bar{\mathcal{S}}|}{2} \sum_{e \in \bar{\mathcal{E}}} \tilde{\xi}_e^T A(e)\tilde{\mu}_e,$$

where $\tilde{\xi}_e = \nabla(\xi^T \omega)(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi$ and $\tilde{\mu}_e = \nabla(\mu^T \omega) + \frac{1}{|\bar{\mathcal{S}}|}\mu$. In particular,

$$\xi^T B \xi = \frac{|\bar{\mathcal{S}}|}{2} \sum_{e \in \bar{\mathcal{E}}} \tilde{\xi}_e^T A(e)\tilde{\xi}_e = \frac{|\bar{\mathcal{S}}|}{2} \sum_{e \in \bar{\mathcal{E}}} \tilde{\xi}_e^T (\nu_e \nu_e^T \lambda_e)\tilde{\xi}_e = \frac{|\bar{\mathcal{S}}|}{2} \sum_{e \in \bar{\mathcal{E}}} \lambda_e (\nu_e^T \tilde{\xi}_e)^2.$$

$\square$

Lemma 5.7. *K is positive definite if and only if for all nonzero $\xi \in \mathbb{R}^d$ there exists some $e \in \bar{\mathcal{E}}$ such that*

$$\left(\omega(\partial_+ e) - \omega(\partial_- e) + \frac{1}{|\bar{\mathcal{S}}|}\nu_e \right)^T \xi \neq 0.$$

Proof. This follows immediately from Lemma 5.6. $\square$

5.6 Minimization of energy

For any fixed $\xi \in \mathbb{R}^d$ and scalar node function $\phi \in \mathbb{R}^{\bar{\mathcal{S}}}$, define the *energy*

$$E_\xi(\phi) := \frac{1}{2} \left(A(e)\big((\nabla\phi)(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi\big), (\nabla\phi)(e) + \frac{1}{|\bar{\mathcal{S}}|}\xi \right).$$

From Lemma 5.6 we see that $E_\xi(\Upsilon_\xi) = \xi^T K \xi$.

Theorem 5.8 (Variational Formulation). *Fix $\xi \in \mathbb{R}^d$. Then ϕ^* minimizes the energy:*

$$E_\xi(\phi^*) = \min_{\phi \in \mathbb{R}^{\bar{\mathcal{S}}}} E_\xi(\phi)$$

if and only if ϕ^* is a solution to the unit-cell problem (15) and thus $\phi^* = \Upsilon_\xi$.

Proof. Let $\phi, \psi \in \mathbb{R}^{\bar{\mathcal{S}}}$. Then

$$E_\xi(\phi) = \frac{1}{2} \left(A\big(\nabla\phi + \frac{1}{|\bar{\mathcal{S}}|}\xi\big), \nabla\phi + \frac{1}{|\bar{\mathcal{S}}|}\xi \right)$$

and we can differentiate to get

$$DE_\xi(\phi)(\psi) = \frac{1}{2} \left(\nabla\psi, A\big(\nabla\phi + \frac{1}{|\bar{\mathcal{S}}|}\xi\big) \right) + \frac{1}{2} \left(\nabla\phi + \frac{1}{|\bar{\mathcal{S}}|}\xi, A\nabla\psi \right) = \left(\nabla\psi, A\big(\nabla\phi + \frac{1}{|\bar{\mathcal{S}}|}\xi\big) \right)$$

where the last equality follows from symmetry of A. Then $DE_\xi(\phi^*)(\psi) = 0$ if and only if

$$\left(\nabla\psi, A(\nabla\phi^* + \frac{1}{|\bar{\mathcal{S}}|}\xi) \right) = 0.$$

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By Lemma 5.2, this is equivalent to

$$\left(\psi, \operatorname{div}\left(A(\nabla\phi^* + \frac{1}{|\mathcal{S}|}\xi))\right)\right) = 0.$$

That is, $\nabla\phi^*$ is an optimal point of E if and only if

$$\operatorname{div}\left(A(\nabla\phi^* + \frac{1}{|\mathcal{S}|}\xi)\right) = 0.$$

By Theorem 5.3, the desired result follows. Note that the Hessian of E is positive semi-definite and thus ϕ^* is a minimizer. $\qquad\square$

6 Rigorous convergence result

Consider a weighted, directed graph $(\mathcal{S}, \mathcal{E}, \lambda)$ satisfying assumptions in Section 2. Recall the random time change representation of Z (2):

$$Z(t) = z_0 + \sum_{e \in \bar{\mathcal{E}}} \nu_e R_e\left(\lambda_e \int_0^t 1_{\{\partial_- e\}}(Y(s))ds\right).$$

For the remainder of this discussion, we assume without loss of generality $z_0 = 0$. We aim to show that, under certain conditions, the scaled process

$$Z_\varepsilon(t) := \varepsilon Z(t/\varepsilon^2) \tag{31}$$

converges to a Brownian motion whose covariance matrix is $2Kt$. Define

$$\tilde{R}_e(t) := R_e(t) - t. \tag{32}$$

Then

$$
\begin{aligned}
Z_\varepsilon(t) &= \varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e \tilde{R}_e\left(\lambda_e \int_0^{t/\varepsilon^2} 1_{\{\partial_- e\}}(Y(s))ds\right) + \varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e \lambda_e \int_0^{t/\varepsilon^2} 1_{\{\partial_- e\}}(Y(s))ds \\
&= \varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e M_e^\varepsilon(t) + \varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e S_e^\varepsilon(t),
\end{aligned}
\tag{33}
$$

where

$$S_e^\varepsilon(t) := \lambda_e \int_0^{t/\varepsilon^2} 1_{\{\partial_- e\}}(Y(s))ds \tag{34}$$

and

$$M_e^\varepsilon(t) := \tilde{R}_e(S_e^\varepsilon(t)). \tag{35}$$

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6.1 Pure drift limit of $\varepsilon^2 Z(t/\varepsilon^2)$

Consider the process

$$W_\varepsilon(t) := \varepsilon^2 Z(t/\varepsilon^2) = \varepsilon^2 \sum_{e \in \bar{\mathcal{E}}} \nu_e M_e^\varepsilon(t) + \varepsilon^2 \sum_{e \in \bar{\mathcal{E}}} \nu_e S_e^\varepsilon(t). \tag{36}$$

We aim to show that $W_\varepsilon(t) \to t \sum_{e \in \bar{\mathcal{S}}} \nu_e \lambda_e \pi(\partial_- e)$ as $\varepsilon \to 0$.

Lemma 6.1 (Second term). *For $t > 0$,*

$$\lim_{\varepsilon \to 0} \varepsilon^2 S_e^\varepsilon(t) = t \lambda_e \pi(\partial_- e) \ \ a.s.$$

Thus,

$$\lim_{\varepsilon \to 0} \varepsilon^2 \sum_{e \in \bar{\mathcal{E}}} \nu_e S_e^\varepsilon(t) = t \sum_{e \in \bar{\mathcal{E}}} \nu_e \lambda_e \pi(\partial_- e) \ \ a.s. \tag{37}$$

Proof. We have

$$\lim_{\varepsilon \to 0} \varepsilon^2 S_e^\varepsilon(t) = t \lambda_e \lim_{\varepsilon \to 0} \frac{1}{t/\varepsilon^2} \int_0^{t/\varepsilon^2} 1_{\{\partial_- e\}}(Y(s)) ds = t \lambda_e \pi(\partial_- e) \ \ \text{a.s.}$$

where the almost sure limit follows from ergodicity of Y. Multiply by ν_e and sum over $e \in \bar{\mathcal{E}}$ to get (37). $\square$

Lemma 6.2 (First term). *For all $T > 0$,*

$$\lim_{\varepsilon \to 0} \sup_{t \in [0,T]} \varepsilon^2 |M_e^\varepsilon(t)| = 0 \ \ a.s.$$

Also,

$$\lim_{\varepsilon \to 0} \varepsilon^2 R_e(S_e^\varepsilon(t)) = \lim_{\varepsilon \to 0} \varepsilon^2 S_e^\varepsilon(t) = t \lambda_e \pi(\partial_- e) \ \ a.s.$$

Proof. Notice that $0 \leq \varepsilon^2 S_e^\varepsilon(t) \leq \lambda_e t$ a.s. for all t. Then

$$\sup_{t \in [0,T]} |\varepsilon^2 M_e^\varepsilon(t)| = \sup_{t \in [0,T]} |\varepsilon^2 \tilde{R}_e(S_e^\varepsilon(t))| = \sup_{t \in [0,T]} |\varepsilon^2 R_e(S_e^\varepsilon(t)) - \varepsilon^2 S_e^\varepsilon(t)|$$

$$= \sup_{t \in [0, S_e^\varepsilon(T)]} |\varepsilon^2 R_e\left(\frac{t}{\varepsilon^2}\right) - t| \leq \sup_{t \in [0, \lambda_e T]} |\varepsilon^2 R_e\left(\frac{t}{\varepsilon^2}\right) - t| \to 0 \text{ a.s. as } \varepsilon \to 0,$$

where the inequality follows from Lemma 6.1 and the limit follows from the functional law of large numbers for Poisson processes [8]. $\square$

Lemma 6.3. *Fix $T > 0$. For all $t \in [0,T]$,*

$$\lim_{\varepsilon \to 0} W_\varepsilon(t) = t \sum_{e \in \bar{\mathcal{E}}} \nu_e \lambda_e \pi(\partial_- e) \ \ a.s.$$

If the unit-cell problem (15) is solvable, then

$$\lim_{\varepsilon \to 0} W_\varepsilon(t) = 0 \ \ a.s.$$

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Proof. The first result follows immediately from Lemmas 6.2 and 6.1. The second result follows from Lemma 3.1. $\qquad\square$

We remark that the above limit is uniform on compact (time) subintervals of $(0, \infty)$. We also note that Lemma 6.3 says W_ε has a deterministic limit, which is a pure drift some direction when the unit-cell problem is not solvable. Otherwise, the limit of W_ε is 0 and we must scale space by ε rather than ε^2. This is the case that is of interest to us and we will demonstrate that the corresponding weak limit is a Brownian motion.

6.2 Limiting behavior of Z_ε

Henceforth we will assume the unit-cell problem is solvable and we define $\psi \in (\mathbb{R}^d)^{\bar{S}}$ by

$$L\psi = \rho \tag{38}$$

where ρ (19) is the drift field. The following Lemma ensures such a ψ exists and we note that ψ is unique only up to an additive constant.

Lemma 6.4. *The unit-cell problem (15) is solvable if and only if $\rho \in R(L)$.*

Proof. Recall that L^T has a one-dimensional null space by ergodicity of Y. Hence the following equivalent statements:

$$\rho \in R(L) \iff \rho \perp N(L^T) \iff \sum_{y \in \bar{S}} \rho(y)\pi(y) = 0 \iff \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \nu_e \lambda_e \pi(y) = 0$$

$$\iff \text{ the unit-cell problem is solvable,}$$

where the last equivalence follows from Lemma 3.1. $\qquad\square$

Define Dynkin's martingale

$$N(t) := \psi(Y(t)) - \psi(Y(0)) - \int_0^t (L\psi)(Y(s))ds. \tag{39}$$

Writing Z_ε as

$$Z_\varepsilon(t) = \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e R_e \Big(\lambda_e \int_0^{t/\varepsilon^2} 1_{\{\partial_- e\}}(Y(s))ds \Big)$$

$$- \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e \lambda_e \int_0^{t/\varepsilon^2} 1_{\{\partial_- e\}}(Y(s))ds + \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e \lambda_e \int_0^{t/\varepsilon^2} 1_{\{\partial_- e\}}(Y(s))ds$$

$$- \varepsilon[\psi(Y(t/\varepsilon^2)) - \psi(Y(0))] + \varepsilon[\psi(Y(t/\varepsilon^2)) - \psi(Y(0))],$$

notice that the third term on the RHS is $\varepsilon \int_0^{t/\varepsilon^2} (L\psi)(Y(s))ds$. Substituting various definitions yields

$$Z_\varepsilon(t) = \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(t) - \varepsilon N(t/\varepsilon^2) + \varepsilon[\psi(Y(t/\varepsilon^2)) - \psi(Y(0))].$$

Notice that M_e^ε and N are martingales and

$$\lim_{\varepsilon \to 0} \varepsilon[\psi(Y(t/\varepsilon^2)) - \psi(Y(0))] = 0 \quad \text{a.s.} \tag{40}$$

because ψ is bounded. We aim to find the quadratic variation of the first two terms, which can be expanded as follows:

$$
\begin{aligned}
&\left[\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot) - \varepsilon N(\cdot/\varepsilon^2) \right](t) \\
&= [\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot), \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot)](t) - [\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot), \varepsilon N(\cdot/\varepsilon^2)](t) \\
&\quad - [\varepsilon N(\cdot/\varepsilon^2), \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot)](t) + [\varepsilon N(\cdot/\varepsilon^2), \varepsilon N(\cdot/\varepsilon^2)](t).
\end{aligned}
\tag{41}
$$

Before demonstrating convergence of (41), we note the following result from [14]:

Lemma 6.5. *Let $f, g : \mathbb{R} \to \mathbb{R}$. If f is continuous and g is of finite variation, then their covariation is zero: $[f, g](t) = 0$.*

The following three lemmas examine convergence of the right hand side of (41).

Lemma 6.6. *For every $t > 0$, the quadratic variation converges almost surely:*

$$\lim_{\varepsilon \to 0} [\varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e M_e^\varepsilon(\cdot), \varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e M_e(\cdot)](t) = t \sum_{e \in \bar{\mathcal{E}}} \lambda_e \nu_e \nu_e^T \pi(\partial_- e).$$

Proof. Let $a, b \in \bar{\mathcal{E}}$. Then

$$
\begin{aligned}
[\varepsilon M_a^\varepsilon(\cdot), \varepsilon M_b^\varepsilon(\cdot)](t) &= \varepsilon^2 \Big[\tilde{R}_a(S_a^\varepsilon(\cdot)), \tilde{R}_b(S_b^\varepsilon(\cdot)) \Big](t) \\
&= \varepsilon^2 \Big[R_a(S_a^\varepsilon(\cdot)), R_b(S_b^\varepsilon(\cdot)) \Big](t) - \varepsilon^2 \Big[R_a(S_a^\varepsilon(\cdot)), S_b^\varepsilon(\cdot) \Big](t) \\
&\quad - \varepsilon^2 \Big[S_a^\varepsilon(\cdot), R_b(S_b^\varepsilon(\cdot)) \Big](t) + \varepsilon^2 \Big[S_a^\varepsilon(\cdot), S_b^\varepsilon(\cdot) \Big](t).
\end{aligned}
\tag{42}
$$

For all $\varepsilon > 0$ and $e \in \bar{\mathcal{E}}$, $S_e^\varepsilon(t)$ is an a.s. continuous finite variation process and $R_e(S_e^\varepsilon(t))$ is a.s. a finite variation process. Thus by Theorem 6.5, the last 3 terms in (42) are all 0 and so

$$[\varepsilon M_a^\varepsilon(\cdot), \varepsilon M_b^\varepsilon(\cdot)](t) = \varepsilon^2 \Big[R_a(S_a^\varepsilon(\cdot)), R_b(S_b^\varepsilon(\cdot)) \Big](t).$$

For a process $A(t)$, let $\Delta A(t)$ denote the size of the jump at time t. For each $e \in \mathcal{E}$, define

$$T_e = \{t \in [0, \infty) \mid \Delta R_e(S_e^\varepsilon(t)) \neq 0\}, \tag{43}$$

the collection of all jump times of $R_e(S_e^\varepsilon(t))$. The number of jumps is a.s. countable because R_e is a unit Poisson process and $S_e^\varepsilon(t) \leq \lambda_e t/\varepsilon^2$.

If $a \neq b$,

$$[\varepsilon M_a^\varepsilon(\cdot), \varepsilon M_b^\varepsilon(\cdot)](t) = \varepsilon^2 \sum_{\substack{s \in T_a \cup T_b \\ s \leq t}} \Delta R_a(S_a^\varepsilon(s)) \Delta R_b(S_b^\varepsilon(s)) = 0 \quad \text{a.s.}$$

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where the last equality follows because R_a and R_b are independent processes whose jumps do not coincide almost surely.

Now suppose $a = b$. Then fix $T > 0$ and apply Lemma 6.1 to get

$$\lim_{\varepsilon \to 0} [\varepsilon M_a^\varepsilon(\cdot), \varepsilon M_a^\varepsilon(\cdot)](t) = \lim_{\varepsilon \to 0} \varepsilon^2 \sum_{t \in T_e} \left(\Delta R_a(S_a^\varepsilon(t)) \right)^2$$

$$= \lim_{\varepsilon \to 0} \varepsilon^2 R_a(S_a^\varepsilon(t)) = t\lambda_a \pi(\partial_- a) \text{ a.s.}$$

Hence,

$$\lim_{\varepsilon \to 0} [\varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e M_e^\varepsilon(\cdot), \varepsilon \sum_{e \in \bar{\mathcal{E}}} \nu_e M_e(\cdot)](t) = \lim_{\varepsilon \to 0} \sum_{e \in \bar{\mathcal{E}}} \sum_{e' \in \bar{\mathcal{E}}} \nu_e \nu_{e'}^T [\varepsilon M_e^\varepsilon(\cdot), \varepsilon M_{e'}^\varepsilon(\cdot)](t)$$

$$= t \sum_{e \in \bar{\mathcal{E}}} \lambda_e \nu_e \nu_e^T \pi(\partial_- e) \text{ a.s.}$$

$\square$

Lemma 6.7. *Fix $t > 0$. Let ψ satisfy (38). Then the quadratic covariation converges almost surely:*

$$\lim_{\varepsilon \to 0} [\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot), \varepsilon N(\cdot/\varepsilon^2)](t) = t \sum_{e \in \bar{\mathcal{E}}} \nu_e \left(\psi(\partial_+ e) - \psi(\partial_- e) \right)^T \lambda_e \pi(\partial_- e).$$

Proof. Substituting the definition of N,

$$\left[\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot), \varepsilon N(\cdot/\varepsilon^2) \right](t)$$

$$= \sum_{e \in \bar{\mathcal{E}}} \varepsilon^2 \left[\nu_e R_e(S_e^\varepsilon(\cdot)) - \nu_e S_e^\varepsilon(\cdot), \psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)) - \int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s))ds \right](t)$$

$$= \sum_{e \in \bar{\mathcal{E}}} \varepsilon^2 \left[\nu_e R_e(S_e^\varepsilon(\cdot)), \psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)) \right](t)$$

$$- \sum_{e \in \bar{\mathcal{E}}} \varepsilon^2 \left[\nu_e R_e(S_e^\varepsilon(\cdot)), \int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s))ds \right](t)$$

$$- \sum_{e \in \bar{\mathcal{E}}} \varepsilon^2 \left[\nu_e S_e^\varepsilon(\cdot), \psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)) \right](t)$$

$$+ \sum_{e \in \bar{\mathcal{E}}} \varepsilon^2 \left[\nu_e S_e^\varepsilon(\cdot), \int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s))ds \right](t).$$

Notice that $R_e(S_e^\varepsilon(t))$ and $\psi(Y(t/\varepsilon^2)) - \psi(Y(0))$ are finite variation processes. Also, $S_e^\varepsilon(t)$ and $\int_0^{t/\varepsilon^2} (L\psi)(Y(s))ds$ are continuous finite variation processes. Applying Lemma 6.5 to each of the second, third, and fourth terms above and noting that $\psi(Y(0))$ is constant,

$$\left[\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot), \varepsilon N(\cdot/\varepsilon^2) \right](t) = \sum_{e \in \bar{\mathcal{E}}} \varepsilon^2 \left[\nu_e R_e(S_e^\varepsilon(\cdot)), \psi(Y(\cdot/\varepsilon^2)) \right](t).$$

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Fix an edge $e \in \mathcal{E}$. Because R_e and ψ are jump processes,

$$\varepsilon^2 \Big[\nu_e R_e(S_e^\varepsilon(\cdot)), \psi(Y(\cdot/\varepsilon^2)) \Big](t) = \varepsilon^2 \nu_e \Big[R_e(S_e^\varepsilon(\cdot)), \psi(Y(\cdot/\varepsilon^2)) \Big](t)$$
$$= \varepsilon^2 \nu_e \sum_{0 \leq s \leq t} \Delta R_e(S_e^\varepsilon(s)) \Delta \psi(Y(s/\varepsilon^2))^T,$$

where we are summing over the countably many simultaneous jumps of the two processes. Notice that the $\Delta R_e(S_e^\varepsilon(t)) \neq 0$ if and only if $t \in T_e$ and if $\Delta \psi(t) \neq 0$ then $t \in \cup_{e \in \bar{\mathcal{E}}} T_e$. Therefore, if $\Delta R_e(S_e^\varepsilon(t)) \Delta \psi(Y(t/\varepsilon^2)) \neq 0$ then $t \in T_e$.

Because R_e increments by 1 at each jump, $R_e(S_e^\varepsilon(t)) = \#([0, t/\varepsilon^2] \cap T_e)$. Thus,

$$\varepsilon^2 \nu_e \sum_{0 \leq s \leq t} \Delta R_e(S_e^\varepsilon(s)) \Delta \psi(Y(s/\varepsilon^2))^T = \varepsilon^2 \nu_e \sum_{\substack{s \in T_e \\ 0 \leq s \leq t}} \Delta R_e(S_e^\varepsilon(s)) \Delta \psi(Y(s/\varepsilon^2))^T$$

$$= \varepsilon^2 \nu_e \sum_{\substack{s \in T_e \\ 0 \leq s \leq t/\varepsilon^2}} \Delta \psi(Y(s))^T = \varepsilon^2 \nu_e \sum_{\substack{s \in T_e \\ 0 \leq s \leq t/\varepsilon^2}} (\psi(\partial_+ e) - \psi(\partial_- e))^T$$

$$= \varepsilon^2 \nu_e (\psi(\partial_+ e) - \psi(\partial_- e))^T R_e(S_e^\varepsilon(t))$$

$$\to t \nu_e (\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(\partial_- e) \text{ as } \varepsilon \to 0 \text{ a.s.},$$

where the final limit follows from Lemma 6.2. Summing over $e \in \bar{\mathcal{E}}$ yields the result. Note that ψ is only defined up to some element in $N(L)$. However, $N(L)$ only contains constant functions and shifting ψ by a constant clearly yields the same limit. $\square$

Lemma 6.8. *Define N as in (39). Let ψ satisfy (38). Then the quadratic variation converges almost surely:*

$$\lim_{\varepsilon \to 0} [\varepsilon N(\cdot/\varepsilon^2), \varepsilon N(\cdot/\varepsilon^2)](t) = t \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(\partial_- e).$$

Proof. First, we have

$$[\varepsilon N(\cdot/\varepsilon^2), \varepsilon N(\cdot/\varepsilon^2)](t) = \varepsilon^2 \Big[\psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)) - \int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s)),$$

$$\psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)) - \int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s)) \Big](t)$$

$$= \varepsilon^2 [\psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)), \psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0))](t)$$

$$- 2\varepsilon^2 [\psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)), \int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s))](t)$$

$$+ \varepsilon^2 \Big[\int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s)), \int_0^{\cdot/\varepsilon^2} (L\psi)(Y(s)) \Big](t)$$

$$= \varepsilon^2 [\psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)), \psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0))](t).$$

The last equality follows from application of Lemma 6.5 (ψ is finite variation and $\int_0^{t/\varepsilon^2}(L\psi)(Y(s))$ is continuous and finite variation). Next, because ψ is a jump process and $\psi(Y(0))$ is constant,

$$\varepsilon^2[\psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0)), \psi(Y(\cdot/\varepsilon^2)) - \psi(Y(0))](t)$$
$$= \varepsilon^2[\psi(Y(\cdot/\varepsilon^2)), \psi(Y(\cdot/\varepsilon^2))](t) = \varepsilon^2 \sum_{0 \le s \le t} \Delta\psi(Y(s/\varepsilon^2))\psi(Y(s/\varepsilon^2))^T,$$

where we are summing over countably many jumps of ψ. Next notice that ψ only jumps when Y jumps along an edge and two jumps almost surely do not occur simultaneously. Recall that if $\Delta\psi(t) \ne 0$ then $t \in \cup_{e \in \bar{\mathcal{E}}} T_e$ and thus

$$\varepsilon^2 \sum_{0 \le s \le t} \Delta\psi(Y(s/\varepsilon^2))\psi(Y(s/\varepsilon^2))^T = \varepsilon^2 \sum_{0 \le s \le t/\varepsilon^2} \Delta\psi(Y(s))\psi(Y(s))^T$$

$$= \varepsilon^2 \sum_{e \in \bar{\mathcal{E}}} \sum_{\substack{s \in \cup_{e \in \bar{\mathcal{E}}} T_e \\ 0 \le s \le t/\varepsilon^2}} \Delta\psi(Y(s))\psi(Y(s))^T$$

$$= \varepsilon^2 \sum_{e \in \bar{\mathcal{E}}} \sum_{\substack{s \in \cup_{e \in \bar{\mathcal{E}}} T_e \\ 0 \le s \le t/\varepsilon^2}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T$$

$$= \varepsilon^2 \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T R_e(S_e^\varepsilon(t))$$

$$= \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \left(\varepsilon^2 R_e(S_e^\varepsilon(t)) - \varepsilon^2 S_e^\varepsilon(t) + \varepsilon^2 S_e^\varepsilon(t)\right).$$

Taking the limit of ε tending to 0 and applying Lemmas 6.2 and 6.1 we have

$$\lim_{\varepsilon \to 0} \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \left(\varepsilon^2 R_e(S_e^\varepsilon(t)) - \varepsilon^2 S_e^\varepsilon(t) + \varepsilon^2 S_e^\varepsilon(t)\right)$$

$$= \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \left(\lim_{\varepsilon \to 0} \varepsilon^2 M_e^\varepsilon(t) + \lim_{\varepsilon \to 0} \varepsilon^2 S_e^\varepsilon(t)\right)$$

$$= t \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(\partial_- e).$$

Combining the above chain of inequalities, we have

$$\lim_{\varepsilon \to 0} [\varepsilon N(\cdot/\varepsilon^2), \varepsilon N(\cdot/\varepsilon^2)](t) = t \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(\partial_- e).$$

Once again, ψ is only defined up to some element in $N(L)$. However, shifting ψ by a constant clearly yields the same limit. $\square$

Now we state our main result.

Theorem 6.9. *The process $Z_\varepsilon(t)$ (2) converges weakly*

$$Z_\varepsilon(t) \Rightarrow \mathbf{Z}(t) \ \text{in} \ D^d[0, T] \ \text{as} \ \varepsilon \to 0,$$

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where $\mathbf{Z}(t)$ is a Brownian motion with

$$\mathbb{E}\mathbf{Z}(t) = 0,$$
$$\mathbb{E}[\mathbf{Z}(t)\mathbf{Z}(t)^T] = 2Ct.$$

Here,

$$C := \frac{1}{2} \sum_{e \in \bar{\mathcal{E}}} \alpha_e \alpha_e^T \lambda_e \pi(\partial_- e) \tag{44}$$

is well defined where

$$\alpha_e := \nu_e - (\psi(\partial_+ e) - \psi(\partial_- e)). \tag{45}$$

and ψ satisfies (38).

Proof. We first show that the maximum jump of $\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(t) - \varepsilon N(t/\varepsilon^2)$ is asymptotically negligible. Note that M_e^ε has a maximum jump size of 1 because R_e is a Poisson process and S_e^ε is continuous. Also, the jumps of $N(t/\varepsilon^2)$ are bounded above by some constant k because ψ is bounded. Thus,

$$\lim_{\varepsilon \to 0} \mathbb{E}\left[\sup_{s \leq t} \Big| \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(s) - \varepsilon N(s/\varepsilon^2) - \Big(\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(s-) - \varepsilon N(s-/\varepsilon^2) \Big) \Big| \right]$$

$$= \lim_{\varepsilon \to 0} \varepsilon \mathbb{E}\left[\sup_{s \leq t} \Big| \sum_{e \in \bar{\mathcal{E}}} \big(\nu_e M_e^\varepsilon(s) - \nu_e M_e^\varepsilon(s-) \big) - \big(N(s/\varepsilon^2) - N(s-/\varepsilon^2) \big) \Big| \right]$$

$$\leq \lim_{\varepsilon \to 0} \varepsilon \mathbb{E}\left[\sum_{e \in \bar{\mathcal{E}}} |\nu_e| + k \right] = 0.$$

Next, applying Lemmas 6.6, 6.7, and 6.8, the limit of the quadratic covariation is

$$\lim_{\varepsilon \to 0} \left[\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot) - \varepsilon N(\cdot/\varepsilon^2) \right](t)$$

$$= \lim_{\varepsilon \to 0} \left[\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot), \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(\cdot) \right](t) - 2 \lim_{\varepsilon \to 0} \left[\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e \nu_e^T M_e^\varepsilon(\cdot), \varepsilon N(\cdot/\varepsilon^2) \right](t)$$

$$+ \lim_{\varepsilon \to 0} [\varepsilon N(\cdot/\varepsilon^2), \varepsilon N(\cdot/\varepsilon^2)](t).$$

$$= t \sum_{e \in \bar{\mathcal{E}}} \lambda_e \nu_e \nu_e^T \pi(\partial_- e) - t \sum_{e \in \bar{\mathcal{E}}} \nu_e \big(\psi(\partial_+ e) - \psi(\partial_- e) \big)^T \lambda_e \pi(\partial_- e)$$

$$- t \sum_{e \in \bar{\mathcal{E}}} \big(\psi(\partial_+ e) - \psi(\partial_- e) \big) \nu_e^T \lambda_e \pi(\partial_- e)$$

$$+ t \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(\partial_- e)$$

$$= t \sum_{e \in \bar{\mathcal{E}}} \alpha_e \alpha_e^T \lambda_e \pi(\partial_- e).$$

Hence we can apply the martingale functional central limit theorem from [8] to the martingale $\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(t) - \varepsilon N(t/\varepsilon^2)$ to get the following weak convergence:

$$\sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(t) - \varepsilon N(t/\varepsilon^2) \Rightarrow \mathbf{Z}(t) \text{ in } D^d[0, T] \text{ as } \varepsilon \to 0.$$

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Recall that

$$Z_\varepsilon(t) = \sum_{e \in \bar{\mathcal{E}}} \varepsilon \nu_e M_e^\varepsilon(t) - \varepsilon N(t/\varepsilon^2) + \varepsilon[\psi(Y(t/\varepsilon^2)) - \psi(Y(0))].$$

Because the first two terms converge weakly to a Brownian motion, **Z**, and the terms involving ψ converge a.s. to 0, the entire process $Z_\varepsilon(t)$ converges weakly to **Z**. See [3] for a proof of this result. □

In the Appendix we prove that this result agrees with the formal derivation (i.e., $K = C$).

Lemma 6.10. *The covariance matrix C (44) is symmetric semi-positive definite. Moreover, if $\{\alpha_e\}_{e \in \bar{\mathcal{E}}}$ (45) spans $\mathbb{R}^d$, then C is symmetric positive definite.*

Proof. From Theorem 6.9, C is clearly symmetric positive semi-definite. This can also be seen directly since for any nonzero $x \in \mathbb{R}^d$,

$$x^T C x = \sum_{e \in \bar{\mathcal{E}}} x^T \alpha_e \alpha_e^T x \lambda_e \pi(\partial_- e) = \sum_{e \in \bar{\mathcal{E}}} |x^T \alpha_e|^2 \lambda_e \pi(\partial_- e) \geq 0.$$

Now, suppose $\{\alpha_e\}_{e \in \bar{\mathcal{E}}}$ spans $\mathbb{R}^d$. Then for some $e \in \bar{\mathcal{E}}$, $x^T \alpha_e \neq 0$. That is, $|x^T \alpha_e|^2 > 0$ and thus $x^T C x > 0$. □

7 Numerical experiments

Throughout this section, we fix a periodic obstruction geometry in two dimensions where a quarter of the periodic cell is obstructed. More precisely, the plane is periodically tiled by a unit square whose upper right quadrant is obstructed. Thus the obstructed region is given by

$$\mathcal{O} = \bigcup_{z \in \mathbb{Z}^2} \{z + [3/4, 1] \times [3/4, 1]\}.$$

Given this geometry, consider a randomly walking solute that undergoes specular reflections at the obstruction boundaries $\partial \mathcal{O}$. In the following subsections we explore different aspects of this random walk with the geometry fixed.

Throughout the following sections, let $(\mathcal{S}_h, \mathcal{E}_h, \lambda_h)$ denote a directed, weighted graph where $h > 0$ is a scaling parameter and

$$\begin{aligned}
\mathcal{S}_h &= h\mathbb{Z}^2 \backslash \mathcal{O}, \\
\mathcal{E}_h &= \{(x, y) \in \mathcal{S}_h \times \mathcal{S}_h \mid x - y = \pm(h, 0) \text{ or } x - y = \pm(0, h)\}.
\end{aligned} \tag{46}$$

That is, the node set excludes the obstructed region $\mathcal{O}$ and edges exist between each node and its nearest neighbors. The jump rate function λ_h varies depending on the effects under investigation. Figure 2 depicts the quotiented node and edge sets of $\mathcal{S}_h$ and $\mathcal{E}_h$ for $h = 1/2, 1/4, 1/8$, and $1/16$.

7.1 Nonzero path length effects

If the mean path length of the random walk is negligible relative to the spacing between obstructions, then one may approximate the random walk by a Brownian motion with reflections. In this case, the probability density function satisfies the diffusion equation with no flux boundary conditions
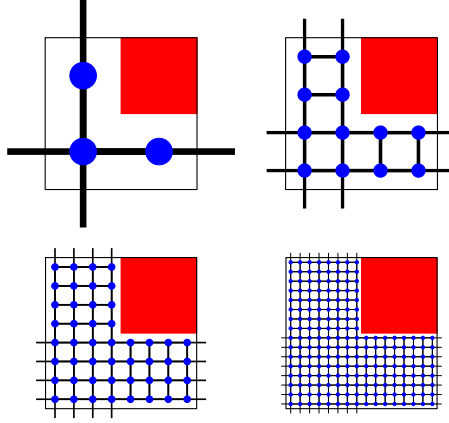
Figure 2: Periodic cells of graphs with nodes and edges defined in (46) for $h = 1/2, 1/4, 1/8$, and $1/16$. The blue circles represent edges, the thick black lines represent edges, and the shaded red region represents the "obstructed" region $\mathcal{O}$ where nodes are removed.

on the obstruction boundaries. This will justify the use of PDE homogenization theory. However, if the mean path length is not sufficiently smaller than the obstruction spacing, the nonzero path length effects need to be investigated. We consider this case by examining a random walk on a subset of a lattice where the jump size is comparable to the obstruction spacing (see Figure 2). We calculate the effective diffusivity coefficients for the graph in (46) with successively decreasing path (edge) lengths. Let

$$\lambda_h(e) = 1/h^2 \text{ for all } e \in \mathcal{E}_h.$$

The obstructed area remains constant but the path length is repeatedly halved. The results in Figure 3 show that D_e varies significantly for different h and thus the choice of path length is meaningful. Additionally, the effective diffusivity coefficients appear to converge that the effective diffusivity predicted by PDE homogenization. This suggests a "backdoor" approach wherein one might approximate PDE homogenization via homogenizing a graph with a very fine mesh or path length.

7.2 Modeling an interaction

This section explores the impact of an interaction (e.g., attraction, repulsion, or bonding) between the particle and obstruction boundaries on the effective diffusivity. We fix $h = 1/8$ and suppress dependence on h. The lower left graph in Figure 3 depicts a periodic cell of the graph of interest, $(\mathcal{S}, \mathcal{E}, \lambda)$. We choose various rate functions to model four different types of interactions between the random walker and the square obstruction. In the "Neutral" case, we simply set $\lambda(e) = 1/h^2$ for all $e \in \mathcal{E}$.

Define the set of nodes bordering the obstructed region,

$$\mathcal{B}_h = \{x \in \mathcal{S}_h \mid x + y \in \mathcal{O} \text{ for some } ||y||_\infty < h\}. \tag{47}$$
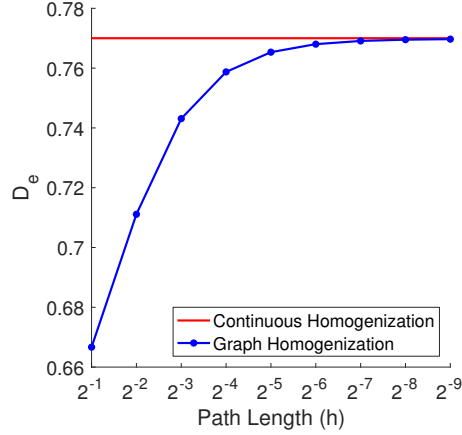
Figure 3: Effective diffusivity coefficients of the graphs depicted in Figure 2 and the effective diffusivity yielded by PDE homogenization. The effective diffusivity varies significantly for different path lengths ($h = 1/2, 1/4, \ldots, 1/512$) and appears to converge to the prediction of PDE homogenization.

In the "Bonding" case, the jump rate function is given by

$$\lambda(x, y) = \begin{cases} 1/(2h^2) & x \in \mathcal{B}_h \\ 1/h^2 & \text{otherwise.} \end{cases}$$

This rate function slows the random walker whenever it is near the boundary of an obstruction. In the "Repulsion" case,

$$\lambda(x, y) = \begin{cases} 2/h^2 & x \in \mathcal{B}_h, y \notin \mathcal{B}_h \\ 1/(2h^2) & x \notin \mathcal{B}_h, y \in \mathcal{B}_h \\ 1/h^2 & \text{otherwise,} \end{cases}$$

which causes the random walker to be pushed away from the obstructions. In the "Attraction" case,

$$\lambda(x, y) = \begin{cases} 2/h^2 & x \notin \mathcal{B}_h, y \in \mathcal{B}_h \\ 1/(2h^2) & x \in \mathcal{B}_h, y \notin \mathcal{B}_h \\ 1/h^2 & \text{otherwise.} \end{cases}$$

This rate function pulls the random walker towards the obstructions.

The latter three rate functions illustrate how one might account for interactions between a particle and the obstructions. The effective diffusivity coefficients for each regime are shown in Figure 4. The Bonding rate function yielded the most significant reduction in diffusion. Notably, diffusion in the Attraction regime was faster than the Repulsion regime.

7.3   Approximating continuous space

Note that our graph framework confines the particle to discrete spatial locations, which may not reflect reflect physical reality. A more accurate model would consider a random walk with finite
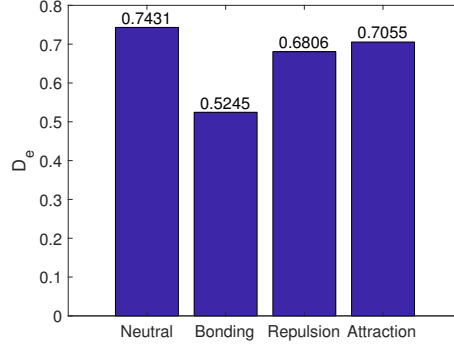
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Figure 4: Effective diffusivity coefficients for graphs with nodes and edges given by (46) and various rate functions. The rates are chosen to model four settings: 1) no interaction, 2) a bonding/sticking effect near the obstruction, 3) an obstruction that repels the random walker, and 4) an obstruction that attracts the random walker.

path length and *continuous state space* consisting of all points in the unobstructed region. The current graph model does not accommodate continuous space and thus we compare (via Monte Carlo simulations) the continuous space model's predictions with those of the graph model.

Define the process $X_h(t) \in \mathbb{R}^2 \backslash \mathcal{O}$ where X_h waits at a location for time $h^2/4$ and then moves along a straight path of length h in a uniformly chosen random direction. If the path intersects the obstructed region $\mathcal{O}$, then X undergoes a specular (mirror-like) reflection to ensure its path does not intersect $\mathcal{O}$. Because $X_h(t)$ exhibits normal diffusion, the effective diffusivity and mean squared displacement $MSD(t)$ are related by

$$D_e = \lim_{t \to \infty} \frac{MSD(t)}{4t}.$$

We use Monte Carlo simulation to compute an estimate $\widetilde{MSD}(t)$ of $MSD(t)$ at equally spaced points in time $\{t_i\}_{i=1}^N$. Let α denote the slope of the line of best fit (with 0 intercept) through the points $\left\{\left(t_i, \widetilde{MSD}(t_i)\right)\right\}_{i=1}^N$. We then estimate D_e as

$$D_e \approx \alpha/4$$

and calculate the 95% confindence intervals appropriately.

We can approximate X_h via the graph $(\mathcal{S}_h, \mathcal{E}_h, \lambda_h)$ where $\lambda_h(e) = 1/h^2$. We also introduce a slightly more sophisticated graph $(\widetilde{\mathcal{S}}_h, \widetilde{\mathcal{E}}_h, \widetilde{\lambda}_h)$ that accounts for jumps to diagonal neighbors and thus ought to better approximate X_h. Let

$$\widetilde{\mathcal{S}}_h = \mathcal{S}_h,$$
$$\widetilde{\mathcal{E}}_h = \mathcal{E}_h \cup \{(x,y) \in \widetilde{\mathcal{S}}_h \times \widetilde{\mathcal{S}}_h \mid x - y = \pm(h,h)\}.$$

The rate function $\widetilde{\lambda}_h$ should replicate the dynamics of X_h reflecting off of an obstruction. Specifically, when the solute has an approximately diagonal collision with an obstruction, the solute will experience a non-negligible displacement (rather than returning to its original location). We therefore double the jump rates along edges that begin and end on the obstruction boundaries $\mathcal{B}_h$ (47).
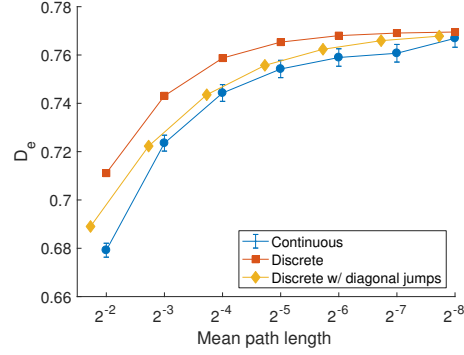
28

Figure 5: Effective diffusivity coefficients for the continuous process X_h ("Continuous"), the graph $(\mathcal{S}_h, \mathcal{E}_h, \lambda_h)$ ("Discrete"), and the graph $(\widetilde{\mathcal{S}}_h, \widetilde{\mathcal{E}}_h, \widetilde{\lambda}_h)$ ("Discrete w/ diagonal jumps") for $h = 2^{-2}, 2^{-3}, \ldots, 2^{-8}$.

Thus we define

$$\widetilde{\lambda}_h(x, y) = \begin{cases} 1/h^2 & x, y \in \mathcal{B}_h \\ 1/(2h^2) & \text{otherwise.} \end{cases}$$

The effective diffusivity coefficients (for $h = 2^{-2}, 2^{-3}, \ldots, 2^{-8}$) of the continuous process X_h, the graph $(\mathcal{S}_h, \mathcal{E}_h, \lambda_h)$, and the graph $(\widetilde{\mathcal{S}}_h, \widetilde{\mathcal{E}}_h, \widetilde{\lambda}_h)$ are shown in Figure 5. Incorporating diagonal jumps and thoughtful jump rates in $(\widetilde{\mathcal{S}}_h, \widetilde{\mathcal{E}}_h, \widetilde{\lambda}_h)$ yields a superior approximation of the continuous setting. In all three settings, D_e appears to converge to the same value as $h \to 0$.

A Validity of the formal result

In this section we show that the diffusivities of the formal asymptotics and the rigorous convergence theory are equal. That is, $K = C$ (see (18), (44) and Theorems 6.9). First, we show two auxiliary results.

Lemma A.1. *Let ω be a solution to the unit-cell problem (15) and ψ satisfy (38). Then*

$$\sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e \omega(y)^T \lambda_e = \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \psi(\partial_+ e) \nu_e^T \lambda_e \pi(y).$$

Proof. The result follows easily:

$$\sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e^i \omega_j(y) \lambda_e = \left(\rho_i, \omega_j \right) = \left(L\psi_i, \omega_j \right) = \left(\psi_i, L^T \omega_j \right) = \left(\psi_i, \sigma_j \right)$$

$$= \sum_{y \in \bar{\mathcal{S}}} \psi_i(y) \sum_{e \in \mathcal{E}'_y} \nu_e^j \pi(\partial_- e) \lambda_e = \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}'_y} \psi_i(\partial_+ e) \nu_e^j \pi(\partial_- e) \lambda_e$$

$$= \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \psi_i(\partial_+ e) \nu_e^j \lambda_e \pi(y).$$

$\square$

Lemma A.2. *The drift field ρ and ψ (see (38)) satisfy:*

$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(y)$$

$$= -\sum_{y \in \bar{S}} \psi(y)\rho(y)^T \pi(y) - \sum_{y \in \bar{S}} \rho(y)\psi(y)^T \pi(y) \tag{48}$$

Proof. First, notice that

$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))\psi(\partial_+ e)^T \lambda_e \pi(y) + \sum_{y \in \bar{S}} \psi(y)\rho(y)^T \pi(y)$$

$$= \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))\psi(\partial_+ e)^T \lambda_e \pi(y) + \sum_{y \in \bar{S}} \psi(y)(L\psi)(y)^T \pi(y)$$

$$= \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))\psi(\partial_+ e)^T \lambda_e \pi(y) + \sum_{y \in \bar{S}} \psi(y) \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(y)$$

$$= \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \Big((\psi(\partial_+ e) - \psi(\partial_- e))\psi(\partial_+ e)^T + (\psi(\partial_+ e) - \psi(\partial_- e))\psi(\partial_- e)^T \Big) \lambda_e \pi(\partial_- e)$$

$$= \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \Big(\psi(\partial_+ e)\psi(\partial_+ e)^T - \psi(\partial_- e)\psi(\partial_+ e)^T$$

$$\qquad + \psi(\partial_+ e)\psi(\partial_- e)^T - \psi(\partial_- e)\psi(\partial_- e)^T \Big) \lambda_e \pi(\partial_- e)$$

$$= \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \Big(\psi(\partial_+ e)\psi(\partial_+ e)^T - \psi(\partial_- e)\psi(\partial_- e)^T \Big) \lambda_e \pi(\partial_- e)$$

$$= \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \psi(\partial_+ e)\psi(\partial_+ e)^T \lambda_e \pi(\partial_- e) - \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} \psi(\partial_- e)\psi(\partial_- e)^T \lambda_e \pi(\partial_- e)$$

$$= \sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}'_y} \psi(\partial_+ e)\psi(\partial_+ e)^T \lambda_e \pi(\partial_- e) - \sum_{y \in \bar{S}} \psi(y)\psi(y)^T \pi(y) \sum_{e \in \mathcal{E}_y} \lambda_e$$

$$= \sum_{y \in \bar{S}} \psi(y)\psi(y)^T \Big(\sum_{e \in \mathcal{E}'_y} \pi(y - \nu_e)\lambda_e - \pi(y)\lambda^0(y) \Big) \sum_{y \in \bar{S}} \psi(y)\psi(y)^T (L^T \pi)(y) = 0.$$

That is,

$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))\psi(\partial_+ e)^T \lambda_e \pi(y) = -\sum_{y \in \bar{S}} \psi(y)\rho(y)^T \pi(y).$$

Combine this equality with

$$\sum_{y \in \bar{S}} \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))\psi(\partial_- e)^T \lambda_e \pi(y)$$

$$= \sum_{y \in \bar{S}} \Big(\sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))\lambda_e \Big) \psi(y)^T \pi(y)$$

$$= \sum_{y \in \bar{S}} (L\psi)(y)\psi(y)^T \pi(y) = \sum_{y \in \bar{S}} \rho(y)\psi(y)^T \pi(y).$$

to get the desired result. $\qquad \square$

Theorem A.3. *The effective diffusivities derived from the formal and rigorous derivation are equal. That is, $K = C$ where K and C are defined in (18) and (44), respectively.*

Proof. Expanding the definition of C (44),

$$
C = \frac{1}{2} \sum_{e \in \bar{\mathcal{E}}} \lambda_e \nu_e \nu_e^T \pi(\partial_- e) - \frac{1}{2} \sum_{e \in \bar{\mathcal{E}}} \nu_e \big(\psi(\partial_+ e) - \psi(\partial_- e)\big)^T \lambda_e \pi(\partial_- e)
$$

$$
- \frac{1}{2} \sum_{e \in \bar{\mathcal{E}}} \big(\psi(\partial_+ e) - \psi(\partial_- e)\big) \nu_e^T \lambda_e \pi(\partial_- e)
$$

$$
+ \frac{1}{2} \sum_{e \in \bar{\mathcal{E}}} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(\partial_- e).
$$

The first terms of K (18) and C (above) are identical and so they can be ignored. Scale the remaining terms by 2 and the desired result holds if and only if

$$
\sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e \omega(y)^T \lambda_e + \omega(y) \nu_e^T \lambda_e
$$

$$
= \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e \big(\psi(\partial_+ e) - \psi(\partial_- e)\big)^T \lambda_e \pi(\partial_- e) + \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \big(\psi(\partial_+ e) - \psi(\partial_- e)\big) \nu_e^T \lambda_e \pi(\partial_- e)
$$

$$
- \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} (\psi(\partial_+ e) - \psi(\partial_- e))(\psi(\partial_+ e) - \psi(\partial_- e))^T \lambda_e \pi(\partial_- e).
$$

From Lemmas A.1 and A.2, this is equivalent to

$$
\sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \psi(\partial_+ e) \nu_e^T \pi(y) \lambda_e + \nu_e \psi(\partial_+ e)^T \pi(y) \lambda_e
$$

$$
= \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e \big(\psi(\partial_+ e) - \psi(\partial_- e)\big)^T \lambda_e \pi(y) + \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \big(\psi(\partial_+ e) - \psi(\partial_- e)\big) \nu_e^T \lambda_e \pi(y)
$$

$$
+ \sum_{y \in \bar{\mathcal{S}}} \psi(y) \rho(y)^T \pi(y) + \sum_{y \in \bar{\mathcal{S}}} \rho(y) \psi(y)^T \pi(y).
$$

Expanding terms and substituting the definition of ρ (19), this is equivalent to

$$
\sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \psi(\partial_+ e) \nu_e^T \pi(y) \lambda_e + \nu_e \psi(\partial_+ e)^T \pi(y) \lambda_e
$$

$$
= \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e \psi(\partial_+ e)^T \lambda_e \pi(y) - \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \nu_e \psi(\partial_- e)^T \lambda_e \pi(y)
$$

$$
+ \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \psi(\partial_+ e) \nu_e^T \lambda_e \pi(y) - \sum_{y \in \bar{\mathcal{S}}} \sum_{e \in \mathcal{E}_y} \psi(\partial_- e) \nu_e^T \lambda_e \pi(y)
$$

$$
+ \sum_{y \in \bar{\mathcal{S}}} \psi(y) \Big(\sum_{e \in \mathcal{E}_y} \nu_e \lambda_e \Big)^T \pi(y) + \sum_{y \in \bar{\mathcal{S}}} \Big(\sum_{e \in \mathcal{E}_y} \nu_e \lambda_e \Big) \psi(y)^T \pi(y).
$$

Some simple bookkeeping demonstrates that this equality holds. Hence, the desired result. $\square$

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References

[1] A. Bensoussan, J.-L. Lions, and G. Papanicolaou, *Asymptotic analysis for periodic structures*, vol. 374, American Mathematical Soc., 2011.

[2] N. Berger and M. Biskup, *Quenched invariance principle for simple random walk on percolation clusters*, Probability theory and related fields, 137 (2007), pp. 83–120.

[3] P. Billingsley, *Convergence of probability measures*, Wiley, 2011.

[4] M. Biskup, *Recent progress on the random conductance model*, Probability Surveys, 8 (2011), pp. 294–373.

[5] P. Caputo and D. Ioffe, *Finite volume approximation of the effective diffusion matrix: the case of independent bond disorder*, in Annales de l'Institut Henri Poincare (B) Probability and Statistics, vol. 39, Elsevier, 2003, pp. 505–525.

[6] P. Donovan, Y. Chehreghanianzabi, M. Rathinam, and S. P. Zustiak, *Homogenization theory for the prediction of obstructed solute diffusivity in macromolecular solutions*, Plos One, 11 (2016).

[7] A.-C. Egloffe, A. Gloria, J.-C. Mourrat, and T. N. Nguyen, *Random walk in random environment, corrector equation and homogenized coefficients: from theory to numerics, back and forth*, IMA journal of numerical analysis, 35 (2014), pp. 499–545.

[8] S. N. Ethier and T. G. Kurtz, *Markov processes characterization and convergence*, Wiley-Interscience, 2005.

[9] A. Faggionato, *Random walks and exclusion processes among random conductances on random infinite clusters: homogenization and hydrodynamic limit*, Electronic Journal of Probability, 13 (2008), pp. 2217–2247.

[10] A. Gloria and J. Nolen, *A quantitative central limit theorem for the effective conductance on the discrete torus*, Communications on Pure and Applied Mathematics, 69 (2016), pp. 2304–2348.

[11] A. Gloria, F. Otto, et al., *An optimal variance estimate in stochastic homogenization of discrete elliptic equations*, The annals of probability, 39 (2011), pp. 779–856.

[12] J. B. Keller, *Effective behavior of heterogeneous media*, in Statistical mechanics and statistical methods in theory and application, Springer, 1977, pp. 631–644.

[13] C. Kipnis and S. S. Varadhan, *Central limit theorem for additive functionals of reversible markov processes and applications to simple exclusions*, Communications in Mathematical Physics, 104 (1986), pp. 1–19.

[14] F. C. Klebaner, *Introduction to stochastic calculus with applications*, Imperial College Press, 2012.

[15] S. Kozlov, *Averaging of difference schemes*, Mathematics of the USSR-Sbornik, 57 (1987), p. 351.

[16] S. Kozlov, O. Olenik, and V. Zhikov, *Homogenization of differential operators*, Russian Mathem. Surveys, 35 (1980), p. 254.

[17] R. Künnemann, *The diffusion limit for reversible jump processes onz d with ergodic random bond conductivities*, Communications in Mathematical Physics, 90 (1983), pp. 27–68.

[18] P. Mathieu, *Quenched invariance principles for random walks with random conductances*, Journal of Statistical Physics, 130 (2008), pp. 1025–1046.

[19] H. Owhadi, *Approximation of the effective conductivity of ergodic media by periodization*, Probability theory and related fields, 125 (2003), pp. 225–258.