RANDOM WALK IN RANDOM ENVIRONMENT, CORRECTOR EQUATION, AND HOMOGENIZED COEFFICIENTS: FROM THEORY TO NUMERICS, BACK AND FORTH

A.-C. EGLOFFE, A. GLORIA, J.-C. MOURRAT, AND T. N. NGUYEN

Abstract. This article is concerned with numerical methods to approximate effective coefficients in stochastic homogenization of discrete linear elliptic equations, and their numerical analysis — which has been made possible by recent contributions on quantitative stochastic homogenization theory by two of us, and by Neukamm and Otto. This article makes the connection between our theoretical results and computations. We give a complete picture of the numerical methods found in the literature, compare them in terms of known (or expected) convergence rates, and empirically study them. Two types of methods are presented: methods based on the corrector equation, and methods based on random walks in random environments. The numerical study confirms the sharpness of the analysis (which it completes by making precise the prefactors, next to the convergence rates), supports some of our conjectures, and calls for new theoretical developments.

Keywords: stochastic homogenization, discrete elliptic equations, effective coefficients, random walk, random environment, Monte-Carlo method, quantitative estimates.

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1. Introduction

In many applications in mechanics and flows in porous media, one faces the problem of heterogeneous coefficients which vary at a very small scale compared to the typical size of the domain. One generally addresses the numerical simulation of such problems by appealing to homogenization methods. In the literature, the periodic case has been widely studied, and both qualitative and quantitative (in the sense of convergence rates) numerical analysis have been successfully conducted, see e. g. [HW97, HWC99, Ar00, Ab05, EMZ05, EH09, BLB09, E12]. Yet, naturally-occuring (and even manly manufactured) materials are rarely periodic. A natural assumption to depart from periodicity — while still ensuring a proper homogenization theory — is to consider a random field that is stationarity and ergodic. In that case however, most of the results in the literature are either qualitative [Ow03, EP03, Gl06] or suboptimal in terms of convergence rates [Yu, CI03, BP04, EMZ05]. A first question that arises in numerical homogenization methods is typically the approximation of effective coefficients (although this is only part of the problem, since fine-scale features of the flux are also of utmost importance for flows in porous media). Many methods have been proposed in the literature to approximate homogenized coefficients: either using approximations of the corrector equation (in which case artificial boundary conditions are needed, see for instance the numerical studies in [EY07, KFGMJ]) or using random walks in random environments as suggested by Papanicolaou in [Pa83].

The aim of this paper is twofold. First, we give a complete numerical analysis of these numerical approximation methods in the case of discrete elliptic equations with independent and identically distributed coefficients (and motivate some conjectures in a few cases), which are a prototypical example of elliptic equations with random coefficients. This part is mainly a review of results obtained by two of us, and Otto and Neukamm in a recent series of papers [GO11, GO12, Mo11, GNOa, Gl12a, GM12, GM13, GNOb], but written this time in view of applications and in a way accessible to probabilists, analysts, and numerical analysts. To this end, since we treat both the corrector equation and the random walks in random environments points of view, we display a short comprehensive review of the well-known qualitative results of stochastic homogenization. Since they require rather different mathematical techniques, they are indeed rarely presented together. To make the review of our recent results more interesting than a mere summary, we also display informal proofs in the simpler case of small ellipticity contrast (that is, when the coefficients are a random perturbation of the identity), which allows us to put in evidence the main arguments without treating the difficulties raised by the general case. This forms the survey part of this paper.

As will be clear in the core of the text, when analyzing numerical methods, we only obtain convergence rates: our methods do not allow one to quantify prefactors. In practice however, prefactors can drastically change the performance of numerical methods. Getting an insight on the values of these prefactors is the aim of the second part of this paper, which displays a systematic empirical study of the methods analyzed in the first part (taking advantage of the analysis itself). This study both confirms the sharpness of our analysis and gives a clear picture of the prefactors, thus allowing us to identify the best performer for the cases addressed in this manuscript. In addition, the outputs of some numerical tests challenge our understanding of some phenomena related to symmetry and display faster convergence than expected in general. This calls for new mathematical insight.

Let us emphasize that this article is not a survey of the literature on quantitative stochastic homogenization or numerical homogenization. For general references on quantitative stochastic homogenization, we refer the reader to the introduction of [GNOa]. For numerical homogenization methods in general, we refer the reader to [Gl12b] and the references therein. Last, let us mention a recent contribution of Costaouec, Le Bris, and Legoll [CLL10]. There the authors address the interesting question of reducing the variance of approximations of homogenized coefficients (which are still random since not yet at the ergodic limit). Their approach may indeed reduce one of the prefactors that appear in the numerical analysis presented here (as will be made clear in the text), and can therefore be used on top of the methods analyzed in this contribution.

2. Stochastic homogenization: corrector equation and RWRE

There have always been strong connections between stochastic homogenization of linear elliptic PDEs and random walks in random environments (RWRE). In the first case, the central object is the random elliptic operator which can be replaced on large scales by a deterministic elliptic operator characterized by the so-called homogenized matrix. In the second case, the distribution of the rescaled random walk can be replaced by the distribution of a Brownian motion, the covariance matrix of which is deterministic (and corresponds to twice the homogenized matrix).

In this section, we start with the description of discrete diffusion coefficients, first present the discrete elliptic point of view, and then turn to the random walk in random environment viewpoint. The aim of this section is to introduce a formalism, and give an intuition on both points of view.

The results recalled here are essentially due to Papanicolaou and Varadhan [PV79], Künnemann [Kü83], Kozlov [Ko87], and Kipnis and Varadhan [KV86].

We present the results in the case of independent and identically distributed (i.i.d.) conductivities, although everything in this section remains valid provided the conductivities lie in a compact set of $(0,+\infty)$, are stationary, and ergodic. In particular, we shall apply this theory (and its quantitative counterpart) to i.i.d. coefficients in this presentation.

2.1. **Random environment.** We say that x, y in $\mathbb{Z}^d$ are neighbors, and write $x \sim y$, whenever $|y-x| = 1$. This relation turns $\mathbb{Z}^d$ into a graph, whose set of (non-oriented) edges is denoted by $\mathbb{B}$.

Definition 2.1 (environment)**.** *Let $0 < \alpha \leqslant \beta < +\infty$, and $\Omega = [\alpha,\beta]^{\mathbb{B}}$. An element $\omega = (\omega_e)_{e\in\mathbb{B}}$ of Ω is called an* environment*. With any edge $e = (x,y) \in \mathbb{B}$, we associate the* conductance *$\omega_{(x,y)} := \omega_e$ (by construction $\omega_{(x,y)} = \omega_{(y,x)}$). Let ν be a probability measure on $[\alpha,\beta]$. We endow Ω with the product probability measure $\mathbb{P} = \nu^{\otimes\mathbb{B}}$. In other words, if ω is distributed according to the measure $\mathbb{P}$, then $(\omega_e)_{e\in\mathbb{B}}$ are independent random variables of law ν. We denote by $L^2(\Omega)$ the set of real square integrable functions on Ω for the measure $\mathbb{P}$, and write $\langle\cdot\rangle$ for the expectation associated with $\mathbb{P}$.*

We then introduce the notion of stationarity.

Definition 2.2 (stationarity)**.** *For all $z \in \mathbb{Z}^d$, we let $\theta_z : \Omega \to \Omega$ be such that for all $\omega \in \Omega$ and $(x,y) \in \mathbb{B}$, $(\theta_z\ \omega)_{(x,y)} = \omega_{(x+z,y+z)}$. This defines an additive action group $\{\theta_z\}_{z\in\mathbb{Z}^d}$ on Ω which preserves the measure $\mathbb{P}$, and is ergodic for $\mathbb{P}$.*

We say that a function $f : \Omega \times \mathbb{Z}^d \to \mathbb{R}$ is stationary *if and only if for all $x, z \in \mathbb{Z}^d$ and $\mathbb{P}$-almost every $\omega \in \Omega$,*

$$f(x+z,\omega) \ = \ f(x,\theta_z\ \omega).$$

In particular, with all $f \in L^2(\Omega)$, one may associate the stationary function (still denoted by f) : $\mathbb{Z}^d \times \Omega \to \mathbb{R}, (x,\omega) \mapsto f(\theta_x\ \omega)$. In what follows we will not distinguish between $f \in L^2(\Omega)$ and its stationary extension on $\mathbb{Z}^d \times \Omega$.

2.2. **Corrector equation.**

Definition 2.3 (conductivity matrix)**.** *Let Ω, $\mathbb{P}$, and $\{\theta_z\}_{z\in\mathbb{Z}^d}$ be as in Definitions 2.1 and 2.2. The stationary diffusion matrix $A : \mathbb{Z}^d \times \Omega \to \mathcal{M}_d(\mathbb{R})$ is defined by*

$$A : (x,\omega) \mapsto \mathrm{diag}(\omega_{(x,x+\mathbf{e}_i)}, \dots, \omega_{(x,x+\mathbf{e}_d)}).$$

For each $\omega \in \Omega$, we consider the discrete elliptic operator L defined by

$$L = -\nabla^* \cdot A(\cdot,\omega)\nabla, \tag{2.1}$$

where ∇ and ∇^* are the forward and backward discrete gradients, acting on functions $u : \mathbb{Z}^d \to \mathbb{R}$ as

$$\nabla u(x) := \begin{bmatrix} u(x+\mathbf{e}_1) - u(x) \\ \vdots \\ u(x+\mathbf{e}_d) - u(x) \end{bmatrix}, \quad \nabla^* u(x) := \begin{bmatrix} u(x) - u(x-\mathbf{e}_1) \\ \vdots \\ u(x) - u(x-\mathbf{e}_d) \end{bmatrix}, \tag{2.2}$$

and we denote by $\nabla^*\cdot$ the backward divergence. In particular, for all $u : \mathbb{Z}^d \to \mathbb{R}$,

$$Lu : \mathbb{Z}^d \to \mathbb{R}, \; z \mapsto \sum_{z' \sim z} \omega_{(z,z')}(u(z) - u(z')). \tag{2.3}$$

The standard stochastic homogenization theory for such discrete elliptic operators (see for instance [Kü83], [Ko87]) ensures that there exist homogeneous and deterministic coefficients A_{hom} such that the solution operator of the continuum differential operator $-\nabla \cdot A_{\mathrm{hom}} \nabla$ describes $\mathbb{P}$-almost surely the large scale behavior of the solution operator of the discrete differential operator $-\nabla^* \cdot A(\cdot,\omega)\nabla$. As for the periodic case, the definition of A_{hom} involves the so-called correctors. Let $\xi \in \mathbb{R}^d$ be a fixed direction. The corrector $\phi : \mathbb{Z}^d \times \Omega \to \mathbb{R}$ in direction ξ is the unique solution (in a sense made precise below) o the equation

$$-\nabla^* \cdot A(x,\omega)(\xi + \nabla\phi(x,\omega)) \;=\; 0, \qquad x \in \mathbb{Z}^d. \tag{2.4}$$

The following lemma gives the existence and uniqueness of this corrector ϕ.

Lemma 2.4 (corrector)**.** *Let Ω, $\mathbb{P}$, $\{\theta_z\}_{z\in\mathbb{Z}^d}$, and A be as in Definitions 2.1, 2.2, and 2.3. Then, for all $\xi \in \mathbb{R}^d$, there exists a unique measurable function $\phi : \mathbb{Z}^d \times \Omega \to \mathbb{R}$ such that $\phi(0,\cdot) \equiv 0$, $\nabla\phi$ is stationary, $\langle \nabla\phi \rangle = 0$, and ϕ solves* (2.4) *$\mathbb{P}$-almost surely. Moreover, the symmetric homogenized matrix A_{hom} is characterized by*

$$\xi \cdot A_{\mathrm{hom}}\xi \;=\; \langle (\xi + \nabla\phi) \cdot A(\xi + \nabla\phi) \rangle \,. \tag{2.5}$$

The standard proof of Lemma 2.4 makes use of the regularization of (2.4) by a zero-order term $\mu > 0$:

$$\mu\phi_\mu(x,\omega) - \nabla^* \cdot A(x,\omega)(\xi + \nabla\phi_\mu(x,\omega)) \;=\; 0, \qquad x \in \mathbb{Z}^d. \tag{2.6}$$

Lemma 2.5 (regularized corrector)**.** *Let Ω, $\mathbb{P}$, $\{\theta_z\}_{z\in\mathbb{Z}^d}$, and A be as in Definitions 2.1, 2.2, and 2.3. Then, for all $\mu > 0$ and $\xi \in \mathbb{R}^d$, there exists a unique stationary function $\phi_\mu \in L^2(\Omega)$ with $\langle \phi_\mu \rangle = 0$ which solves* (2.6) *$\mathbb{P}$-almost surely.*

To prove Lemma 2.5, we follow [PV79], and introduce difference operators on $L^2(\Omega)$: for all $u \in L^2(\Omega)$, we set

$$\mathrm{D}\, u(\omega) := \begin{bmatrix} u(\theta_{\mathbf{e}_1}\omega) - u(\omega) \\ \vdots \\ u(\theta_{\mathbf{e}_d}\omega) - u(\omega) \end{bmatrix}, \quad \mathrm{D}^*\, u(\omega) := \begin{bmatrix} u(\omega) - u(\theta_{-\mathbf{e}_1}\omega) \\ \vdots \\ u(\omega) - u(\theta_{-\mathbf{e}_d}\omega) \end{bmatrix}. \tag{2.7}$$

These operators play the same roles as the finite differences ∇ and ∇^* — this time for the variable ω. In other words, they define a difference calculus in $L^2(\Omega)$. They allow us to define the counterpart on $L^2(\Omega)$ of the operator L of (2.1):

Definition 2.6. *Let Ω, $\mathbb{P}$, $\{\theta_z\}_{z\in\mathbb{Z}^d}$, and A be as in Definitions 2.1, 2.2, and 2.3. We define $\mathcal{L} : L^2(\Omega) \to L^2(\Omega)$ by*

$$\begin{aligned} \mathcal{L}u(\omega) &= -\,\mathrm{D}^* \cdot A(\omega)\,\mathrm{D}\,u(\omega) \\ &= \sum_{z\sim 0} \omega_{0,z}(u(\omega) - u(\theta_z\,\omega)) \end{aligned}$$

where D *and* D^* *are as in* (2.7)*.*

The fundamental relation between L and $\mathcal{L}$ is the following identity for stationary fields $u : \mathbb{Z}^d \times \Omega \to \mathbb{R}$: for all $z \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$,

$$Lu(z,\omega) \,=\, \mathcal{L}u(\theta_z\omega).$$

In particular, the regularized corrector ϕ_μ is also the unique weak solution in $L^2(\Omega)$ of the equation

$$\mu\phi_\mu(\omega) - \mathrm{D}^* \cdot A(\omega)(\xi + \mathrm{D}\,\phi_\mu(\omega)) \,=\, 0, \quad \omega \in \Omega,$$

and its existence simply follows from the Riesz representation theorem in $L^2(\Omega)$.

The regularized corrector ϕ_μ is an approximation of the corrector ϕ in the following sense:

Lemma 2.7. *Let Ω, $\mathbb{P}$, $\{\theta_z\}_{z\in\mathbb{Z}^d}$, and A be as in Definitions 2.1, 2.2, and 2.3. For all $\mu > 0$ and $\xi \in \mathbb{R}^d$, let ϕ and ϕ_μ be the corrector and regularized corrector of Lemmas 2.4 and 2.5. Then, we have*

$$\lim_{\mu\to 0} \left\langle |\,\mathrm{D}\,\phi_\mu - \nabla\phi|^2 \right\rangle \,=\, 0.$$

Proof of Lemma 2.4. From the elementary a priori estimates

$$\left\langle |\nabla\phi_\mu|^2 \right\rangle \,=\, \left\langle |\,\mathrm{D}\,\phi_\mu|^2 \right\rangle \,\leqslant\, C, \qquad \left\langle \phi_\mu^2 \right\rangle \,\leqslant\, C\mu^{-1},$$

for some C independent of μ, we learn that $\mathrm{D}\,\phi_\mu$ is bounded in $L^2(\Omega, \mathbb{R}^d)$ uniformly in μ, so that up to extraction it converges weakly in $L^2(\Omega, \mathbb{R}^d)$ to some random field Φ. Let us denote by $L^2_{\mathrm{pot}}(\Omega, \mathbb{R}^d)$ the closure of gradient fields in $L^2(\Omega, \mathbb{R}^d)$. Then, $\Phi \in L^2_{\mathrm{pot}}(\Omega, \mathbb{R}^d)$. This allows one to pass to the limit in the weak formulations and obtain the existence of a field $\Phi = (\Phi_1, \dots, \Phi_d) \in L^2_{\mathrm{pot}}(\Omega, \mathbb{R}^d)$ such that for all $\psi \in L^2(\Omega)$,

$$\langle \mathrm{D}\,\psi \cdot A(\xi + \Phi) \rangle \,=\, 0. \tag{2.8}$$

Using the following weak Schwarz commutation rule

$$\begin{aligned} \forall j,k \in \{1,\dots,d\}, \quad \langle (\mathrm{D}_j\,\psi)\Phi_k \rangle &= \lim_{\mu\to 0} \langle (D_j\psi)(D_k\phi_\mu) \rangle \\ &= \lim_{\mu\to 0} \langle (D_k\psi)(D_j\phi_\mu) \rangle \,=\, \langle (\mathrm{D}_k\,\psi)\Phi_j \rangle \end{aligned}$$

one may uniquely define $\phi : \mathbb{Z}^d \times \Omega \to \mathbb{R}$ such that $\nabla\phi$ is the stationary extension of Φ, and $\phi(0,\omega) = 0$ for almost every $\omega \in \Omega$. By definition this function ϕ is not stationary. It is indeed a priori not clear (and even wrong in dimension $d \leqslant 2$) whether there exists some function $\varphi \in L^2(\Omega)$ such that $\mathrm{D}\,\varphi = \Phi$ (this is a major difference with the periodic case). Let us check that for all $\chi : \mathbb{Z}^d \to \mathbb{R}$ with compact support, ϕ satisfies almost surely the weak form of (2.4):

$$\sum_{z\in\mathbb{Z}^d} \nabla\chi(z)\cdot A(z,\omega)(\xi+\nabla\phi(z,\omega)) \;=\; 0. \tag{2.9}$$

Let $\zeta \in L^2(\Omega)$ and test the equation for Φ with test-function $\sum_{z\in\mathbb{Z}^d}\chi(z)\zeta(\theta_{-z}\omega)$ (which is well-defined since χ is compactly supported). This yields after resummation in z (discrete integration by parts):

$$0 \;=\; \left\langle \sum_{z\in\mathbb{Z}^d} \chi(z)\,\mathrm{D}\,\zeta(\theta_{-z}\cdot)\cdot A(\xi+\Phi)\right\rangle \;=\; \left\langle \sum_{z\in\mathbb{Z}^d} \nabla\chi(z)\zeta(\theta_{-z}\cdot)\cdot A(\xi+\Phi)\right\rangle.$$

Since θ_{-z} preserves the measure, this turns into

$$\left\langle \zeta\sum_{z\in\mathbb{Z}^d} \nabla\chi(z)\cdot A(\theta_z\cdot)(\xi+\Phi(\theta_z\cdot))\right\rangle \;=\; 0,$$

which implies (2.9) by arbitrariness of ζ and definition of stationary extensions. This proves the existence of a corrector ϕ. We now turn to uniqueness. There are at least three different proofs. All of them rely on ergodicity:

(i) a proof based on spectral theory (using that ergodicity implies that $t\mapsto \exp(t\,\mathrm{D}\cdot\mathrm{D})\chi$ converges to $\langle\chi\rangle$ as $t\to\infty$), see [PV79];
(ii) a proof based on the sublinearity of quadratic averages of the corrector at infinity, see [SS04] and [ADS13];
(iii) a proof based on a characterization of potential fields in probability through the Weyl decomposition of $L^2(\Omega,\mathbb{R}^d)$, see [JKO94].

The last two approaches imply it is enough to prove uniqueness of potential fields $\Psi \in L^2_{\mathrm{pot}}(\Omega,\mathbb{R}^d)$ that satisfy for all $\zeta\in L^2(\Omega)$,

$$\langle \mathrm{D}\,\zeta\cdot A(\xi+\Psi)\rangle \;=\; 0.$$

Indeed, if $\nabla\phi$ is a stationary field with bounded second moment, there exists $\Psi\in L^2(\Omega,\mathbb{R}^d)$ such that $\nabla\phi(x,\omega)=\Psi(\theta_x\omega)$, and both (ii) and (iii) imply that $\Psi\in L^2_{\mathrm{pot}}(\Omega,\mathbb{R}^d)$. Let us conclude. The field Φ is a solution of this problem by construction. Let Ψ be another solution. If there were some $\varphi,\psi\in L^2(\Omega)$ with $\Phi=\mathrm{D}\,\varphi$ and $\Psi=\mathrm{D}\,\psi$, we would simply test the equation with $\varphi-\psi$. Here, instead we test the equation with functions of $L^2(\Omega)$ whose gradients are arbitrarily close to Φ and Ψ. To this aim we consider the unique weak solution $\psi_\mu\in L^2(\Omega)$ of

$$\mu\psi_\mu - \mathrm{D}^*\cdot\mathrm{D}\,\psi_\mu \;=\; -\,\mathrm{D}^*\cdot\Psi.$$

From the same a priori estimates as for ϕ_μ, i. e.

$$\left\langle|\,\mathrm{D}\,\psi_\mu|^2\right\rangle \;\leqslant\; C, \qquad \left\langle\psi_\mu^2\right\rangle \;\leqslant\; C\mu^{-1},$$

we learn that $\mathrm{D}\,\psi_\mu$ is bounded in $L^2(\Omega,\mathbb{R}^d)$, and that $\mu\psi_\mu$ converges weakly to 0 in $L^2(\Omega)$. Hence, there exists $\tilde\Psi\in L^2_{\mathrm{pot}}(\Omega,\mathbb{R}^d)$ such that up to extraction, we have for all $\zeta\in L^2(\Omega)$,

$$\left\langle \mathrm{D}\,\zeta\cdot\tilde\Psi\right\rangle \;=\; \lim_{\mu\to 0}\,\langle\mu\psi_\mu\zeta+\mathrm{D}\,\zeta\cdot\mathrm{D}\,\psi_\mu\rangle \;=\; \langle \mathrm{D}\,\zeta\cdot\Psi\rangle\,.$$

Since $\tilde{\Psi}$ and Ψ are both potential fields, this yields $\tilde{\Psi}=\Psi$ by the arbitrariness of ζ, so that the entire sequence $\mathrm{D}\,\psi_\mu$ converges weakly in $L^2(\Omega,\mathbb{R}^d)$ to Ψ. We then substract the weak formulations of the equations for Φ and Ψ with test-function $\phi_\mu-\psi_\mu$. This yields

$$\langle \mathrm{D}(\phi_\mu-\psi_\mu)\cdot A(\Phi-\Psi)\rangle \;=\; 0.$$

Since $\lim_{\mu\to 0}\mathrm{D}(\phi_\mu-\psi_\mu)=\Phi-\Psi$ weakly in $L^2(\Omega)^d$, we conclude that

$$\left\langle |\Phi-\Psi|^2\right\rangle \;=\; 0,$$

which is the desired uniqueness result. □

We conclude this section by the proof of the strong convergence (2.11), which is the adaptation to the discrete setting of the corresponding proof of [PV79] in the continuum setting.

Proof of Lemma 2.7. The operator $\mathcal{L}$ of Definition 2.6 is bounded, self-adjoint, and non-negative on $L^2(\Omega)$. Indeed, for all $\psi,\chi\in L^2(\Omega)$, we have by direct computations

$$\left\langle (\mathcal{L}\psi)^2\right\rangle^{1/2} \;\leqslant\; 4d\sqrt{\beta}\left\langle \psi^2\right\rangle^{1/2}, \quad \langle (\mathcal{L}\psi)\chi\rangle \;=\; \langle \psi(\mathcal{L}\chi)\rangle\,, \quad \langle \psi\mathcal{L}\psi\rangle \geqslant 2d\alpha\left\langle \psi^2\right\rangle.$$

Hence, $\mathcal{L}$ admits a spectral resolution on $L^2(\Omega)$. For all $g\in L^2(\Omega)$ we denote by e_g the projection of the spectral measure of $\mathcal{L}$ on g. This defines the following spectral calculus: for any bounded continuous function $\Psi:[0,+\infty)\to\mathbb{R}_+$,

$$\langle (\Psi(\mathcal{L})g)g\rangle \;=\; \int_{\mathbb{R}^+}\Psi(\lambda)de_g(\lambda).$$

Let $\xi\in\mathbb{R}^d$ with $|\xi|=1$ be fixed, and define the local drift by $\mathfrak{d}\;=\;\mathrm{D}^*\cdot A\xi\in L^2(\Omega)$. For all $\mu\geqslant\nu>0$ we have $\phi_\mu=(\mu+\mathcal{L})^{-1}\mathfrak{d}$ and $\phi_\nu=(\nu+\mathcal{L})^{-1}\mathfrak{d}$, so that by the Cauchy-Schwarz inequality,

$$\begin{aligned}
\left\langle |\mathrm{D}\,\phi_\mu-\mathrm{D}\,\phi_\nu|^2\right\rangle &\leqslant \alpha^{-1}\langle (\phi_\mu-\phi_\nu)\mathcal{L}(\phi_\mu-\phi_\nu)\rangle\\
&= \alpha^{-1}\langle \phi_\mu\mathcal{L}\phi_\mu\rangle-2\alpha^{-1}\langle \phi_\mu\mathcal{L}\phi_\nu\rangle+\alpha^{-1}\langle \phi_\nu\mathcal{L}\phi_\nu\rangle\\
&= \alpha^{-1}\left\langle \mathfrak{d}(\mu+\mathcal{L})^{-1}\mathcal{L}(\mu+\mathcal{L})^{-1}\mathfrak{d}\right\rangle-2\alpha^{-1}\left\langle \mathfrak{d}(\mu+\mathcal{L})^{-1}\mathcal{L}(\nu+\mathcal{L})^{-1}\mathfrak{d}\right\rangle\\
&\quad +\alpha^{-1}\left\langle \mathfrak{d}(\nu+\mathcal{L})^{-1}\mathcal{L}(\nu+\mathcal{L})^{-1}\mathfrak{d}\right\rangle.
\end{aligned}$$

By the spectral formula with functions

$$\Psi(\lambda)\;=\;\frac{\lambda}{(\mu+\lambda)^2},\frac{\lambda}{(\mu+\lambda)(\nu+\lambda)},\frac{\lambda}{(\nu+\lambda)^2},$$

we obtain

$$\begin{aligned}
\left\langle |\mathrm{D}\,\phi_\mu-\mathrm{D}\,\phi_\nu|^2\right\rangle &\leqslant \alpha^{-1}\int_{\mathbb{R}^+}\left(\frac{\lambda}{(\mu+\lambda)^2}-2\frac{\lambda}{(\mu+\lambda)(\nu+\lambda)}+\frac{\lambda}{(\nu+\lambda)^2}\right)de_{\mathfrak{d}}(\lambda)\\
&= \alpha^{-1}\int_{\mathbb{R}^+}\frac{\lambda(\nu-\mu)^2}{(\mu+\lambda)^2(\nu+\lambda)^2}de_{\mathfrak{d}}(\lambda) \qquad (2.10)\\
&\leqslant \alpha^{-1}\int_{\mathbb{R}^+}\frac{\mu^2}{(\mu+\lambda)^2\lambda}de_{\mathfrak{d}}(\lambda),
\end{aligned}$$

since $0<\nu\leqslant\mu$. Since the upper bound is independent of ν, we have proved the claim if we can show that it tends to zero as μ vanishes. This is a consequence of the Lebesgue dominated convergence theorem provided we show that

$$\int_{\mathbb{R}^+} \frac{1}{\lambda} de_{\mathfrak{d}}(\lambda) \,<\, \infty. \tag{2.11}$$

On the one hand, by the a priori estimate of $\mathrm{D}\,\phi_\mu$,

$$\langle \phi_\mu \mathcal{L} \phi_\mu \rangle \,\leqslant\, \beta \left\langle |\,\mathrm{D}\,\phi_\mu|^2 \right\rangle \,\leqslant\, \beta C.$$

On the other hand, we have already proved that

$$\langle \phi_\mu \mathcal{L} \phi_\mu \rangle \,=\, \int_{\mathbb{R}^+} \frac{\lambda}{(\mu+\lambda)^2} de_{\mathfrak{d}}(\lambda).$$

Estimate (2.11) then follows from the monotone convergence theorem. □

2.3. **Random walk in random environment.** We now turn our attention to the probabilistic aspects of homogenization. This presentation is informal. It aims at being accessible to non-specialists of probability theory, and at highlighting the inner similarities with the corrector approach of subsection 2.2.

2.3.1. *The continuous-time random walk.* Let the environment ω be fixed for a while (that is, we have picked a realization of the conductivities $\omega_e \in [\alpha, \beta]$, $e \in \mathbb{B}$). The random walk $(X_t)_{t\in\mathbb{R}_+}$ is a random process whose behavior is influenced by the environment.

To the specialist, it is the Markov process whose transition rates are given by $(\omega_e)_{e\in\mathbb{B}}$. The Markov property means that given any time $t \geqslant 0$, the behavior of the process after time t depends on its past only through its location at time t. In other words, the process "starts afresh" at time t given its current location. In order to give a complete description of the process, it thus suffices to describe its behavior over a time interval $[0, t]$, for some $t > 0$, no matter how small. As t tends to 0, this behavior is given by

$$\mathbf{P}_z^\omega \left[X_t = z'\right] = \left| \begin{array}{ll} t\omega_{z,z'} + o(t) & \text{if } z' \sim z, \\ 1 - \sum_{y\sim z} t\omega_{z,y} + o(t) & \text{if } z' = z, \\ o(t) & \text{otherwise,} \end{array} \right. \tag{2.12}$$

where $\mathbf{P}_z^\omega$ is the probability measure corresponding to the walk started at z, that is, $\mathbf{P}_z^\omega[X_0 = z] = 1$. Equation (2.12) shows that $\omega_{z,z'}$ is the jump rate from z to z'.

A more constructive way to represent the random walk is as follows. Let the walk be at some site $z \in \mathbb{Z}^d$ at time t, and start an "alarm clock" that rings after a random time T following an exponential distribution of parameter

$$p_\omega(z) := \sum_{z'\sim z} \omega_{z,z'}. \tag{2.13}$$

This means that for any $s \geqslant 0$, the probability that $T > s$ is equal to $e^{-p_\omega(z)s}$. When the clock rings, the walk randomly moves to one (out of the $2d$) neighboring site z' with probability

$$p(z \rightsquigarrow z') := \frac{\omega_{z,z'}}{p_\omega(z)}, \tag{2.14}$$

and this random choice is made independently of the value of T.

Note that by the Markov property, the fact that the walk has not moved during the time interval $[t, t+s]$ should give no information on the time of the next jump. Only exponential distributions have this memoriless property.

Let us see why the so-defined random walk satisfies (2.12). The probability that the clock rings during the time interval $[0, t]$ is

$$1 - e^{-p_\omega(z)t} = p_{\omega(z)}t + o(t).$$

Since $p_\omega(z)$ is bounded by $2d\beta$ uniformly over z, the probability that the walk makes two or more jumps is $o(t)$. The probability that it ends up at $z' \sim z$ at time t is thus

$$\big(p_{\omega(z)}t + o(t)\big)\, p(z \rightsquigarrow z') - o(t) = \omega_{z,z'}t + o(t),$$

and the probability that it stays still is indeed as in (2.12).

The link between the random walk and the elliptic operators of the previous subsection is as follows. We let $(P_t^\omega)_{t \in \mathbb{R}_+}$ be the semi-group associated with the random walk, that is, for any $t \geqslant 0$ and any bounded function $f : \mathbb{Z}^d \to \mathbb{R}$, we let

$$P_t^\omega f(z) \;=\; \mathbf{E}_z^\omega[f(X_t)],$$

where $\mathbf{E}_z^\omega$ denotes the expectation associated with the probability measure $\mathbf{P}_z^\omega$, under which the random walk starts at $z \in \mathbb{Z}^d$ in the environment ω. This is a semi-group since X has the Markov property. As we now show, the infinitesimal generator of this semi-group is the elliptic operator $-L$ (where L is defined in (2.1)). Recall that the infinitesimal generator of a semi-group, applied to f, is given by

$$\lim_{t \to 0} \left(\frac{P_t^\omega f - f}{t} \right),$$

for any f for which the limit exists. From the description (2.12), this limit is easily computed. Indeed,

$$\begin{aligned} P_t^\omega f(z) &= \mathbf{E}_z^\omega[f(X_t)] \\ &= (1 - p_\omega(z)t)f(z) + t \sum_{z' \sim z} \omega_{(z,z')} f(z') + o(t) \qquad (2.15) \\ &= f(z) + t \sum_{z' \sim z} \omega_{(z,z')}(f(z') - f(z)) + o(t), \qquad (2.16) \end{aligned}$$

so that by (2.3),

$$\lim_{t \to 0} \left(\frac{P_t^\omega f(z) - f(z)}{t} \right) \;=\; \sum_{z' \sim z} \omega_{(z,z')}(f(z') - f(z)) \;=\; -Lf(z), \qquad (2.17)$$

and we have identified the infinitesimal generator to be $-L$, as announced.

An important feature of this random walk is that the jump rates are symmetric: the probability to go from z to z' in an "infinitesimal" amount of time is equal to the probability to go from z' to z, as can be seen on (2.12). One then says that the counting measure on $\mathbb{Z}^d$ (which puts mass 1 to every site) is *reversible* for the random walk, that is, for every $f, g \in L^2(\mathbb{Z}^d)$,

$$\sum_{x \in \mathbb{Z}^d} f(x)\; Lg(x) = \sum_{x \in \mathbb{Z}^d} Lf(x)\; g(x).$$

In the previous section, we moved from the operator L to its "environmental" version, the operator $\mathcal{L}$. This takes a very enlightening probabilistic meaning. Instead of considering the random walk itself, we may consider the *environment viewed by the particle*, which is the random process defined by

$$t \mapsto \omega(t) := \theta_{X(t)}\omega,$$

where $(\theta_x)_{x\in\mathbb{Z}^d}$ are the translations of Definition 2.2. As the name suggests, $\omega(t)$ is the environment of conductances centered at the position occupied by the walk at time t. One can convince oneself that $(\omega(t))_{t\in\mathbb{R}_+}$ is a Markov process, and the important point is that its infinitesimal generator is precisely $-\mathcal{L}$. An elementary computation shows that the reversibility of the counting measure for the random walk translates into the reversibility of the measure $\mathbb{P}$ for the process $(\omega(t))_{t\in\mathbb{R}_+}$, that is, for every $f, g \in L^2(\Omega)$,

$$\langle f \ \mathcal{L}g\rangle = \langle \mathcal{L}f \ g\rangle \,.$$

2.3.2. *Central limit theorem for the random walk.* The aim of this paragraph is to sketch the proof of the following result of [KV86], highlighting the connections with subsection 2.2. A more complete presentation of this and of many more related problems and ideas can be found in the very recent monograph [KLO]. We write $\mathbb{P}_0$ for the ("annealed") probability measure $\mathbb{P}\mathbf{P}_0^\omega[\cdot]$, and $\mathbb{E}_0$ for the associated expectation.

Theorem 2.8 ([KV86])**.** *Under the measure $\mathbb{P}_0$ and as ε tends to 0, the rescaled random walk $X^{(\varepsilon)} := (\sqrt{\varepsilon}X_{t/\varepsilon})_{t\in\mathbb{R}_+}$ converges in distribution (for the Skorokhod topology) to a Brownian motion with covariance matrix $2A_{\text{hom}}$, where A_{hom} is as in (2.5). In other words, for any bounded continuous functional F on the space of cadlag functions, one has*

$$\mathbb{E}_0\left[F(X^{(\varepsilon)})\right] \xrightarrow[\varepsilon\to 0]{} E[F(B)], \tag{2.18}$$

where B is a Brownian motion started at the origin and with covariance matrix $2A_{\text{hom}}$, and E denotes averaging over B. Moreover, for any $\xi \in \mathbb{R}^d$, one has

$$t^{-1}\mathbb{E}_0\left[(\xi\cdot X_t)^2\right] \xrightarrow[t\to+\infty]{} 2\xi\cdot A_{\text{hom}}\xi. \tag{2.19}$$

Note that the convergence of the rescaled mean square displacement in (2.19) does not follow from (2.18), since the square function is not bounded.

Sketch of proof of Theorem 2.8. From now on, we focus on the one-dimensional projections of X. As in subsection 2.2, we let ξ be a fixed vector of $\mathbb{R}^d$. The idea is to decompose $\xi\cdot X_t$ as

$$\xi\cdot X_t = M_t + R_t, \tag{2.20}$$

where $(M_t)_{t\geqslant 0}$ is a martingale and R_t is a (hopefully small) remainder. We recall that $(M_t)_{t\geqslant 0}$ is a martingale under $\mathbf{E}_0^\omega$ if for all $t \geqslant 0$ and $s \geqslant 0$,

$$\mathbf{E}_0^\omega[M_{t+s}|\mathcal{F}_t] \;=\; M_t, \tag{2.21}$$

where in our context, it is natural to choose $\mathcal{F}_t$ as the σ-algebra generated by $(X_\tau)_{\tau\in[0,t]}$.

We look for a martingale of the form $M_t = \chi^\omega(X_t)$ for some function χ^ω. By the Markov property of X_t, such a $(M_t)_{t\geqslant 0}$ is a martingale if and only if, for any $z \in \mathbb{Z}^d$ and any $t \geqslant 0$,

$$\mathbf{E}_z^\omega[\chi^\omega(X_t)] \;=\; \chi^\omega(z). \tag{2.22}$$

From (2.12), we learn that

$$\mathbf{E}_z^\omega[\chi^\omega(X_t)] = \chi^\omega(z) - tL\chi^\omega(z) + O(t^2).$$

Hence, a necessary condition is that $L\chi^\omega(z) = 0$, and in fact, this condition is also sufficient. Keeping in mind that we also want the remainder term to be small, we would like χ^ω to be a perturbation of the function $z \mapsto \xi \cdot z$, so that a right choice for χ^ω should be

$$\chi^\omega(z) \;=\; \xi \cdot z + \phi(z, \omega),$$

where ϕ is the corrector of Lemma 2.4 (compare equation (2.4) to $L\chi^\omega(z) = 0$). The link between the corrector equation and the RWRE appears precisely there. We thus define the martingale M_t by

$$M_t = \xi \cdot X_t + \phi(X_t, \omega), \tag{2.23}$$

and the remainder term $R_t = -\phi(X_t, \omega)$.

Martingales are interesting for our purpose since they are "Brownian motions in disguise". To make this idea more precise, let us point out that any one-dimensional continuous martingale can be represented as a time-change of Brownian motion (this is the Dubins-Schwarz theorem, see [RY, Theorem V.1.6]). If $(B_t)_{t\geqslant 0}$ is a Brownian motion, a time-change of it is for instance $M_t = B_{t^7}$. Note that in this example, the time-change can be recovered by computing $E[M_t^2] = t^7$. Here, the martingale we consider has jumps (since X itself has), which complicates the matter a little, but let us keep this under the rug. Intuitively, in order to justify the convergence to a Brownian motion, we should show that the underlying time-change grows linearly at infinity. One can check that two increments of a martingale over disjoint time intervals are always orthogonal in L^2 (provided integration is possible). In our case, the martingale M_t has stationary increments since $\nabla\phi$ is a stationary function. Letting $\sigma^2(\xi) = \mathbb{E}_0[M_1^2]$, it thus follows that

$$\mathbb{E}_0[M_t^2] = \sigma^2(\xi)\ t, \tag{2.24}$$

so we are in a good position (i.e. on a heuristic level, it indicates that the underlying time-change indeed grows linearly). Letting $f : z \mapsto (x \cdot \xi + \phi(x, \omega) \cdot \xi)^2$ and using (2.12), one can write

$$\begin{aligned} \mathbf{E}_0^\omega[(M_t \cdot \xi)^2] \;&=\; \mathbf{E}_0^\omega[f(X_t)] \\ &=\; f(0) + t \sum_{z' \sim 0} \omega_{(z,z')} \big(z' \cdot \xi + \phi(z', \omega)\big)^2 + o(t) \\ &=\; \underbrace{2t(\xi + \nabla\phi(0, \omega)) \cdot A(0, \omega)(\xi + \nabla\phi(0, \omega))}_{=: t\ v(\omega)} + o(t), \end{aligned}$$

since $\phi(0, \omega) = 0$. From the definition of A_{hom} in (2.5), we thus get

$$\sigma^2(\xi) = \langle v \rangle = 2\xi \cdot A_{\text{hom}} \xi. \tag{2.25}$$

Provided we can show that the remainder is negligible, this already justifies (2.19). In order to prove that $(\sqrt{\varepsilon} M_{\varepsilon^{-1}t})_{t\geqslant 0}$ converges to a Brownian motion of variance $\sigma^2(\xi)$ as ε tends to 0, knowing (2.24) is however not sufficient: one does not recover all the information about the time-change by computing $\mathbb{E}_0[M_t^2]$ alone. This can be understood from the fact that in the Dubins-Schwarz theorem, the time-change that appears can be random itself, and is in fact the quadratic variation of the martingale. We will not go into explaining what the quadratic variation of a martingale is in general, but simply state that in our case, it is given by

$$V_t = \int_0^t v(\omega(s))\ \mathrm{d}s,$$

and one needs to prove that

$$t^{-1}V_t = t^{-1}\int_0^t v(\omega(s))\ \mathrm{d}s \xrightarrow[t\to+\infty]{\text{a.s.}} \sigma^2(\xi) = 2\xi\cdot A_{\text{hom}}\xi. \tag{2.26}$$

One can show that the process $(\omega(t))_{t\geqslant 0}$ is ergodic under the measure $\mathbb{P}_0$ (see for instance [Mo10, Proposition 3.1]), and thus the convergence in (2.26) is a consequence of the ergodic theorem. Note the surprising fact that the proof of this central limit theorem was reduced to a law of large numbers.

In order to obtain a central limit theorem for $\xi\cdot X$ itself (instead of the martingale part), we need to argue that the remainder term is small. In order to do so, and following [KV86], we will rely on spectral theory. We recall that since the operator $\mathcal{L}$ of Definition 2.6 is a bounded non-negative self-adjoint operator on $L^2(\Omega)$, it admits a spectral decomposition in $L^2(\Omega)$. For any $g\in L^2(\Omega)$ the characterizing property of the spectral measure e_g previously defined is that for any continuous function $\Psi:[0,+\infty)\to\mathbb{R}_+$, one has

$$\langle g\ \Psi(\mathcal{L})g\rangle \ =\ \int_{\mathbb{R}^+}\Psi(\lambda)\ \mathrm{d}e_g(\lambda).$$

We now argue that

$$\frac{1}{t}\mathbb{E}_0[R_t^2]\ =\ 2\int_{\mathbb{R}^+}\frac{1-e^{-t\lambda}}{t\lambda^2}\ \mathrm{d}e_{\mathfrak{d}}(\lambda) \xrightarrow[t\to+\infty]{} 0, \tag{2.27}$$

where $\mathfrak{d}$ is the local drift in the direction ξ, that is,

$$\mathfrak{d} = \nabla^*\cdot A(0,\omega)\xi = \mathrm{D}^*\cdot A\xi = \sum_{z\sim 0}\omega_{0,z}\xi\cdot z. \tag{2.28}$$

We start by showing the identity in (2.27), and will later show that the spectral integral tends to 0 as t tends to infinity. Recall that

$$R_t = -\phi(X_t,\omega) = \phi(0,\omega)-\phi(X_t,\omega), \tag{2.29}$$

and that $\phi(0,\omega)-\phi(x,\omega)$ can be obtained as the limit of $\phi_\mu(0,\omega)-\phi_\mu(x,\omega)$ (this can indeed be written as a sum of discrete gradients along a path between 0 and x). To make things easier, we display the computations below as if ϕ was a stationary ϕ_μ. The argument can be made rigorous through spectral analysis as in [Mo11, Theorem 8.1], or using Lemma 2.7. We expand the square:

$$\mathbb{E}_0[R_t^2] = \mathbb{E}_0[(\phi(0,\omega))^2]+\mathbb{E}_0[(\phi(X_t,\omega))^2]-2\mathbb{E}_0[\phi(0,\omega)\phi(X_t,\omega)].$$

Note that, by the simplifying assumption,

$$\mathbb{E}_0[(\phi(X_t,\omega))^2] = \mathbb{E}_0[(\phi(0,\theta_{X_t}\ \omega))^2] = \mathbb{E}_0[(\phi(0,\omega(t)))^2].$$

Since $(\omega(t))_{t\in\mathbb{R}_+}$ is stationary under $\mathbb{P}_0$, the last expectation is equal to $\mathbb{E}_0[(\phi(0,\omega))^2] = \langle\phi^2\rangle$. Since $\mathcal{L}\phi=\mathfrak{d}$, we have

$$\langle\phi^2\rangle = \langle\mathcal{L}^{-1}\mathfrak{d}\ \mathcal{L}^{-1}\mathfrak{d}\rangle = \langle\mathfrak{d}\ \mathcal{L}^{-2}\mathfrak{d}\rangle = \int\lambda^{-2}\ \mathrm{d}e_{\mathfrak{d}}(\lambda).$$

For the cross-product,

$$\mathbb{E}_0[\phi(0,\omega)\phi(X_t,\omega)] = \langle\phi(0,\omega)\ \mathbf{E}_0^\omega\left[\phi(0,\omega(t))\right]\rangle, \tag{2.30}$$

and $\mathbf{E}_0^\omega\,[\phi(0,\omega(t))]$ is the image ϕ by the semi-group associated to $-\mathcal{L}$, that is, $e^{-t\mathcal{L}}$. Using also the fact that $\mathcal{L}\phi = \mathfrak{d}$, we can rewrite the r.h.s. of (2.30) as

$$\left\langle \phi \; e^{-t\mathcal{L}}\phi \right\rangle = \left\langle \mathcal{L}^{-1}\mathfrak{d} \; e^{-t\mathcal{L}}\mathcal{L}^{-1}\mathfrak{d} \right\rangle = \int \lambda^{-2} e^{-t\lambda} \; \mathrm{d}e_{\mathfrak{d}}(\lambda),$$

and this justifies the equality (2.27). The fact that the spectral integral in (2.27) tends to zero follows from (2.11) and the dominated convergence theorem. □

Before concluding this section, let us point out the differences between the present arguments and the original arguments in [KV86]. Here, we used the existence of the corrector, borrowed from subsection 2.2, to construct the martingale. In [KV86], the martingale is constructed directly, by considering

$$\xi \cdot X_t + \phi_\mu(\omega(t)) - \phi_\mu(\omega(0)) - \mu \int_0^t \phi_\mu(\omega(s)) \; \mathrm{d}s,$$

and showing that for each fixed t, it is a Cauchy sequence in $L^2(\mathbb{P}_0)$ (and thus converges) as μ tends to 0. This is achieved through spectral analysis, using the estimate (2.11). This estimate is obtained by a general argument of (anti-) symmetry (see the proof of [KV86, Theorem 4.1]), which has been systemized in [DFGW89]. Another difference is that the arguments of [KV86] apply to general reversible Markov processes.

3. Numerical approximation of the homogenized coefficients using the corrector equation

3.1. **General approach.**

Let $\xi \in \mathbb{R}^d$ be a fixed unit vector. In order to approximate A_{hom} using the corrector ϕ, we first replace the expectation in (2.5) by a spatial average appealing to ergodicity: almost surely

$$\xi \cdot A_{\mathrm{hom}}\xi \;=\; \lim_{N\to\infty} \fint_{Q_N} (\xi + \nabla\phi) \cdot A(\xi + \nabla\phi), \tag{3.1}$$

where $Q_N = [0,N)^d$ and $\fint_{Q_N} := N^{-d}\sum_{Q_N\cap\mathbb{Z}^d}$.

Recall that ϕ is the solution to (2.4), which is a problem posed on $\mathbb{Z}^d$. In order to turn (3.1) into a practical formula, one needs a computable approximation $\tilde{\phi}_N$ of ϕ on Q_N, which would allow us to define an approximation A_N of A_{hom} by

$$\xi \cdot A_N\xi \;=\; \fint_{Q_N} (\xi + \nabla\tilde{\phi}_N) \cdot A(\xi + \nabla\tilde{\phi}_N).$$

Although A_{hom} is deterministic, this approximation A_N is a random variable. Provided the chosen approximation $\tilde{\phi}_N$ is "consistent",

$$\lim_{N\to\infty} \xi \cdot A_N\xi \;=\; \xi \cdot A_{\mathrm{hom}}\xi$$

almost surely.

The starting point for a quantitative convergence analysis is the following identity:

$$\left\langle (\xi \cdot A_N\xi - \xi \cdot A_{\mathrm{hom}}\xi)^2 \right\rangle \;=\; \mathrm{var}\,[\xi \cdot A_N\xi] + (\xi \cdot \langle A_N\rangle\,\xi - \xi \cdot A_{\mathrm{hom}}\xi)^2. \tag{3.2}$$

The square root of the first term of the r. h. s. is called the *random error* or *statistical error*. It measures the fluctuations of A_N around its expectation. As we shall see it can often be estimated optimally by $\mathrm{var}\,[\xi \cdot A_N\xi] \leqslant CN^{-d}$ (the central limit theorem scaling) for some $C > 0$. The method introduced in [CLL10] is a way to reduce the prefactor C

in practice (using variance reduction techniques); note that it has no effect on the second term of the r. h. s. of (3.2). The square root of this second term is the *systematic error.* It measures the fact that $\nabla\tilde{\phi}_N$ is only an approximation of $\nabla\phi$ on Q_N. In order to give quantitative estimates of these errors, we need to make assumptions on the statistics of A, and shall assume in most of this section that the entries of A are independent and identically distributed.

In the following subsection, we introduce three approximation methods based on the above strategy, and recall the known (or expected) convergence rates for both errors. The third subsection is dedicated to a empirical study which completes the analysis in two respects: it allows to confirm (or not) the expected convergence rates (if they are not precisely known), and it allows to make explicit the prefactors.

3.2. **Methods and theoretical analysis.**

3.2.1. *Homogeneous Dirichlet boundary conditions.* The simplest approximation of the corrector ϕ on Q_N for $N \geqslant 1$ is given by the unique solution $\phi_N \in L^2(Q_N \cap \mathbb{Z}^d)$ of

$$-\nabla^* \cdot A(\xi + \nabla\phi_N) \,=\, 0 \qquad \text{in } Q_N, \tag{3.3}$$

completed by the boundary conditions $\phi_N(x) = 0$ for all $x \in \mathbb{Z}^d \setminus Q_N$.

The approximation A_N of A_{hom} is then defined by

$$\xi \cdot A_N\xi \,:=\, \fint_{Q_N} (\xi + \nabla\phi_N) \cdot A(\xi + \nabla\phi_N).$$

As a direct consequence of homogenization, we have the almost sure convergence:

$$\lim_{N\to\infty} |A_N - A_{\mathrm{hom}}| \,=\, 0.$$

In terms of convergence rates, the starting point is identity (3.2). We expect the random error to scale as the central limit theorem, that is:

$$\mathrm{var}\,[\xi \cdot A_N\xi]^{1/2} \,\sim\, N^{-d/2}, \tag{3.4}$$

and the systematic error to scale as a surface effect (the corrector is perturbed on the boundary):

$$|\xi \cdot \langle A_N\rangle\, \xi - \xi \cdot A_{\mathrm{hom}}\xi| \,\sim\, N^{-1}. \tag{3.5}$$

For a proof of (3.4), we refer to [GMO]. Let us give an informal argument for (3.4) when the ellipticity ratio β/α is close to 1 (that is, for A a perturbation of Id) in the form of the following proposition.

Proposition 3.1. *If ϕ_N satisfies*

$$-\nabla^* \cdot \nabla\phi_N \,=\, \nabla^* \cdot A\xi \qquad \text{in } Q_N,$$

completed by homogeneous Dirichlet boundary conditions on ∂Q_N, in place of (3.3) *(which corresponds to the linearization of* (3.3) *as $\beta/\alpha \to 1$), then* (3.4) *holds.*

Proof of Proposition 3.1. Let G denote the Green's function of the discrete Laplace equation on Q_N with homogeneous Dirichlet boundary conditions. Then, by the Green representation formula,

$$\phi_N(x) = \int_{Q_N} \nabla_y G(x,y)\cdot A(y)\xi dy, \tag{3.6}$$

$$\nabla\phi_N(x) = \int_{Q_N} \nabla_x\nabla_y G(x,y)\cdot A(y)\xi dy. \tag{3.7}$$

We then appeal to the following spectral gap inequality (which is at the core [GO11]): for any function X of a finite number of the i.i.d. random variables ω_e, we have:

$$\mathrm{var}\,[X] \leqslant \sum_e \left\langle \sup_{\omega_e}\left|\frac{\partial X}{\partial \omega_e}\right|^2\right\rangle \mathrm{var}\,[\omega]\,, \tag{3.8}$$

where the supremum is taken w. r. t. the variable ω_e, and $\mathrm{var}\,[\omega]$ is the variance of the i.i.d. conductances. Such spectral gap estimates (and variants) have been extensively used in statistical physics (see for instance [GNOa, Introduction]). The use of such estimates in stochastic homogenization is inspired by the work of Naddaf and Spencer [NS98] (who used the Brascamp-Lieb inequality instead). We shall apply this inequality to $X = \xi\cdot A_N\xi$. We first note that the weak formulation of the equation yields

$$X = \xi\cdot A_N\xi = \fint_{Q_N} \xi\cdot A(\xi+\nabla\phi_N),$$

so that by (3.7), we have for all $e=(z,z+e_i)$

$$\frac{\partial X}{\partial\omega_e} = \frac{1}{N^d}\xi_i(\xi_i+\nabla_i\phi_N(z)) + \frac{1}{N^d}\int_{Q_N}\xi\cdot A(x)\nabla_x\nabla_{z_i}G(x,z)\xi_i dx,$$

which, by symmetry of A and of G, we rewrite as

$$\frac{\partial X}{\partial\omega_e} = \frac{1}{N^d}\xi_i(\xi_i+\nabla_i\phi_N(z)) + \frac{1}{N^d}\xi_i\nabla_{z_i}\int_{Q_N}\nabla_x G(z,x)\cdot A(x)\xi dx.$$

Using (3.6), this turns into

$$\frac{\partial X}{\partial\omega_e} = \frac{1}{N^d}\xi_i(\xi_i+2\nabla_i\phi_N(z)).$$

It remains to take the supremum of this quantity w. r. t. ω_e. In view of (3.6), we have for all j

$$\operatorname*{osc}_{\omega_e}\nabla_j\phi(z) = \sup_{\omega_e}\nabla_j\phi(z) - \inf_{\omega_e}\nabla_j\phi(z) \leqslant |\nabla_{x_j}\nabla_{z_i}G(x,z)|,$$

which is bounded by a universal constant (in the discrete setting, the Green's function is bounded). We thus have the desired variance estimate:

$$\begin{aligned}
\operatorname{var}[X] &\leqslant \frac{1}{N^{2d}} \sum_e \left\langle C(1+|\nabla_i \phi_N(z)|^2) \right\rangle \operatorname{var}[\omega] \\
&= \frac{1}{N^{2d}} \left\langle \sum_e C(1+|\nabla_i \phi_N(z)|^2) \right\rangle \operatorname{var}[\omega] \\
&= \frac{1}{N^d} \frac{1}{N^d} \left\langle dCN^d + C\|\nabla \phi_N\|^2_{L^2(Q_N)} \right\rangle \operatorname{var}[\omega] \\
&\lesssim \frac{1}{N^d},
\end{aligned}$$

since an elementary deterministic estimate yields

$$\int_{Q_N} |\nabla \phi_N|^2 \leqslant \beta^2 |Q_N| = \beta^2 N^d.$$

□

In the case of general ellipticity ratio the difficulty is to treat the dependence of the Green's function with respect to ω_e, which yields additional terms of the form $|\nabla \phi_N|^4$ which we do not control a priori (see [GNOa] in the case of periodic approximations), see [GMO] for the proof in the general case.

Note that the convergence rate of the random error (3.4) is expected to depend on the dimension whereas the convergence rate of the systematic error (3.5) does not. The combination of these (conjectured) estimates would yield the following convergence rate in any dimension

$$\left\langle (\xi \cdot A_N \xi - \xi \cdot A_{\mathrm{hom}} \xi)^2 \right\rangle \sim N^{-2}.$$

3.2.2. *Regularized corrector and filtering.* In [GO11, GO12, Gl12a], the following strategy was used. Instead of considering an approximation of the corrector ϕ, we consider an approximation of the regularized corrector ϕ_μ of Lemma 2.5. The advantage of the regularized corrector is that the Green's function associated with the operator $\mu - \nabla^* \cdot A \nabla$ decays exponentially fast in terms of the distance measured in units of $\mu^{-1/2}$. Let $N > 0$. We denote by $\phi_{\mu,N}$ the unique solution in $L^2(Q_N \cap \mathbb{Z}^d)$ of

$$\mu \phi_{\mu,N} - \nabla^* \cdot A(\xi + \nabla \phi_{\mu,N}) = 0 \qquad \text{in } Q_N,$$

completed by the boundary conditions $\phi_{\mu,N}(x) = 0$ for all $x \in \mathbb{Z}^d \setminus Q_N$.

To define an approximation of A_{hom}, we introduce for all $L \in \mathbb{N}$ an averaging mask $\eta_L : \mathbb{Z}^d \to \mathbb{R}^+$, with support in Q_L, and such that $\int_{Q_L} \eta_L = 1$ and $\sup_{\mathbb{Z}^d} |\nabla \eta_L| \lesssim L^{-(d+1)}$. The idea of using an averaging mask is rather natural and appears for instance in [EY07] and [BLB09]. For all $N \geqslant L > 0$ and $\mu > 0$, we then set:

$$\xi \cdot A_{\mu,N,L} \xi := \int_{Q_L} (\xi + \nabla \phi_{\mu,N}) \cdot A(\xi + \nabla \phi_{\mu,N}) \eta_L. \tag{3.9}$$

We have the following almost sure convergence:

$$\lim_{\mu \to 0} \lim_{N \geqslant L \to \infty} |A_{\mu,N,L} - A_{\mathrm{hom}}| = 0.$$

Following the general approach, we have using the triangle inequality, and expanding the square:

$$\left\langle (\xi\cdot(A_{\mu,N,L}-A_{\text{hom}})\xi)^2\right\rangle^{1/2} \leqslant \left\langle (\xi\cdot(A_{\mu,N,L}-A_{\mu,L})\xi)^2\right\rangle^{1/2} + \text{var}\,[A_{\mu,L}]^{1/2} + |A_\mu - A_{\text{hom}}|, \tag{3.10}$$

where:

$$\begin{aligned} \xi\cdot A_{\mu,L}\xi &:= \int_{Q_L} (\xi+\nabla\phi_\mu)\cdot A(\xi+\nabla\phi_\mu)\eta_L, \\ \xi\cdot A_\mu\xi &:= \langle (\xi+\nabla\phi_\mu)\cdot A(\xi+\nabla\phi_\mu)\rangle\,. \end{aligned} \tag{3.11}$$

The first term is the error due to the fact that we replace ϕ_μ by the computable approximation $\phi_{\mu,N}$ on Q_L. As shown in [Gl12a] the function $\phi_{\mu,N}$ is a good approximation of ϕ_μ in the sense that we have the following deterministic estimate: there exists $c>0$ such that for all $0<L\leqslant N$, we have almost surely

$$|A_{\mu,N,L}-A_{\mu,L}| \lesssim \mu^{-3/4}\left(\frac{N}{L}\right)^{d/2}\left(\frac{N}{N-L}\right)^{d-1/2}\exp\left(-c\sqrt{\mu}(N-L)\right). \tag{3.12}$$

This estimate essentially follows from the exponential decay of the Green's function measured in units of $\mu^{-1/2}$. Hence, provided $\sqrt{\mu}(N-L)\gg 1$, the error between $A_{\mu,N,L}$ and $A_{\mu,L}$ is negligible.

If A is iid, [GO11, Theorem 2.1] (using [GNOa, Proposition 2 (a)] to obtain the optimal power on the logarithmic term for $d=2$) yields

$$\text{var}\,[\xi\cdot A_{\mu,L}\xi] \lesssim \left| \begin{array}{lcl} d=2 &:& L^{-2}|\ln\mu| + \mu^2|\ln\mu|, \\ d>2 &:& L^{-d}+\mu^2L^{2-d}, \end{array}\right. \tag{3.13}$$

that is the central limit theorem scaling (up to a logarithmic correction in dimension 2) provided $\mu L\lesssim 1$. (We expect this convergence rate to be optimal in general, the term μ^2L^{2-d} is due to the zero-order term in the modified corrector equation, this is to be compared to (3.4).)

In [GO12] (see also [GNOa] for $d=2$), it is proved that

$$|\xi\cdot A_\mu\xi - \xi\cdot A_{\text{hom}}\xi| \lesssim \left| \begin{array}{lcl} d=2 &:& \mu, \\ d=3 &:& \mu^{3/2}, \\ d=4 &:& \mu^2|\ln\mu|, \\ d>4 &:& \mu^2. \end{array}\right. \tag{3.14}$$

Note that this scaling depends on the dimension and saturates at dimension $d=4$. The proof of this estimate is interesting because similar arguments are used to analyze methods based on RWRE. It relies on spectral calculus and an observation of [Mo11]. Recall that for a fixed unit vector $\xi\in\mathbb{R}^d$ we denote by $\mathfrak{d} = \text{D}^*\cdot A\xi$ the local drift and by $e_{\mathfrak{d}}$ the projection of the spectral measure of $\mathcal{L}$ onto $\mathfrak{d}$. By definition,

$$\begin{aligned}\xi\cdot A_\mu\xi-\xi\cdot A_{\hom}\xi &= \langle(\xi+\mathrm{D}\,\phi_\mu)\cdot A(\xi+\mathrm{D}\,\phi_\mu)-(\xi+\nabla\phi)\cdot A(\xi+\nabla\phi)\rangle\\ &= \langle(\mathrm{D}\,\phi_\mu-\nabla\phi)\cdot A(\xi+\nabla\phi)+(\xi+\mathrm{D}\,\phi_\mu)\cdot A(\mathrm{D}\,\phi_\mu-\nabla\phi)\rangle\,.\end{aligned}$$

Using the weak form of the corrector equation (2.8), one has for all $\psi\in L^2(\Omega)$,

$$\langle \mathrm{D}\,\psi\cdot A(\xi+\nabla\phi)\rangle \,=\, 0.$$

Taking $\psi=\phi_\mu-\phi_\nu$ for $\nu>0$, and using the symmetry of A, one obtains

$$\langle(\mathrm{D}\,\phi_\mu-\mathrm{D}\,\phi_\nu)\cdot A(\xi+\nabla\phi)\rangle \,=\, 0 \,=\, -\langle(\xi+\nabla\phi)\cdot A(\mathrm{D}\,\phi_\mu-\mathrm{D}\,\phi_\nu)\rangle\,.$$

Taking the limit $\nu\to 0$ and using the strong convergence of $\mathrm{D}\,\phi_\nu$ to $\nabla\phi$ given by Lemma 2.7, this finally yields

$$\xi\cdot A_\mu\xi-\xi\cdot A_{\hom}\xi \,=\, \langle(\mathrm{D}\,\phi_\mu-\nabla\phi)\cdot A(\mathrm{D}\,\phi_\mu-\nabla\phi)\rangle\,.$$

Hence, by spectral calculus and taking the limit $\nu\to 0$ in (2.10), we obtain

$$0\,\leqslant\,\xi\cdot A_\mu\xi-\xi\cdot A_{\hom}\xi \,=\, \mu^2\int_{\mathbb{R}^+}\frac{1}{(\mu+\lambda)^2\lambda}de_{\mathfrak{d}}(\lambda).$$

This immediately implies that $\xi\cdot A_\mu\xi-\xi\cdot A_{\hom}\xi\sim\mu^2$ if $\lambda\mapsto\lambda^{-3}$ is $de_{\mathfrak{d}}$-integrable on $\mathbb{R}^+$. More precisely, what matters in this spectral integral is the behavior at the bottom of the spectrum. We cannot expect a spectral gap (which would hold in the periodic case since there is a Poincaré's inequality on the torus) but we expect the bottom of the spectrum to be sufficiently thin to yield the result. It is convenient to rewrite the spectral integral as

$$\int_{\mathbb{R}^+}\frac{1}{(\mu+\lambda)^2\lambda}de_{\mathfrak{d}}(\lambda)\,\leqslant\,\int_0^1\frac{1}{(\mu+\lambda)^2\lambda}de_{\mathfrak{d}}(\lambda)+\int_{\mathbb{R}^+}\frac{1}{\lambda}de_{\mathfrak{d}}(\lambda).$$

By (2.11) the second term of the r. h. s. is bounded, and an elementary calculation shows that (3.14) is a consequence of the following optimal estimate of the so-called "spectral exponents": for all $0<\nu\leqslant 1$ and $d\geqslant 2$,

$$\int_0^\nu de_{\mathfrak{d}}(\lambda)\,\lesssim\,\nu^{d/2+1}. \tag{3.15}$$

Suboptimal bounds with exponents $d/2-2$ were first obtained for d large in [Mo11, Theorem 2.4] using probabilistic arguments, optimal bounds up to dimension 4 (and up to some logarithm in dimension 2) in [GO12] using the spectral gap estimate (3.8) and elliptic regularity theory, up to dimension 6 in [GM12] by pushing forward the method of [GO12] (see [GM13] for a generalization of this strategy which would yield the optimal exponents for all $d>2$), and in any dimension in [GNOa] using the spectral gap estimate and parabolic regularity theory to obtain first bounds on the semi-group which turn after integration in time into bounds on the spectral exponents.

Altogether, if we take $N-L\sim N\sim L$, and $\mu\sim N^{-\gamma}$ with $1\leqslant\gamma<2$ (so that (3.12) is of infinite order in N), the combination of the three estimates (3.12), (3.13), and (3.14) yields:

$$\left\langle |A_{\mu,N,L} - A_{\mathrm{hom}}|^2 \right\rangle \lesssim \left| \begin{array}{lcl} d=2 & : & N^{-2}\ln N, \\ d=3 & : & N^{-3}, \\ d=4 & : & N^{-4} + N^{-4\gamma}\ln^2 N, \\ d>4 & : & N^{-4}, \end{array} \right. \tag{3.16}$$

which yields the central limit theorem scaling up to dimension 4 at least.

3.2.3. *Periodization method.* The periodization method is a widely used method to approximate homogenized coefficients, which consists in periodizing the random medium, see [Ow03, EY07]. What is less known is that there may be several ways to periodize a random medium:

- the periodization in space,
- the periodization in law.

Both periodization methods coincide in the specific case of i.i.d. conductances. The periodization in law is implicitly used in the very nice contribution [KFGMJ]. In order to distinguish between periodization in law and in space, we shall consider in this paragraph some specific example of correlated conductances for which the quantitative analysis of [GNOa] holds (see below).

Let us begin with the periodization in space. It consists in approximating the corrector ϕ on Q_N by the Q_N-periodic solution ϕ_N^{spa} with zero average of

$$-\nabla \cdot A^{\#,N}(\xi + \nabla\phi_N^{\mathrm{spa}}) \;=\; 0 \text{ in } \mathbb{Z}^d,$$

where $A^{\#,N}$ is the Q_N-periodic extension of $A|_{Q_N}$ on $\mathbb{Z}^d$, that is for all $k \in \mathbb{Z}^d$ and $z \in Q_N$, $A^{\#,N}(kN+z) := A(z)$. The associated approximation A_N^{spa} of A_{hom} is then given by

$$\xi \cdot A_N^{\mathrm{spa}}\xi \;:=\; \fint_{Q_N} (\xi + \nabla\phi_N^{\mathrm{spa}}) \cdot A^{\#,N}(\xi + \nabla\phi_N^{\mathrm{spa}}).$$

As a direct consequence of homogenization (see also [Ow03]), we have almost surely

$$\lim_{N\to\infty} |A_N^{\mathrm{spa}} - A_{\mathrm{hom}}| \;=\; 0. \tag{3.17}$$

In order to define the periodization in law, we have to make specific the structure of A. For all $i \in \{1,\dots,d\}$, let $g_i : [\alpha,\beta]^{\mathbb{B}} \to [\alpha,\beta]$ be a measurable function depending only on a finite number of variables in $\mathbb{B}$ within distance $\mathscr{L}_c$ of 0 (recall that $\mathbb{B}$ is the set of edges), and let $\{\bar\omega_e\}_{e\in\mathbb{B}}$ be a family of i.i.d. random variables in $[\alpha,\beta]$. We assume that the conductances $\{\omega_e\}_{e\in\mathbb{B}}$ are given as follows: For all $z \in \mathbb{Z}^d$ and $i \in \{1,\dots,d\}$,

$$\omega_{(z,z+\mathbf{e}_i)} \;:=\; g_i(\tau_z\bar\omega),$$

where $\tau_z\bar\omega$ is the translation of $\bar\omega$ by z, i. e. for all $e = (z', z'+\mathbf{e}_j)$ with $z' \in \mathbb{Z}^d$ and $j \in \{1,\dots,d\}$, $\tau_z\bar\omega_e := \bar\omega_{(z+z',z+z'+\mathbf{e}_j)}$. The statistics for ω satisfies a spectral gap estimate and the analysis of [GNOa] holds, see [GNOb] for details. The periodization in law consists in periodizing the underlying i.i.d. random variables and then applying the deterministic function g. For all $N \geqslant 1$ we define $\bar\omega^{\#,N}$ by: for all $k \in \mathbb{Z}^d$, $z \in Q_N$, and $i \in \{1,\dots,d\}$, $\bar\omega^{\#,N}_{(k+z,k+z+\mathbf{e}_i)} := \bar\omega_{(z,z+\mathbf{e}_i)}$, and we set for all $z \in \mathbb{Z}^d$

$$A_{\#,N}(z) \,:=\, \mathrm{diag}(g_1(\tau_z\bar\omega^{\#,N}),\dots,g_d(\tau_z\bar\omega^{\#,N})).$$

Note that $A_{\#,N}$ is Q_N-periodic. It does coincide with $A^{\#,N}$ if $g_i(\bar\omega) = \mathcal{G}(\bar\omega_{(0,0+\mathbf{e}_i)})$ for some $\mathcal{G}$, in which case the conductances ω_e are i.i.d. random variables, but not otherwise. We then consider the unique Q_N-periodic solution ϕ_N^{law} with zero average of

$$-\nabla\cdot A_{\#,N}(\xi+\nabla\phi_N^{\mathrm{law}}) \,=\, 0 \text{ in } \mathbb{Z}^d,$$

and define

$$\xi\cdot A_N^{\mathrm{law}}\xi \,:=\, \fint_{Q_N}(\xi+\nabla\phi_N^{\mathrm{law}})\cdot A_{\#,N}(\xi+\nabla\phi_N^{\mathrm{law}}).$$

In order to prove the almost sure convergence

$$\lim_{N\to\infty}|A_N^{\mathrm{law}}-A_{\mathrm{hom}}| \,=\, 0,$$

in view of (3.17), it is enough to show that for large N,

$$\xi\cdot A_N^{\mathrm{spa}}\xi - o(1) \,\leqslant\, \xi\cdot A_N^{\mathrm{law}}\xi \,\leqslant\, \xi\cdot A_N^{\mathrm{spa}}\xi + o(1).$$

By Meyers' estimates, there exists some $p>2$ such that for all N and almost surely,

$$\int_{Q_N}|\nabla\phi_N^{\mathrm{law}}|^p,\int_{Q_N}|\nabla\phi_N^{\mathrm{spa}}|^p \,\lesssim\, N^d. \tag{3.18}$$

Next we use the following alternative formula for A_N^{law} (which holds by symmetry of $A_{\#,N}$):

$$\xi\cdot A_N^{\mathrm{law}}\xi \,=\, \inf\left\{\fint_{Q_N}(\xi+\nabla\phi)\cdot A_{\#,N}(\xi+\nabla\phi), \phi \text{ is } Q_N\text{-periodic}\right\}.$$

Using ϕ_N^{spa} as a test function and the fact that $A_{\#,N}$ and $A^{\#,N}$ coincide on $Q_{N-\mathscr{L}_c}$, where $\mathscr{L}_c$ is the correlation-length of A, we get by Hölder's inequality with exponents $(p/2,p/(p-2))$

$$\begin{aligned}
\xi\cdot A_N^{\mathrm{law}}\xi \;&\leqslant\; \fint_{Q_N}(\xi+\nabla\phi_N^{\mathrm{spa}})\cdot A_{\#,N}(\xi+\nabla\phi_N^{\mathrm{spa}})\\
&=\; \fint_{Q_N}(\xi+\nabla\phi_N^{\mathrm{spa}})\cdot A^{\#,N}(\xi+\nabla\phi_N^{\mathrm{spa}})\\
&\qquad +\fint_{Q_N}(\xi+\nabla\phi_N^{\mathrm{spa}})\cdot(A_{\#,N}-A^{\#,N})(\xi+\nabla\phi_N^{\mathrm{spa}})\\
&\leqslant\; \xi\cdot A_{\#,N}\xi+\beta N^{-d}\int_{Q_N\setminus Q_{N-\mathcal{L}_c}}(1+|\nabla\phi_N^{\mathrm{spa}}|^2)\\
&\leqslant\; \xi\cdot A_N^{\mathrm{spa}}\xi+\beta N^{-d}|Q_N\setminus Q_{N-\mathcal{L}_c}|^{(p-2)/p}\|\nabla\phi_N^{\mathrm{spa}}\|^{2/p}_{L^p(Q_N)}\\
&=\; \xi\cdot A_N^{\mathrm{spa}}\xi+o(1)
\end{aligned}$$

using in addition (3.18). The converse inequality is proved the same way.

Let us turn to convergence rates, and begin with the periodization in law, which is analyzed in [GNOa, GNOb]. The general approach takes the form:

$$\left\langle|\xi\cdot A_N^{\mathrm{law}}\xi-\xi\cdot A_{\mathrm{hom}}\xi|^2\right\rangle \,=\, \mathrm{var}\left[\xi\cdot A_N^{\mathrm{law}}\xi\right]+(\xi\cdot(\langle A_N^{\mathrm{law}}\rangle-A_{\mathrm{hom}})\xi)^2.$$

As shown in [GNOa, GNOb], the random and systematic errors satisfy

$$\mathrm{var}\left[\xi\cdot A_N^{\mathrm{law}}\xi\right]^{1/2} \lesssim N^{-d/2}, \tag{3.19}$$

and

$$|\xi\cdot\langle A_N^{\mathrm{law}}\rangle\xi-\xi\cdot A_{\mathrm{hom}}\xi| \lesssim N^{-d}\ln^d N. \tag{3.20}$$

The proof of (3.20) is subtle.

Sketch of proof of (3.20) *for* $d=2,3$. We treat the case of i.i.d. conductances. The idea consists in introducing a zero-order term as for the regularization, and we consider

$$\xi\cdot A_{\mu,N}^{\mathrm{law}}\xi := \fint_{Q_N}(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}})\cdot A_{\#,N}(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}}),$$

where $\mu>0$, and $\phi_{\mu,N}^{\mathrm{law}}$ is the Q_N-periodic solution to

$$\mu\phi_{\mu,N}^{\mathrm{law}}-\nabla^*\cdot A_{\#,N}(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}}) = 0 \text{ in } \mathbb{Z}^d.$$

We also denote by A_μ the approximation of A_{hom} defined in (3.11). Then by the triangle inequality, for all $\mu>0$,

$$\begin{aligned}|\xi\cdot\langle A_N^{\mathrm{law}}\rangle\xi-\xi\cdot A_{\mathrm{hom}}\xi| \leqslant{}& |\xi\cdot\langle A_N^{\mathrm{law}}\rangle\xi-\xi\cdot\langle A_{\mu,N}^{\mathrm{law}}\rangle\xi|\\ &+|\xi\cdot\langle A_{\mu,N}^{\mathrm{law}}\rangle\xi-\xi\cdot A_\mu\xi|+|\xi\cdot(A_\mu-A_{\mathrm{hom}})|.\end{aligned}$$

The first term of the r. h. s. has the same scaling as the last term (repeating the arguments of spectral theory), that is (3.14), which is independent of N. The only term which relates N to μ is the second term. In the i.i.d. case, we have by periodicity and stationarity

$$\begin{aligned}\xi\cdot\langle A_{\mu,N}^{\mathrm{law}}\rangle\xi &= \left\langle\fint_{Q_N}(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}})\cdot A_{\#,N}(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}})\right\rangle\\ &= \left\langle(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}}(0))\cdot A_{\#,N}^{\mathrm{law}}(0)(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}}(0))\right\rangle.\end{aligned} \tag{3.21}$$

Hence, since $A_{\#,N}^{\mathrm{law}}(0)=A(0)$,

$$\begin{aligned}&\xi\cdot\langle A_{\mu,N}^{\mathrm{law}}\rangle\xi-\xi\cdot A_\mu\xi\\ &\quad=\left\langle(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}}(0))\cdot A(0)(\xi+\nabla\phi_{\mu,N}^{\mathrm{law}}(0))-(\xi+\nabla\phi_\mu(0))\cdot A(0)(\xi+\nabla\phi_\mu(0))\right\rangle,\end{aligned}$$

and we only have to compare $\nabla\phi_\mu$ and $\nabla\phi_{\mu,N}^{\mathrm{law}}$ at the origin. Using deterministic estimates on the Green's function (cf. [GNOa, Proof of Lemma 9]), this yields

$$|\xi\cdot\langle A_{\mu,N}^{\mathrm{law}}\rangle\xi-\xi\cdot A_\mu\xi| \lesssim \frac{1}{\sqrt{\mu}}\exp(-c\sqrt{\mu}N),$$

for some c depending only on α, β, and d. Optimizing the error with respect to μ (taking for instance $\sqrt{\mu}=\frac{d+1}{c}L^{-1}\ln(L/\ln L)$) yields the desired result (3.20). □

Let us make two comments on this proof. First, for $d>3$ this strategy does not allow one to get (3.20) since (3.14) saturates at $d=4$. Instead of comparing A_{hom} to A_μ, we then compare A_{hom} to a family of approximations $A_{k,\mu}$ for which we have

$$\xi\cdot A_{k,\mu}\xi-\xi\cdot A_{\mathrm{hom}}\xi \lesssim \mu^p\int_{\mathbb{R}^+}\frac{1}{\lambda^{p+1}}de_{\mathfrak{d}}(\lambda),$$

for some $p \in \mathbb{N}$ which tends to infinity as k tends to infinity. This allows one to fully exploit (3.15). There are many possible choices for $A_{k,\mu}$, as the one introduced in [GM12] and defined by its spectral formula (and then translated back in physical space), and the one introduced in [GNOa] and defined by Richardson extrapolation in space. Second, the proof presented above crucially relies on the i.i.d. structure when writing (3.21). Indeed this relies on the fact that both statistical ensembles we use (the i.i.d. on $\mathbb{B}$ and on the set of edges of the N-torus) can be coupled (the ensemble on the torus being "included" in the ensemble on $\mathbb{B}$). A similar construction can be made in the case of hidden i.i.d. variables as introduced above — but not in full generality.

We expect these convergence rates to be optimal in general, so that the systematic error would scale as the square of the random error in any dimension (up to logarithmic corrections). Since the fluctuations of A_N^{law} have the scaling of the central limit theorem (3.13), one may wonder whether the distribution of $L^{d/2}(\xi \cdot A_N^{\mathrm{law}}\xi - \xi \cdot \langle A_N^{\mathrm{law}} \rangle \xi)$ converges in law to a Gaussian random variable. Related results were obtained by Nolen [No11], Rossignol [Ro12], and Biskup, Salvi, and Wolff [BSW12]. A full quantitative CLT is proved in [GN], which shows that the Wasserstein distance between $L^{d/2}\dfrac{\xi \cdot A_N^{\mathrm{law}}\xi - \xi \cdot A_{\mathrm{hom}}\xi}{\sigma}$ and a centered Gaussian random variable is of order $L^{-d/2}\ln^d L$ (where σ^2 is the limiting rescaled variance).

In the case of the periodization in space, we still expect the random error to scale as the central limit theorem

$$\mathrm{var}\left[\xi \cdot A_N^{\mathrm{spa}}\xi\right]^{1/2} \lesssim N^{-d/2}. \tag{3.22}$$

Yet, we do not expect the scaling of (3.20) to hold in this case, and we rather conjecture that (unless the entries of A are i.i.d.) the systematic error scales as a surface effect (as for Dirichlet boundary conditions), namely

$$|\xi \cdot \langle A_N^{\mathrm{spa}} \rangle \xi - \xi \cdot A_{\mathrm{hom}}\xi| \sim N^{-1}, \tag{3.23}$$

although we do not have a proof of this. The intuition behing this conjecture is that the imposed periodicity is not compatible with the underlying stationarity. A similar phenomenon occurs when considering a periodic problem and approximating the corrector on a domain which is not a multiple of the period and with periodic boundary conditions (so that the periodicity of the approximated corrector and that of the true corrector do not match), which yields an error which scales again as a surface effect (although the prefactor is usually much smaller than for Dirichlet boundary conditions).

3.3. **Numerical study.**

3.3.1. *Homogeneous Dirichlet boundary conditions (without zero-order term).* We consider the simplest possible example: the case of Bernoulli variables. The conductances $\{\omega_e\}_{e\in\mathbb{B}}$ are i.i.d. random variables taking values $\alpha = 1$ and $\beta = 4$ with probability 1/2.

In dimension $d = 2$, the homogenized matrix satisfies the Dykhne formula $A_{\mathrm{hom}} = \sqrt{\alpha\beta}\mathrm{Id} = 2\mathrm{Id}$ (see [Gl12a] for a proof). Figure 1 displays the plots of the estimates of the random error $N \mapsto \mathrm{var}\,[\xi \cdot A_N\xi]^{1/2}$ and of the systematic error $N \mapsto |\xi \cdot \langle A_N \rangle \xi - \xi \cdot A_{\mathrm{hom}}\xi|$ in logarithmic scale.

These errors are approximated by empirical averages of independent realizations (the intervals represent the empirical standard deviation). The number of independent realizations in function of N is displayed for completeness in Table 1. As can be seen, the

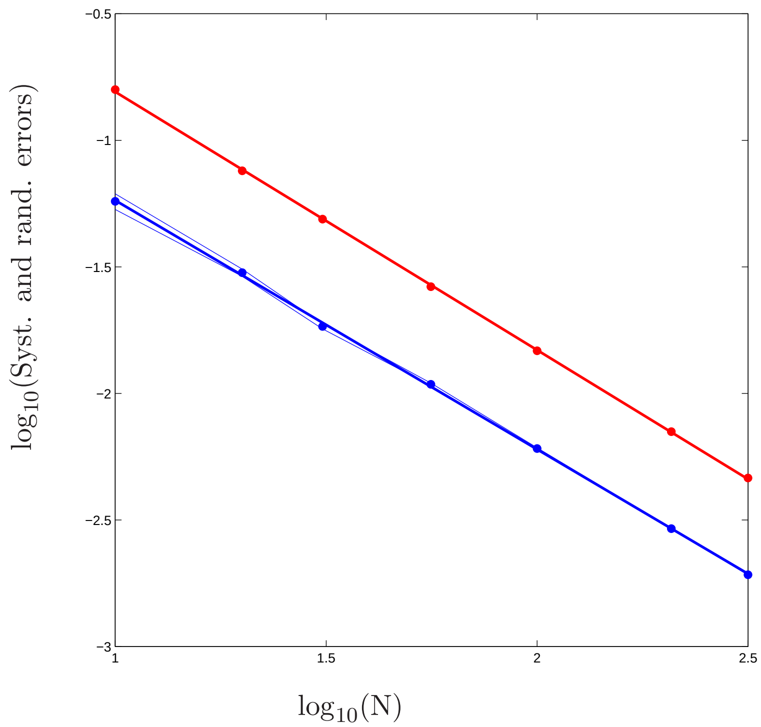

FIGURE 1. Dirichlet boundary conditions (and $\mu = 0$), $d = 2$, statistical error (red) rate 1.02 and prefactor 1.62, systematic error (blue) rate 0.98 and prefactor 0.56.

TABLE 1.

N	10	20	31	56	100	208	316
Number of realizations	1500	6000	14415	47040	150000	648960	1497840

apparent convergence rates of the random error and of the systematic error are 1.02 and 0.98, respectively. This confirms the conjectures (3.4) and (3.5) for $d = 2$.

For numerical tests in dimension $d = 3$, we have to proceed slightly differently since there is no closed formula for the homogenized coefficient (the homogenized matrix is still a multiple of the identity by symmetry arguments). The approximation of the random error $N \mapsto \operatorname{var}[\xi \cdot A_N \xi]^{1/2}$ is unchanged. Yet, instead of plotting the systematic error $N \mapsto |\xi \cdot \langle A_N \rangle \xi - \xi \cdot A_{\hom}\xi|$, we plot an approximation of $N \mapsto |\xi \cdot \langle A_N \rangle \xi - \xi \cdot \left\langle A_N^{\mathrm{law}} \right\rangle \xi|$ via empirical averages, where A_N^{law} is the approximation of $A_{\hom}$ by periodization. In particular, in view of (3.20), we have by the triangle inequality

$$|\xi \cdot \langle A_N \rangle \xi - \xi \cdot A_{\hom}\xi| \geqslant |\xi \cdot \langle A_N \rangle \xi - \xi \cdot \langle A_N^{\mathrm{law}} \rangle \xi| - CN^{-d} \ln^d N$$

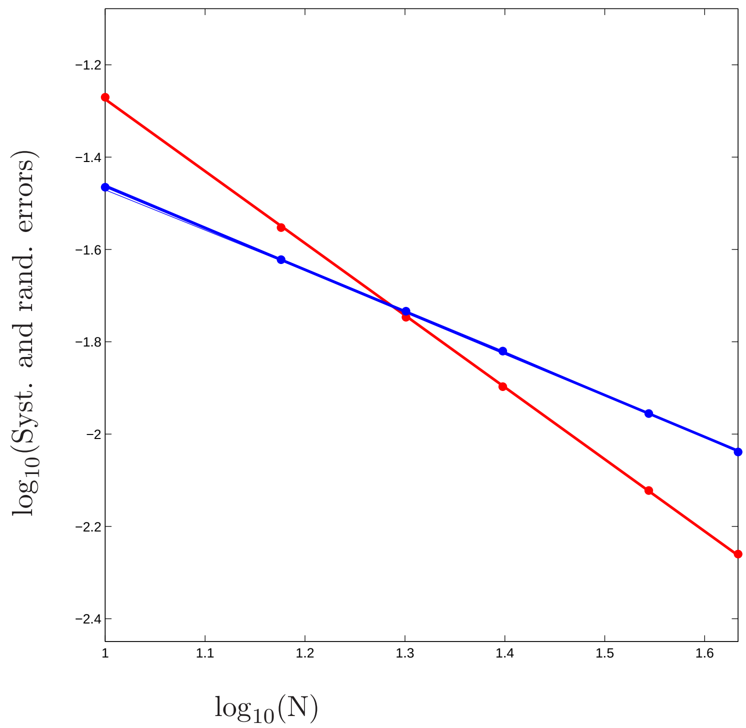

FIGURE 2. Dirichlet boundary conditions, $d = 3$, statistical error (red) rate 1.56 and prefactor 1.91, systematic error (blue) rate 0.90 and prefactor 0.27.

TABLE 2.

N	10	15	20	25	35	43
Number of realizations	15000	50625	120000	234375	643125	1192605

for some $C > 0$, so that $|\xi \cdot \langle A_N \rangle \xi - \xi \cdot A_{\text{hom}}\xi|$ and $|\xi \cdot \langle A_N \rangle \xi - \xi \cdot \langle A_N^{\text{law}} \rangle \xi|$ are of the same order provided $|\xi \cdot \langle A_N \rangle \xi - \xi \cdot \langle A_N^{\text{law}} \rangle \xi| \gtrsim N^{-d} \ln^d N$ (which we indeed observe empirically). These two errors $N \mapsto \text{var}\,[\xi \cdot A_N \xi]^{1/2}$ and $N \mapsto |\xi \cdot \langle A_N \rangle \xi - \xi \cdot \langle A_N^{\text{law}} \rangle \xi|$ are plotted on Figure 2 in logarithmic scale. The number of independent realizations in function of N is displayed for completeness in Table 2. As can be seen, the apparent convergence rate of the random error and of the (modified) systematic error are 1.56 and 0.9, respectively. These exponents are close to the conjectured exponents of (3.4) and (3.5) for $d = 3$.

3.3.2. *Regularized corrector and filtering.* We still consider the two-dimensional example of Paragraph 3.3.1. In order to define $A_{\mu,N,L}$ completely, we need to choose L and μ in function of N, and define the averaging mask η_L. We have taken

- $L = 4N/5$ and $L = 3N/5$,
- $\mu = 125/N^{3/2}$,

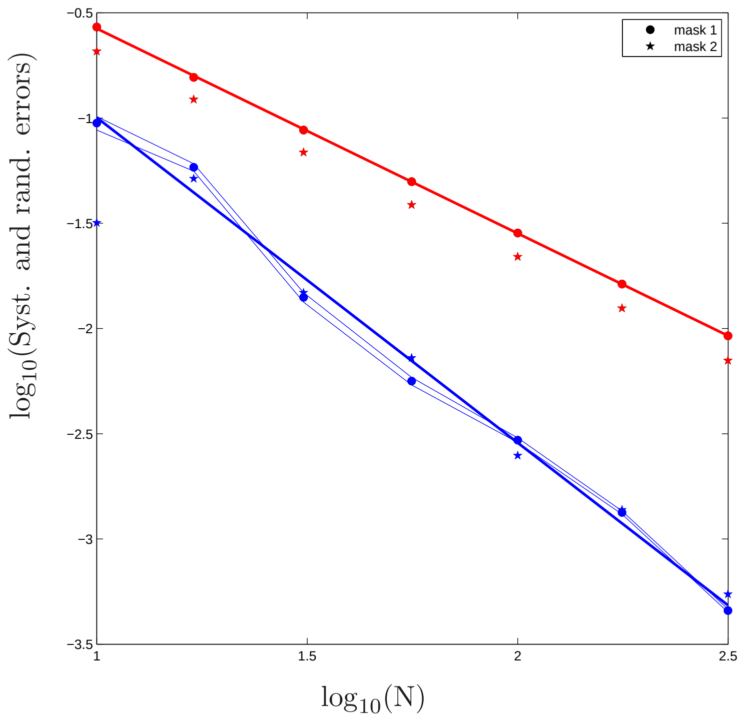

FIGURE 3. Regularized corrector, $d = 2$, i .i. d. case, statistical error (red) rate 0.97 and prefactor 2.51, systematic error (blue) rate 1.55 and prefactor 3.55.

TABLE 3.

N	10	17	31	56	100	177	316
Number of realizations	1500	4335	14415	47040	150000	510081	1480338

- a piecewise affine mask, as plotted on Figure 4 for $N = 10$ (the first one for $L = 4N/5$ and the second one for $L = 3N/5$).

The theoretical predictions (3.13) and (3.14) take the following forms with these parameters:

$$\mathrm{var}\left[\xi \cdot A_{\mu,N,L}\xi\right]^{1/2} \lesssim N^{-1} \ln^{1/2} N \tag{3.24}$$

$$|\xi \cdot \langle A_{\mu,N,L}\rangle\, \xi - \xi \cdot A_{\mathrm{hom}}\xi| \lesssim N^{-3/2}. \tag{3.25}$$

These two errors are plotted on Figure 3 in logarithmic scale. The number of independent realizations in function of N is displayed for completeness in Table 3. As can be seen, the apparent convergence rates for the random and systematic errors are 0.97 and 1.55, respectively. This shows the sharpness of the analysis. These numerical tests also give an idea on the prefactors in (3.13) and (3.14). We observe that the systematic error decays

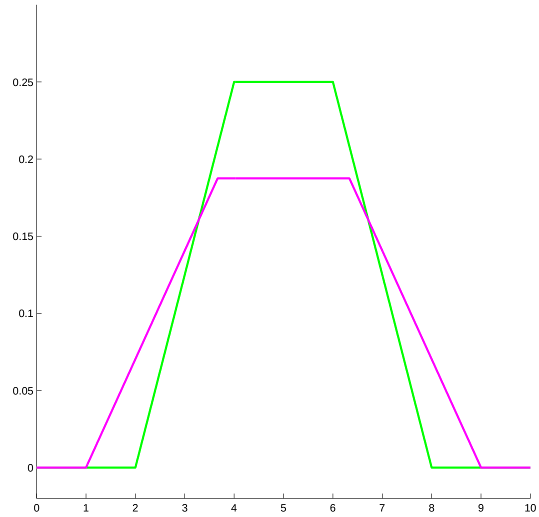

FIGURE 4. Two masks for $N = 10$

faster than the random error, and that the prefactors are of the same order (roughly twice as big for the systematic error).

The second series of tests on the regularization method aims at validating an approach which will be used to compare the two periodization methods. In particular, we consider now a two-dimensional case with correlations of the type considered in Paragraph 3.2.3. In this case we do not have a closed formula for the homogenized coefficients. The statistics of the coefficients is defined as follows. We let $\{\bar\omega_{(z,z+e_i)}\}_{z\in\mathbb{Z}^2,i\in\{1,2\}}$ be i.i.d. variables following a uniform law in $[0,1]$. We define $\omega_{(z,z+e_i)}$ to be $\alpha = 1$ if for all z' such that $\|z'-z\|_\infty \leqslant 2$ we have $\bar\omega_{(z,z+e_i)} \leqslant p$ (that is, if the 25 hidden i.i.d. random variables are less than p), and $\omega_{(z,z+e_i)}$ to be $\beta = 4$ if there exists z' with $\|z'-z\|_\infty \leqslant 2$ such that $\bar\omega_{(z,z+e_i)} > p$, where p is chosen so that $p^{25} = 1/2$ (that is, α and β are equiprobable). The typical realization of such conductances is made of islands of β's of size 4 in a sea of α's. The theoretical predictions (3.24) and (3.25) hold provided we take

- $L = 4N/5$;
- $\mu = 125/N^{3/2}$,
- a piecewise affine mask, as plotted on Figure 4.

Since we do not know A_{hom} a priori, we shall replace the systematic error by $N \mapsto |\xi \cdot \left\langle A_{\mu,N,L} - A_N^{\mathrm{law}}\right\rangle \xi|$, where A_N^{law} is the approximation of A_{hom} by periodization in law. The combination of (3.25) and (3.20) indeed yields

$$|\xi \cdot \langle A_{\mu,N,L} - A_N^{\mathrm{law}}\rangle \xi| \lesssim N^{-3/2},$$

which we want to verify empirically. This modified systematic error is plotted on Figure 5 in logarithmic scale. The number of independent realizations in function of N is reported on in Table 4. As can be seen, the apparent convergence rate for the modified systematic error is close to 3/2, so that the true systematic error $|\xi \cdot \langle A_{\mu,N,L}\rangle - A_{\mathrm{hom}}\xi|$ has the same

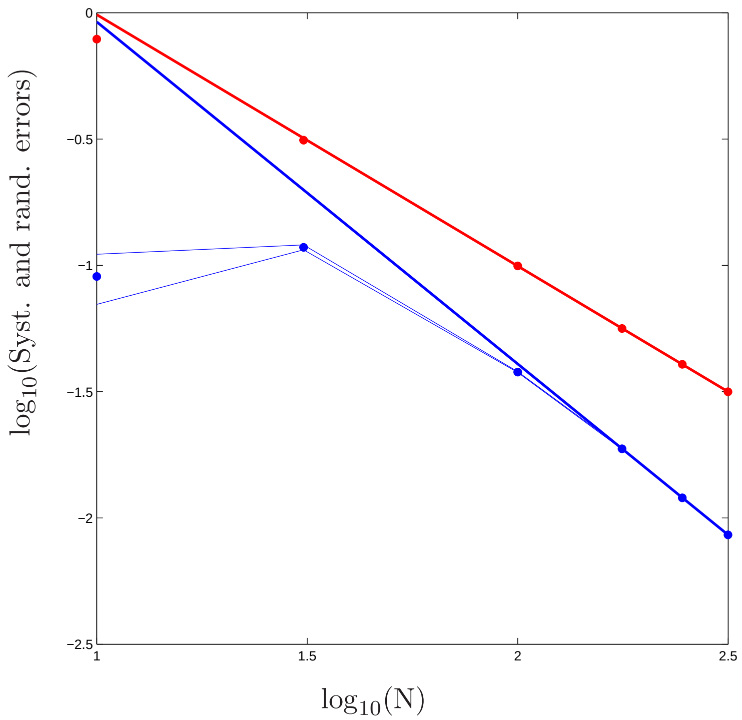

FIGURE 5. Regularized corrector, $d = 2$, correlated case, statistical error (red) rate 1 and prefactor 9.77, systematic error (blue) rate 1.35 and prefactor 20.9.

TABLE 4.

N	10	31	100	177	246	316
Number of realizations	1500	14415	150000	469935	907740	1497840

decay since

$$|\xi \cdot \langle A_{\mu,N,L} \rangle - A_{\text{hom}}\xi| \geqslant |\xi \cdot \left\langle A_{\mu,N,L} - A_N^{\text{law}} \right\rangle \xi| + CN^{-2} \ln^2 N,$$

for some $C > 0$ due to (3.20). Note that the asymptotic regime is more difficult to capture in the correlated case than in the i.i.d. since the typical lengthscale is 4 in the first case (the size of a typical island), and 1 in the second case. Yet these tests show it is possible to observe numerically a convergence with a rate larger than 1 in this correlated case.

3.3.3. *Periodization methods.* In this paragraph we first check empirically the sharpness of (3.19) and (3.20) on the simple two-dimensional example of Paragraph 3.3.1. Figure 6 displays the plots of the estimates of the random error $N \mapsto \text{var}\left[\xi \cdot A_N^{\text{law}}\xi\right]^{1/2}$ and of the systematic error $N \mapsto |\xi \cdot \left\langle A_N^{\text{law}} \right\rangle \xi - \xi \cdot A_{\text{hom}}\xi|$ in logarithmic scale. These errors are

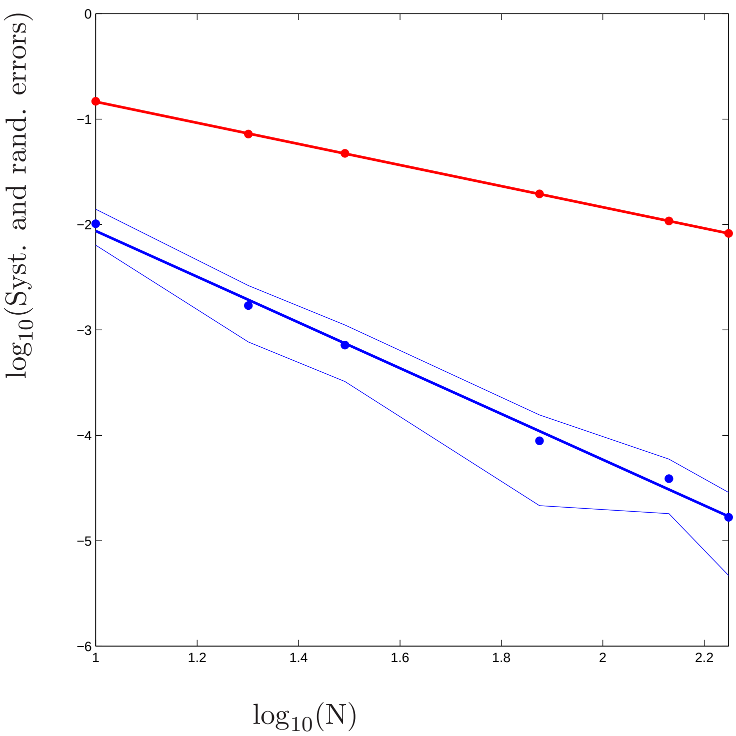

FIGURE 6. Periodization in law, $d = 2$, i.i.d., statistical error (red) rate 1.01 and prefactor 1.48, systematic error (blue) rate 2.17 and prefactor 1.29.

TABLE 5.

N	10	20	31	75	135	177
Number of realizations	1500	14415	498904	469930	780900	1245782

approximated by empirical averages of independent realizations, and intervals of confidence are given for the systematic error (corresponding to the empirical standard deviation). The number of independent realizations in function of N is displayed for completeness in Table 5. As can be seen, the apparent convergence rates of the random error and of the systematic error are 1.01 and 2.17 (note that the fluctuations are more important for the evaluation of the systematic error which is very small), which confirms the predictions. In addition, the prefactors are again of the same order (slightly smaller for the systematic error), so that the systematic error is negligible wrt the random error. This will be further analyzed in the next paragraph.

The second series of tests deals with the correlated two-dimensional example introduced in Paragraph 3.3.2. The aim is to investigate empirically the conjecture (3.23) on the systematic error for periodization in space. As in the previous paragraph we replace the

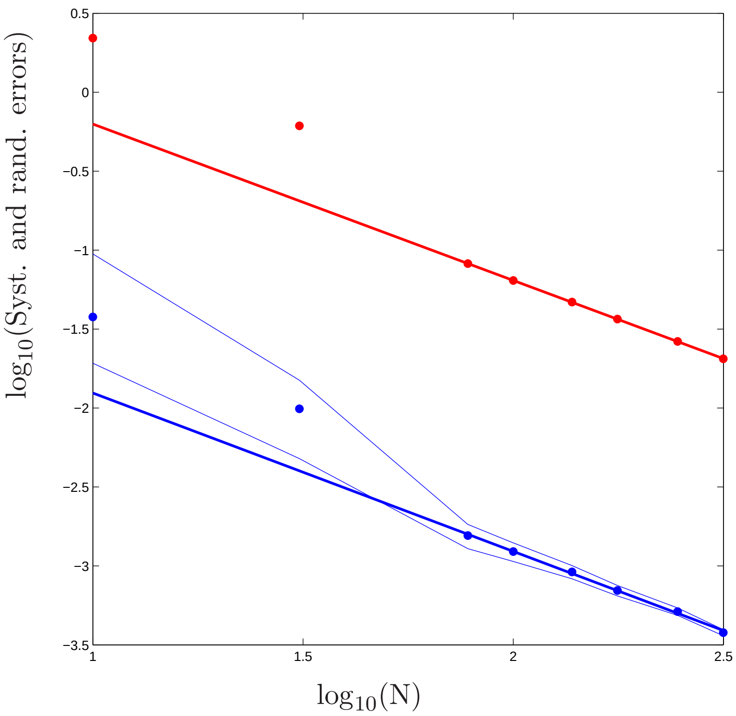

FIGURE 7. Periodization in space, $d = 2$, correlated conductances, statistical error (red) rate 0.99 and prefactor 6.17, modified systematic error (blue) rate 1 and prefactor 0.13.

TABLE 6.

N	10	31	78	100	138	177	246	316
Number of realizations	1500	14415	91260	150000	285660	469935	907740	1497840

systematic error by the modified systematic error $N \mapsto |\xi \cdot \left\langle A_N^{\text{spa}} - A_N^{\text{law}} \right\rangle \xi|$. In view of (3.20), we indeed have

$$|\xi \cdot (\langle A_N^{\text{spa}} \rangle - A_{\text{hom}})\xi| = |\xi \cdot \langle A_N^{\text{spa}} - A_N^{\text{law}} \rangle \xi| + O(N^{-2} \ln^2 N).$$

Figure 7 displays the plots of the estimates of the random error $N \mapsto \text{var}\left[\xi \cdot A_N^{\text{law}} \xi\right]^{1/2}$ and of the modified systematic error $N \mapsto |\xi \cdot \left\langle A_N^{\text{law}} - A_N^{\text{spa}} \right\rangle \xi|$ in logarithmic scale. These errors are approximated by empirical averages of independent realizations, and intervals of confidence are given for the systematic error (corresponding to the empirical standard deviation). The number of independent realizations in function of N is displayed for completeness in Table 6. As can be seen, the slopes of the random error and of the systematic error are 0.99 and 1, which confirms the conjectures (3.22) and (3.23) on the periodization in space method. Yet the prefactor of the systematic error is much

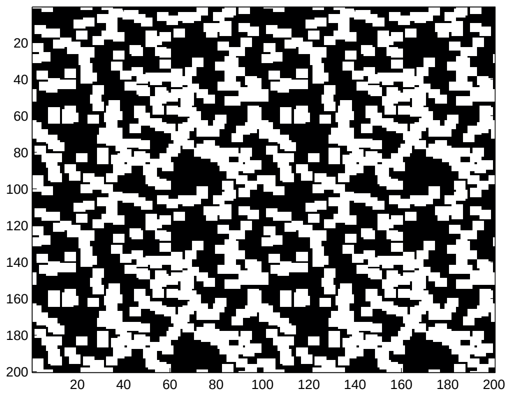

FIGURE 8. Periodization in law of A (four periods)

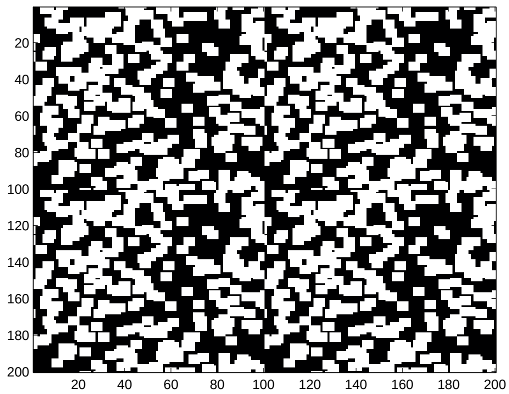

FIGURE 9. Periodization in space of A (four periods)

smaller (roughly 40 times smaller) than the prefactor of the random error. This makes the systematic error hardly observable in practice. This would not be so clear for $d \geqslant 3$ (as on Figure 2).

It is instructive to compare the periodization in law $A_{N,\#}$ of A to the periodization in space $A^{N,\#}$ of A visually. Typical realizations of these periodizations are pictured on Figures 8 and 9 for $N = 100$ — 4 periods are reproduced. A close look at Figure 9 reveals the mismatch between stationarity and enforced periodicity (which does not appear on Figure 8 — this is the core of the "coupling" strategy).

3.3.4. *Optimal numerical strategy.* In this last paragraph, we propose a numerical strategy to obtain an approximation of the homogenized coefficients in the i.i.d. case at a given precision and at the lowest cost. In view of the previous parapraphs, it is clear that periodization (in law) minimizes both the random and systematic errors at N fixed. One feature we have not used yet is the scalability of the variance: if $\{A_i\}_{1\leqslant i\leqslant k}$ are k independent realizations of a random variable A, then

$$\mathrm{var}\left[\frac{1}{k}\sum_{i=1}^{k} A_i\right] \;=\; \frac{1}{\sqrt{k}}\mathrm{var}\left[A\right].$$

While empirical averages of independent realizations do not allow one to reduce the systematic error, they do allow one to reduce the random error. This is particularly interesting since:

- the dominant error is the random error,
- it is computationally cheaper to solve several smaller linear problems than one single large problem (the solution cost of a linear system is always superlinear).

In view of the analysis of periodization in law, in order to approximate homogenized coefficients within a tolerance $\delta > 0$, the cheapest computational way consists in solving k_δ independent periodic problems of size N_δ, and take as approximation the empirical average of these k_δ realizations $A^{\text{law}}_{N_\delta,i}$:

$$\frac{1}{k_\delta}\sum_{i=1}^{k_\delta} A^{\text{law}}_{N_\delta,i}, \tag{3.26}$$

where N_δ is such that

$$\delta/2 \;=\; C_{syst} N_\delta^{-d} \ln^d N_\delta,$$

and k_δ such that

$$\delta/2 \;=\; \frac{1}{\sqrt{k_\delta}} C_{rand} N_\delta^{-d/2}.$$

where C_{syst} and C_{rand} are the optimal prefactors in the estimates (3.20) and (3.19), respectively. Then we have

$$\left\langle \left| A_{\text{hom}} - \frac{1}{k_\delta}\sum_{i=1}^{k_\delta} A^{\text{law}}_{N_\delta,i} \right|^2 \right\rangle^{1/2} \;\leqslant\; \delta.$$

To be precise, the associated computational cost is $k_\delta \gamma_d(N_\delta^d)$, where $M \mapsto \gamma_d(M)$ is the cost of solving a linear problem of order M (order of the matrix of the linear system) in dimension d. Since γ_d is superlinear, one readily convinces oneself that the best one can do is indeed (3.26). In the i.i.d. example of Figure 6, an approximation of these prefactors is

$$C_{syst} = 1.29, \quad C_{rand} = 1.48.$$

4. Numerical approximation of the homogenized coefficients using the RWRE

4.1. **General approach.** We now discuss how to approximate homogenized coefficients by simulating random walks. The simulation of a random walk has a very interesting feature: one does not need to generate a full environment a priori. Rather, it suffices to generate the environment along the trajectory of the random walk. This is particularly interesting in dimensions 3 and higher, where the random walk is transient, and visits only a vanishing fraction of the space. In fact, although the walk is recurrent in dimension 2, this last property still holds, since the time necessary to exit a box of size N is of order N^2, while at such a time, the walk has typically visited a number of distinct sites of order $N^2/\ln(N)$.

The strategy consists in simulating a large number of random walks, each in its own independent environment, and rely on Theorem 2.8 to recover the homogenized coefficients. Keeping the environment fixed would be more difficult to analyse from a theoretical point of view, would certainly lead to larger errors (although we cannot prove this), and would force us to abandon the approach of generating the environment along the trajectory.

4.2. **The discrete-time random walk.** Although it is easier to see the link between the corrector equation and the continuous-time random walk, when it comes to simulations, it is more convenient to work with a discrete-time version of X, since there is no waiting times to compute. We define $(Y_n)_{n\in\mathbb{N}}$ to be the discrete-time Markov chain such that

$\mathbf{P}_z^\omega[X_0 = z] = 1$ and

$$\mathbf{P}_z^\omega[Y_1 = z'] = \left| \begin{array}{ll} p(z \rightsquigarrow z') & \text{if } z' \sim z, \\ 0 & \text{otherwise,} \end{array} \right. \tag{4.1}$$

where $p(z \rightsquigarrow z')$ is as in (2.14). Considering the "constructive" definition of the random variable X given in paragraph 2.3.1, if Y_n is the position of X after n steps, then $(Y_n)_{n\in\mathbb{N}}$ is a discrete-time Markov process satisfying (4.1). As before, it will be convenient to consider the environment viewed by the walk Y, defined by

$$\omega_n = \theta_{Y_n}\, \omega.$$

Note that the probabilities $p(z \rightsquigarrow z')$ and $p(z' \rightsquigarrow z)$ need not be equal, hence it is not true in general that the counting measure is reversible for Y. A reversible measure π for Y should satisfy, for any $z, z' \in \mathbb{Z}^d$,

$$\pi(z)\; p(z \rightsquigarrow z') = \pi(z')\; p(z' \rightsquigarrow z).$$

This relation holds if we choose $\pi(z) = p_\omega(z)$ (recall the definitions of $p_\omega(z)$ and $p(z \rightsquigarrow z')$ given in (2.13) and (2.14) respectively). This means that contrary to the continuous-time random walk, the discrete-time walk will preferably spend time on sites where $p_\omega(z)$ is large. This effect has its counterpart concerning the environment viewed by Y: the initial product measure $\mathbb{P}$ on the conductances is not an invariant measure for the process $(\omega_n)_{n\in\mathbb{N}}$ in general. Indeed, an invariant measure for this process should favor environments for which $p(\omega) := p_\omega(0)$ is large. Precisely, the following "tilted" measure $\tilde{\mathbb{P}}$, defined by

$$\mathrm{d}\tilde{\mathbb{P}}(\omega) = \frac{p(\omega)}{\langle p \rangle}\, \mathrm{d}\mathbb{P}(\omega) \tag{4.2}$$

is invariant for $(\omega_n)_{n\in\mathbb{N}}$. In particular, the measure $\tilde{\mathbb{P}}$ has a density with respect to our initial product measure $\mathbb{P}$. Since $p(\omega)$ is never equal to 0 or infinity, a property holds $\tilde{\mathbb{P}}$-almost surely if and only if it holds $\mathbb{P}$-almost surely.

We write $\tilde{\mathbb{P}}_0$ for the measure $\tilde{\mathbb{P}}\mathbf{P}_0^\omega$, and $\tilde{\mathbb{E}}_0$ for the associated expectation. Adapting slightly the arguments of paragraph 2.3.2, we obtain the following.

Theorem 4.1 ([KV86]). *Under the measure $\tilde{\mathbb{P}}_0$ and as ε tends to 0, the rescaled discrete-time random walk $Y^{(\varepsilon)} := (\sqrt{\varepsilon} Y_{\lfloor t/\varepsilon \rfloor})_{t\in\mathbb{R}_+}$ converges in distribution (for the Skorokhod topology) to a Brownian motion with covariance matrix $2A_{\mathrm{hom}}^{\mathrm{disc}}$, where*

$$A_{\mathrm{hom}}^{\mathrm{disc}} = \langle p \rangle^{-1} A_{\mathrm{hom}} = (2d\, \langle \omega_e \rangle)^{-1} A_{\mathrm{hom}}, \tag{4.3}$$

and A_{hom} is as in (2.5). In other words, for any bounded continuous functional F on the space of cadlag functions, one has

$$\tilde{\mathbb{E}}_0 \left[F(Y^{(\varepsilon)}) \right] \xrightarrow[\varepsilon \to 0]{} E[F(B)], \tag{4.4}$$

where B is a Brownian motion started at the origin and with covariance matrix $2A_{\mathrm{hom}}^{\mathrm{disc}}$. Moreover, for any $\xi \in \mathbb{R}^d$, one has

$$n^{-1} \tilde{\mathbb{E}}_0 \left[(\xi \cdot Y_n)^2 \right] \xrightarrow[n \to +\infty]{} 2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}} \xi. \tag{4.5}$$

Before discussing numerical methods based on this theorem, we introduce some notation. Let $Y^{(1)}, Y^{(2)}, \ldots$ be independent discrete-time random walks evolving in the environments $\omega^{(1)}, \omega^{(2)}, \ldots$ respectively. We write $\mathbf{P}_0^{\overline{\omega}}$ for their joint distribution, all random walks starting from 0, where $\overline{\omega} = (\omega^{(1)}, \omega^{(2)}, \ldots)$. The environments $(\omega^{(1)}, \omega^{(2)}, \ldots)$ are themselves i.i.d. random variables distributed according to $\mathbb{P}$, and we write $\mathbb{P}^{\otimes}$ for their joint distribution. We also write $\mathbb{P}_0^{\otimes}$ as a shorthand for the measure $\mathbb{P}^{\otimes}\mathbf{P}_0^{\overline{\omega}}$. As usual, we simply replace "P" by "E" with the appropriate typography to denote corresponding expectations.

4.3. **Methods and theoretical analysis.** In the following two paragraphs, we discuss numerical methods based on (4.5) and (4.4), respectively. This will allow us to demonstrate the superiority of the method based on the square displacement.

4.3.1. *Method based on the mean square displacement.* We start with a method based on (4.5). Recall that by the definition of the tilted measure $\tilde{\mathbb{P}}$ in (4.2) we have

$$n^{-1}\tilde{\mathbb{E}}_0\left[(\xi \cdot Y_n)^2\right] = \frac{1}{n\langle p\rangle}\mathbb{E}_0\left[p(\omega)(\xi \cdot Y_n)^2\right]. \tag{4.6}$$

By the law of large numbers, for any fixed n, the quantity

$$\hat{A}_k(n) := \frac{p(\omega^{(1)})(\xi \cdot Y_n^{(1)})^2 + \cdots + p(\omega^{(k)})(\xi \cdot Y_n^{(k)})^2}{kn\langle p\rangle} \tag{4.7}$$

converges (almost surely) to the r. h. s. of (4.6) as k tends to infinity. From the convergence in (4.5), we thus obtain

$$\lim_{n\to+\infty}\lim_{k\to+\infty}\hat{A}_k(n) = 2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}}\xi. \tag{4.8}$$

The quantity $\hat{A}_k(n)$ is what we shall compute. It involves k random walks, each simulated in its own environment, up to time n. The formula involves the average $\langle p\rangle = 2d\langle\omega_e\rangle$, which can be easily computed beforehand, so that we assume that we have exact knowledge of this quantity. The convergence in (4.8) can be made quantitative.

Theorem 4.2 ([GM13]). *There exist constants $q, C, c > 0$ such that for any $k \in \mathbb{N}^*$, any $\varepsilon > 0$ and any n large enough,*

$$\mathbb{P}_0^{\otimes}\left[\left|\hat{A}_k(n) - 2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}}\xi\right| \geqslant (C\mu_d(n) + \varepsilon)/n\right] \leqslant \exp\left(-\frac{k\varepsilon^2}{cn^2}\right), \tag{4.9}$$

where

$$\mu_d(n) = \left| \begin{array}{ll} \ln^q n & \text{if } d = 2, \\ 1 & \text{if } d \geqslant 3. \end{array}\right.$$

This theorem ensures that for k larger than a constant times n^2, the difference between $\hat{A}_k(n)$ and $2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}}\xi$ is smaller than C/n (or $C\ln^q(n)/n$ if $d = 2$) for some constant C, with probability close to 1.

Sketched proof of Theorem 4.2. By the triangle inequality,

$$\left|\hat{A}_k(n) - 2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}}\xi\right| \leqslant \left|\hat{A}_k(n) - n^{-1}\tilde{\mathbb{E}}_0\left[(\xi \cdot Y_n)^2\right]\right| + \left|n^{-1}\tilde{\mathbb{E}}_0\left[(\xi \cdot Y_n)^2\right] - 2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}}\xi\right|. \tag{4.10}$$

We call the first term the *statistical error*, and the second term the *systematic error*. The theorem is proved if we show the following two inequalities:

$$\mathbb{P}_0^{\otimes}\left[\left|\hat{A}_k(n) - n^{-1}\tilde{\mathbb{E}}_0\left[(\xi \cdot Y_n)^2\right]\right| \geqslant \varepsilon/n\right] \leqslant \exp\left(-\frac{k\varepsilon^2}{cn^2}\right), \tag{4.11}$$

$$\left|n^{-1}\tilde{\mathbb{E}}_0\left[(\xi \cdot Y_n)^2\right] - 2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}}\xi\right| \leqslant C\mu_d(n)/n. \tag{4.12}$$

Inequality (4.11) follows from classical large deviations theory, noting that $\hat{A}_k(n)$ is a sum of i.i.d. random variables. In the same vein, it is also possible to show (see [GM13, Proposition 5.1]) that for any sequence $k_n \to \infty$,

$$\sqrt{k_n}\left(\hat{A}_{k_n}(n) - n^{-1}\tilde{\mathbb{E}}_0\left[(\xi \cdot Y_n)^2\right]\right) \xrightarrow[n\to+\infty]{\text{(distr.)}} \mathcal{N}(0, \mathsf{v}), \tag{4.13}$$

where $\mathcal{N}(0, \mathsf{v})$ is a Gaussian random variable of variance v given by

$$\mathsf{v} = \left(3\frac{\langle p^2\rangle}{\langle p\rangle^2} - 1\right)(2\xi \cdot A_{\mathrm{hom}}^{\mathrm{disc}}\xi)^2. \tag{4.14}$$

Although the l. h. s. of (4.12) is deterministic, its proof requires a more subtle analysis and a quantitative control of the convergence in (4.5).

To simplify the presentation, we shall prove the continuous-time version of (4.12), that is, a quantitative version of (2.19). Recall from paragraph 2.3.2 that $\xi \cdot X_t = M_t + R_t$, where M_t is a stationary martingale under the measure $\mathbb{P}_0$, and R_t is a remainder. The martingale property and the stationarity of the increments guarantee that $\mathbb{E}_0[M_t^2]$ grows linearly with t, and in fact (see (2.24) and (2.25))

$$\mathbb{E}_0[M_t^2] = 2t\ \xi \cdot A_{\mathrm{hom}}\xi. \tag{4.15}$$

Note that (4.15) is an identity for all t.

Combined with (4.15), the decomposition $\xi \cdot X_t = M_t + R_t$ yields

$$\mathbb{E}_0\left[(\xi \cdot X_t)^2\right] = 2t\xi \cdot A_{\mathrm{hom}}\xi + \mathbb{E}_0\left[R_t^2\right] + 2\mathbb{E}_0\left[M_t R_t\right]. \tag{4.16}$$

In paragraph 2.3.2, we have sketched the argument for the convergence $R_t/\sqrt{t} \to 0$ in $L^2(\mathbb{P}_0)$ (see (2.27)), which reduces to the proof of the integrability of $\lambda \mapsto \frac{1}{\lambda}$ close to 0 for the spectral measure (see (2.11)).

When the conductances are not only ergodic but also satisfy a spectral gap estimate (as in the case of i.i.d. conductances), one can characterize those functions $\psi : (0, \infty) \to \mathbb{R}^+$ which are integrable close to 0 for the spectral measure. This is achieved using the optimal estimates (3.15) of [GNOa]

$$\int_0^{\nu} \mathrm{d}e_{\mathfrak{d}}(\lambda) \lesssim \nu^{d/2+1}.$$

Such a control of the spectral measure at the bottom of the spectrum gives information on the speed of convergence of $t^{-1}\mathbb{E}_0\left[R_t^2\right]$ to 0. Indeed, in view of (2.27),

$$\begin{aligned} \frac{1}{2}\mathbb{E}_0[R_t^2] &= \int_{\mathbb{R}^+} \frac{1 - e^{-t\lambda}}{\lambda^2}\ \mathrm{d}e_{\mathfrak{d}}(\lambda) \\ &= \left(\int_0^{1/t} + \int_{1/t}^{1} + \int_1^{+\infty}\right)\frac{1 - e^{-t\lambda}}{\lambda^2}\ \mathrm{d}e_{\mathfrak{d}}(\lambda). \end{aligned} \tag{4.17}$$

The last integral is bounded by $\int_0^{+\infty} \mathrm{d}e_{\mathfrak{d}}(\lambda) = \|\mathfrak{d}\|_2^2$. Since $1 - e^{-x} \leqslant x$, the first integral is bounded by

$$\begin{aligned}
\int_0^{1/t} \frac{t}{\lambda} \, \mathrm{d}e_{\mathfrak{d}}(\lambda) \quad &= \quad t \int_0^{1/t} \int_\lambda^{+\infty} \frac{1}{\delta^2} \, \mathrm{d}\delta \, \mathrm{d}e_{\mathfrak{d}}(\lambda) \\
&= \quad t \int_0^{+\infty} \frac{1}{\delta^2} \int_0^{\delta \wedge 1/t} \mathrm{d}e_{\mathfrak{d}}(\lambda) \, \mathrm{d}\delta \\
&\overset{(3.15)}{\lesssim} \quad t \int_0^{+\infty} \frac{1}{\delta^2} (\delta \wedge 1/t)^{d/2+1} \, \mathrm{d}\delta \lesssim C.
\end{aligned}$$

The second integral in (4.17) is itself bounded by

$$\begin{aligned}
\int_{1/t}^{1} \frac{1}{\lambda^2} \, \mathrm{d}e_{\mathfrak{d}}(\lambda) \quad &= \quad \int_{1/t}^{1} \int_\lambda^{+\infty} \frac{1}{\delta^3} \, d\delta \, \mathrm{d}e_{\mathfrak{d}}(\lambda) \\
&= \quad \int_{1/t}^{+\infty} \frac{1}{\delta^3} \int_{1/t}^{\delta \wedge 1} \mathrm{d}e_{\mathfrak{d}}(\lambda) \, \mathrm{d}\delta \\
&\overset{(3.15)}{\lesssim} \quad \int_{1/t}^{+\infty} \frac{1}{\delta^3} (\delta \wedge 1)^{d/2+1} \, d\delta,
\end{aligned}$$

which is bounded by a constant if $d > 2$, and diverges logarithmically for $d = 2$. In short, up to logarithmic corrections in dimension 2, we have shown that (3.15) implies that $\mathbb{E}_0 \left[R_t^2 \right]$ remains bounded as t tends to infinity.

In the case of discrete time, our estimates of the bottom of the spectral measure are slightly weaker than (3.15) (we have a logarithmic divergence in dimension 2, and optimal estimates up to dimension 6), see [GM12, Appendix A]. This is however sufficient to prove Theorem 4.2.

In view of (4.16), it only remains to estimate the cross-product $\mathbb{E}_0 [M_t R_t]$. Since $\mathbb{E}_0 \left[R_t^2 \right]$ remains bounded as t tends to infinity (for $d > 2$), a naive use of the Cauchy-Schwarz inequality would ensure that $|\mathbb{E}_0 [M_t R_t] \,|$ grows no faster than $\sqrt{t}$. However, cancellations occur, and this cross-product vanishes identically:

$$\mathbb{E}_0 [M_t R_t] \equiv 0. \tag{4.18}$$

Recall that by (2.23) and (2.29), this cross-product can be written as

$$\mathbb{E}_0 \left[(\xi \cdot X_t + \phi(X_t, \omega) - \phi(0, \omega)) \, (\phi(X_t, \omega) - \phi(0, \omega)) \right]. \tag{4.19}$$

By the Markov property and the stationarity of $(\omega(t))_{t \geqslant 0}$, it suffices to show that the derivative at time 0 of $\mathbb{E}_0 [M_t R_t]$ vanishes to prove (4.18). Using (2.12), this derivative is given by

$$\left\langle \sum_{z \sim 0} \omega_{0,z} \, (\xi \cdot z + \phi(z, \omega) - \phi(0, \omega)) \, (\phi(z, \omega) - \phi(0, \omega)) \right\rangle = \langle A(\xi + \nabla \phi) \cdot \nabla \phi \rangle \,,$$

and the latter vanishes identically by (2.4) (the fact that (4.19) vanishes is also clear from the alternative construction of the corrector based on orthogonal projections, as was done for instance in [MP07]).

This completes our sketch of the proof of the continuous-time analog of Theorem 4.2. For discrete time, we refer the reader to [GM13]. □

4.3.2. *Methods based on other functions of the random walk.* We now turn to numerical methods based on (4.4), and focus in this presentation on its continuous-time analog (2.18). We shall consider a special case of (2.18): for any bounded continuous $f : \mathbb{R}^d \to \mathbb{R}$,

$$\mathbb{E}_0\left[f\left(\frac{X_t}{\sqrt{t}}\right)\right] \xrightarrow[t\to+\infty]{} E[f(B_1)], \tag{4.20}$$

where B_1 is a Gaussian vector with covariance matrix $2A_{\mathrm{hom}}$. In the last paragraph, two important facts made the difference between the l.h.s. of (2.19) and its limit of order t^{-1}: (4.15) and (4.18). Both facts are indeed *specific* to the square function. Although we cannot prove this claim, we only expect the convergence in (4.20) to be of order $t^{-1/2}$ in general. We now recall the known upper bounds on the convergence in (4.20).

Theorem 4.3. *Let B_1 be a Gaussian vector with covariance matrix $2A_{\mathrm{hom}}$.*

(1) [Mo12c] *If f is smooth and bounded, then for any $\delta > 0$, there exist q, C such that*

$$\left|\mathbb{E}_0\left[f\left(\frac{X_t}{\sqrt{t}}\right)\right] - E[f(B_1)]\right| \leqslant C \left| \begin{array}{ll} t^{-1/4} & \text{if } d = 1, \\ \ln^q(t)\ t^{-1/4} & \text{if } d = 2, \\ t^{-1/2+\delta} & \text{if } d \geqslant 3. \end{array}\right. \tag{4.21}$$

(2) [Mo12b] *There exists q, C such that for any $\xi \in \mathbb{R}^d$,*

$$\sup_{x\in\mathbb{R}}\left|\mathbb{P}_0\left[\frac{\xi\cdot X_t}{\sqrt{t}} \leqslant x\right] - P\left[\frac{\xi\cdot B_1}{\sqrt{t}} \leqslant x\right]\right| \leqslant C \left| \begin{array}{ll} t^{-1/10} & \text{if } d = 1, \\ \ln^q(t)\ t^{-1/10} & \text{if } d = 2, \\ \ln(t)\ t^{-1/5} & \text{if } d = 3, \\ t^{-1/5} & \text{if } d \geqslant 4. \end{array}\right. \tag{4.22}$$

Part (2) of Theorem 4.3 considers the function $f(z) = \mathbf{1}_{\xi\cdot z\leqslant x}$, and is often referred to as a *Berry-Esseen* estimate.

For comparison, note that if X_t was replaced by a sum of i.i.d. centered random variables with finite third moment and covariance matrix $2A_{\mathrm{hom}}$, then the left-hand sides of (4.21) and (4.22) would both be $O(t^{-1/2})$ (see for instance [Pe, Theorem 5.5]). We believe that for $d = 2$, it is possible to refine the proof and replace the r. h. s. in (4.21) by $t^{-1/2+\delta}$, for any $\delta > 0$. The conjectured optimal rates in this inequality are

$$\left| \begin{array}{ll} t^{-1/4} & \text{if } d = 1, \\ \ln(t)\ t^{-1/2} & \text{if } d = 2, \\ t^{-1/2} & \text{if } d \geqslant 3. \end{array}\right. \tag{4.23}$$

Remark 4.4. To be precise, if X_t was replaced by a sum of i.i.d. centered random variables, say $Z_1, \ldots, Z_t$ ($t \in \mathbb{N}$ here), then the characteristic function of the normalized sum would satisfy (for any $\zeta \in \mathbb{R}$)

$$\mathbb{E}\left[\exp\left(i\zeta \frac{Z_1 + \cdots + Z_t}{\sqrt{t}}\right)\right] = \mathbb{E}\left[\exp\left(i\zeta \frac{Z_1}{\sqrt{t}}\right)\right]^t = \exp\left(-\frac{\zeta^2 \mathbb{E} Z_1^2}{2} - i\frac{\zeta^3 \mathbb{E} Z_1^3}{\sqrt{t}} + O(t^{-1})\right),$$

where we assumed that Z_1 has finite moments of order 4. The first term in the expansion gives the characteristic function of the limiting Gaussian random variable, and there is indeed a correction of order $t^{-1/2}$. But *this correction vanishes* in the special case when $\mathbb{E} Z_1^3 = 0$, and in particular if the distribution of Z_1 is invariant under the transformation $z \mapsto -z$. Numerical simulations suggest that similar cancellations may also occur for random walks in random environments, as we discuss below.

Sketch of proof of Theorem 4.3. In the case of general functions the two facts (4.15) and (4.18) we used for quadratic functions do not hold. Since $\mathbb{E}_0[R_t^2]$ grows at most logarithmically with t, the orthogonality property (4.18) can be replaced by the Cauchy-Schwarz inequality to control the cross-product $\mathbb{E}_0\left[M_t R_t\right]$ by $\sqrt{t}$ (up to a logarithmic correction for $d = 2$). Finding a substitute for (4.15) is more subtle. The identity (4.15) indeed holds regardless of whether the martingale M_t is actually close to a Brownian motion or not. For a generic function f however, it is no longer true that the difference

$$\left|\mathbb{E}_0\left[f\left(\frac{M_t}{\sqrt{t}}\right)\right] - E[f(B_1)]\right| \tag{4.24}$$

vanishes, and the proof of Theorem 4.3 requires to further control this quantity. Recall that the difference in (4.24) converges to 0 as a consequence of the convergence of $t^{-1}V_t$ in (2.26). The main two remaining main steps of the proof of Theorem 4.3 are as follows:

(i) estimate the speed at which the variance of $t^{-1}V_t$ tends to 0 (i.e. get an L^2 estimate on the speed of convergence in (2.26)), and

(ii) use a general quantitative version of the central limit theorem for martingales to turn the estimate obtained in (i) into an upper bound on (4.24).

At least for $d \geqslant 4$, our control of the variance of $t^{-1}V_t$ is optimal, and the reason for the not-so-intuitive exponent 1/5 appearing in part (2) of Theorem 4.3 is hidden in part (ii) of the proof, that is, in the general quantitative central limit theorem for martingales. Surprisingly, this general result is however optimal [Mo12a]. Yet, we conjecture that the exponents obtained in part (2) of Theorem 4.3 are not optimal, and that the rates obtained in part (1) of the theorem may in fact hold as well in part (2). □

4.4. **Numerical study.** We consider the Bernoulli example of Paragraph 3.3.1 of i.i.d. conductances taking values 1 and 4 with probability 1/2, and recall that $A_{\mathrm{hom}}^{\mathrm{disc}}$ is necessarily a multiple of the identity. For $d = 2$, Dykhne's formula yields $A_{\mathrm{hom}} = 2\,\mathrm{Id}$, and thus by (4.3), $A_{\mathrm{hom}}^{\mathrm{disc}} = 1/5\,\mathrm{Id}$. For $d = 3$, there is no closed formula and we approximate $A_{\mathrm{hom}}^{\mathrm{disc}}$ using periodization in law, cf. Paragraph 3.2.3.

In practice, to simulate the random walk, we generate the environment along its trajectory only. The conductances are generated on the fly. When the value of a conductance is needed, we check whether it has been generated at a previous time, and if not, it is generated. Roughly speaking, the walk up to time n discovers of order n conductances, independently of the dimension $d \geqslant 2$ (except for a logarithmic correction in dimension 2).

The methods based on simulating random walks have two main interesting features. First, their efficiency and cost are fairly insensitive to dimension. Second, the computations

n	10	20	40	80	160	320	640	1280	∞
Variance	0.40	0.39	0.380	0.373	0.369	0.367	0.3653	0.3647	0.3632

TABLE 7. Numerical estimates of (4.26) and theoretical limiting value in dimension 2.

n	10	20	40	80	160	320	640	1280	∞
Variance	0.20	0.19	0.188	0.186	0.184	0.184	0.1836	0.1835	0.1829

TABLE 8. Numerical estimates of (4.26) and theoretical limiting value (computed with a numerical approximation of $A_{\mathrm{hom}}^{\mathrm{disc}}$ by periodization) in dimension 3.

ca be done in parallel, since each *independent* random walk evolves in its own *independent* environment.

4.4.1. *Method based on the mean square displacement.* We start by investigating empirically the method based on the mean square displacement of the random walk. As for the methods based on the corrector, we investigate separately the statistical and systematic errors, that is, the two terms in the sum (4.10). For the statistical error, we focus on

$$\mathbb{E}_0^{\otimes}\left[\left(\hat{A}_k(n) - n^{-1}\tilde{\mathbb{E}}_0\left[(\xi\cdot Y_n)^2\right]\right)^2\right] = \mathbb{V}\mathrm{ar}\left[\hat{A}_k(n)\right],$$

where we write $\mathbb{V}\mathrm{ar}\left[\cdot\right]$ for the variance with respect to the measure $\mathbb{P}_0^{\otimes}$. Since $\hat{A}_k(n)$ is a sum of independent random variables, we have

$$\mathbb{V}\mathrm{ar}\left[\hat{A}_k(n)\right] = \frac{1}{k}\mathbb{V}\mathrm{ar}\left[\frac{p(\omega)}{\langle p\rangle}\left(\frac{\xi\cdot Y_n}{\sqrt{n}}\right)^2\right]. \tag{4.25}$$

A simple variant of the proof of (4.13) shows that

$$\lim_{n\to+\infty}\mathbb{V}\mathrm{ar}\left[\frac{p(\omega)}{\langle p\rangle}\left(\frac{\xi\cdot Y_n}{\sqrt{n}}\right)^2\right] = \mathsf{v},$$

where v is as in (4.14). Table 7 displays the empirical estimates in dimension 2 of

$$\mathbb{V}\mathrm{ar}\left[\frac{p(\omega)}{\langle p\rangle}\left(\frac{\xi\cdot Y_n}{\sqrt{n}}\right)^2\right] \tag{4.26}$$

for several values of n, and the predicted limiting value. As (4.25) shows, the variance of the estimator $\hat{A}_k(n)$ is obtained by dividing this value by the number k of walks we run. Table 8 displays the same results in dimension 3.

For the systematic error, the theoretical prediction is given by (4.12). To investigate empirically the validity of (4.12), we have computed $\hat{A}_{k_n}(n)$ with $k_n = K(n)n^2$, where $K(n)$ is some large number. This choice of k_n ensures that the random fluctuations are

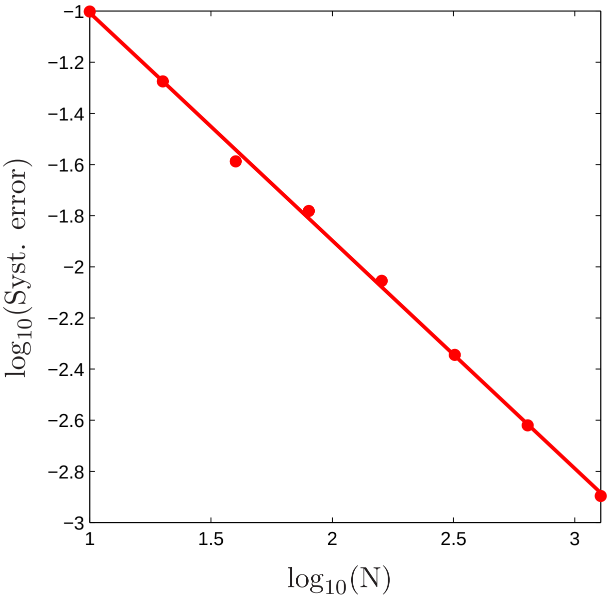

FIGURE 10. Systematic error for $d = 2$, rate 0.89 and prefactor 0.77.

of higher order, so that $\hat{A}_{k_n}(n)$ is very close to its expectation. In practice, we chose $K(n) = 10^4$ for $n \leqslant 320$, and $K(n) = 10^3$ for larger values.

For $d = 2$, the results are reported on in Figure 10. In this case, the theoretical prediction in (4.12) contains a polylogarithmic correction to $1/n$. We conjecture that the systematic error indeed scales as $\ln(n)/n$ (as can be proved for the continuous-time random walk). On the log-log plot, this would yield a correction to the expected slope -1 of the order of $1/\ln(n)$, which is between 0.17 and 0.14 for n between 320 and 1280, and corresponds rather well with the empirical slope.

For $d = 3$, the results are reported on in Figure 11. The empirical estimates match very well with the predicted convergence in $1/n$.

4.4.2. *Methods based on other functions of the random walk.* We finally turn to methods based on other functions of the final position of the random walk than the squared displacement. For any reasonable function f, we can devise an estimator (as we did for $f(x) = (\xi \cdot x)^2$):

$$\hat{A}^f_k(n) := \frac{1}{k\,\langle p\rangle} \sum_{i=1}^{k} p(\omega^{(i)}) f(Y^{(i)}_n/\sqrt{n}). \tag{4.27}$$

We have

$$\mathbb{E}^{\otimes}_0[\hat{A}^f_k(n)] = \tilde{\mathbb{E}}_0[f(Y_n/\sqrt{n})],$$

which (for suitable f) converges to $E[f(B_1)]$, where B_1 is a Gaussian vector with covariance matrix $2A^{\text{disc}}_{\text{hom}}$. Since this more general estimator is still a sum of i.i.d. random variables, the statistical error is easy to understand, as we have

$$\mathbb{V}\text{ar}\left[\hat{A}^f_k(n)\right] = \frac{1}{k}\mathbb{V}\text{ar}\left[\frac{p(\omega)}{\langle p\rangle} f\left(\frac{\xi \cdot Y_n}{\sqrt{n}}\right)\right],$$

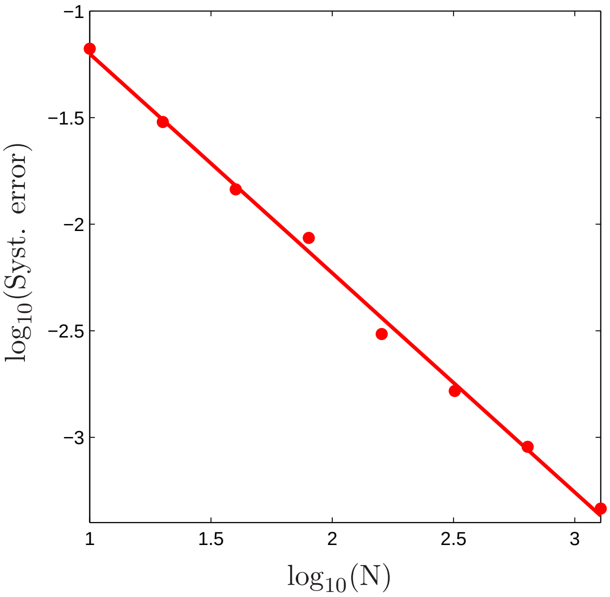

FIGURE 11. Systematic error for $d = 3$, rate 1.03 and prefactor 0.67.

where the last variance converges (for suitable f) to a constant that can be explicitely written. We now focus on the systematic error, that is, the difference between $\tilde{\mathbb{E}}_0[f(Y_n/\sqrt{n})]$ and the limiting value $E[f(B_1)]$. Based on the analogy with the continuous-time case, we expect the systematic error to decay as $n^{-1/2}$ for $d \geqslant 2$, possibly with a logarithmic correction in dimension 2.

In order to test this prediction, we consider the function

$$f(x) = \exp\left(-\frac{\|x\|_2^2}{2}\right). \tag{4.28}$$

Recall that $2A_{\text{hom}}^{\text{disc}} = \sigma^2 \,\text{Id}$ with $\sigma^2 = 2/5$ for $d = 2$. A simple computation shows that in this case and for f defined in (4.28), the limiting value of the variance is given by

$$E[f(B_1)] = (\sigma^2 + 1)^{-d/2},$$

which is equal to $5/7$ for $d = 2$ (and can be approximated by periodization for $d = 3$).

The empirical systematic errors are displayed on Figures 12 and 13 for $d = 2$ and $d = 3$, respectively.

Surprisingly, the observed convergence rates are far better than the predicted ones, being close to 1 in both cases instead of the predicted 1/2. Similar rates where observed for other choices of the function f. We believe that these surprising rates are due to ungeneric cancellations. As discussed in Remark 4.4, such cancellations also occur for sums of i.i.d. random variables in some specific cases, and in particular when the distribution of the random variables is invariant under the transformation $z \mapsto -z$. In the regime of small ellipticity ratio (that is, when β/α close to 1) already considered in this contribution, one indeed observes in the asymptotic expansion that the first contribution is of order $t^{-1/2}$ followed by a contribution of order t^{-1}. If in addition the distribution is invariant under the transformation $z \mapsto -z$, then the prefactor in front of $t^{-1/2}$ vanishes, so that the

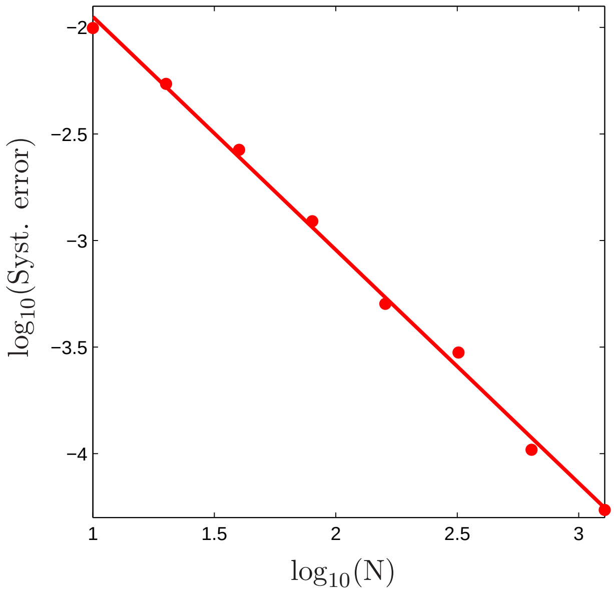

FIGURE 12. The systematic error in two dimensions for f as in (4.28), rate 1.09 and prefactor 0.14.

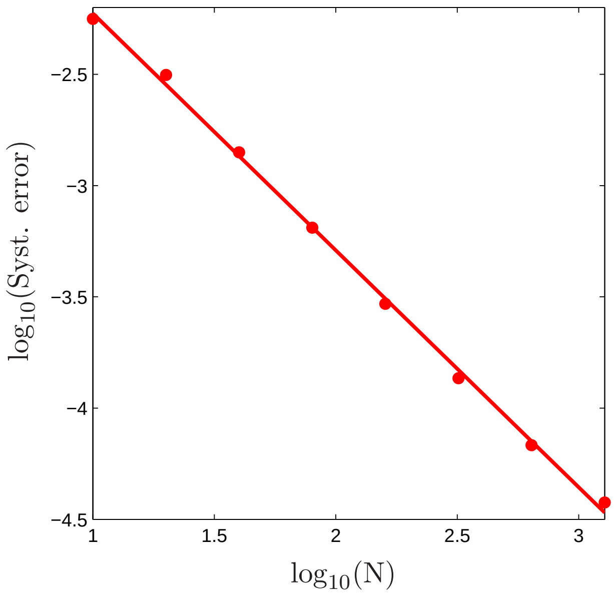

FIGURE 13. The systematic error in three dimensions for f as in (4.28), rate 1.06 and prefactor 0.07.

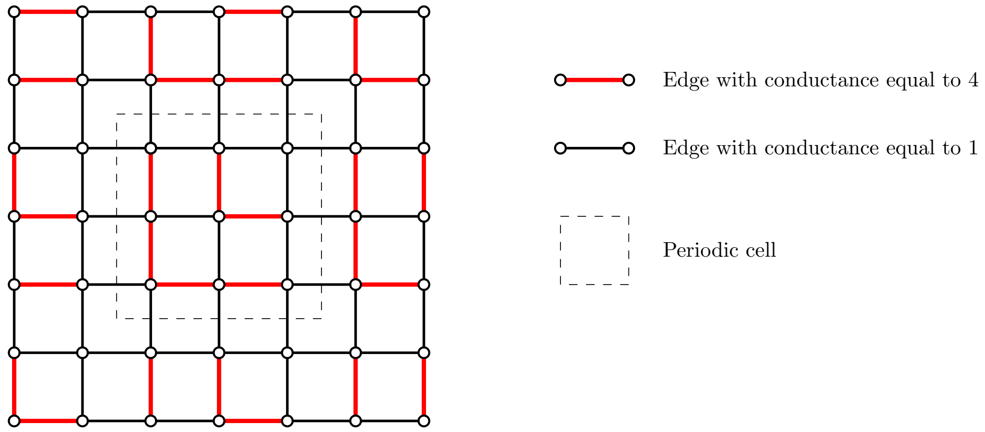

Figure 14. Periodic environment, without $z \mapsto -z$-invariance

leading order term is of order t^{-1}, as in the numerical experiments. In view of these two facts, we believe that the convergence rates observed on Figures 12 and 13 are not generic, and due to the invariance of the distribution of the conductances under the transformation $z \mapsto -z$.

In order to illustrate that the convergence rates observed are non-generic, we turn to a periodic environment that is not symmetric under the transformation $z \mapsto -z$. A periodic environment should provide better convergence rates than any generic and truly random environment (in any dimension). We consider the 3-periodic cell displayed on Figure 14 and take $f(x,y) = \sin(x)$, so that $\tilde{\mathbb{E}}_0[f(Y_n/\sqrt{n})]$ tends to 0 as n tends to infinity (and the knowledge of the homogenized matrix is not needed). The results are reported on in Figure 15. As expected, the empirical convergence rate is 1/2.

To conclude this paragraph, we investigate the convergence rates for the non-smooth function

$$f(x) = \mathbf{1}_{\xi \cdot x \leqslant z}, \tag{4.29}$$

where ξ is the first vector of the canonical basis and $z = 1/2$ or $z = 1/4$. For the systematic error, Theorem 4.3 predicts a convergence rate of 1/10 in dimension 2, and of 1/5 in dimension 3, up to logarithmic corrections. We believe that the exponent can be pushed to 1/5 in dimension 2 with a refined argument, but the proof cannot be pushed to higher exponents [Mo12a]. The aim of these empirical investigations is to check whether the exponent 1/5 is sharp. The results are displayed on Figure 16 for $d = 2$, and on Figure 17 for $d = 3$. While the onset of a nice asymptotic regime is delayed, the results suggest that the convergence rates ultimately settle to a behavior similar to that observed on Figures 12 and 13, that is, close to the value 1.

5. Conclusion

In this article we have recalled qualitative and quantitative results on stochastic homogenization of discrete linear elliptic PDEs and of random walks in random environments on $\mathbb{Z}^d$. This has allowed us to make a rather complete picture of numerical methods to approximate homogenized coefficients, based both on the corrector equation and on the random walk. Numerical tests have confirmed the sharpness of the analysis, supported some conjectures, and put some interesting phenomena into evidence (such as ungenerically fast

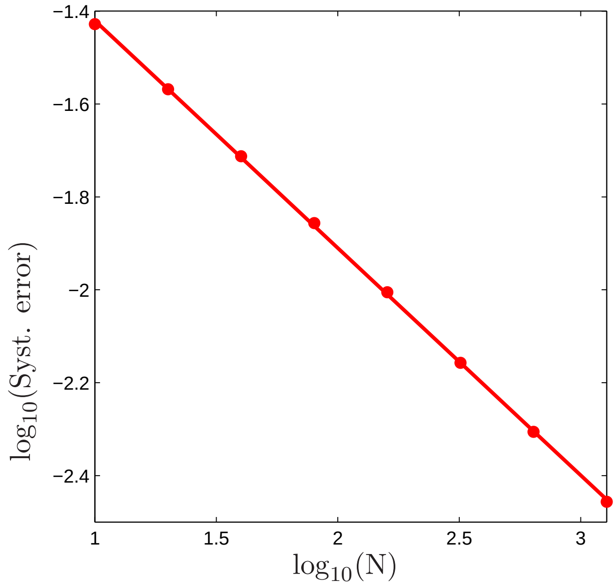

FIGURE 15. Systematic error, periodic environment, $f(x, y) = \sin(x)$, rate 0.49 and prefactor 0.12.

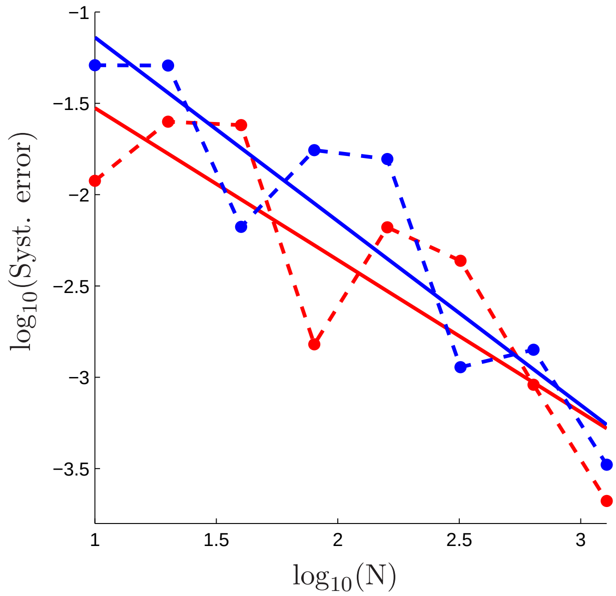

FIGURE 16. The systematic error in two dimensions for f as in (4.29) and $z = 1/2$ (red), rate 0.8 and prefactor 0.2, or $z = 1/4$ (blue), rate 1.0 and prefactor 0.7.

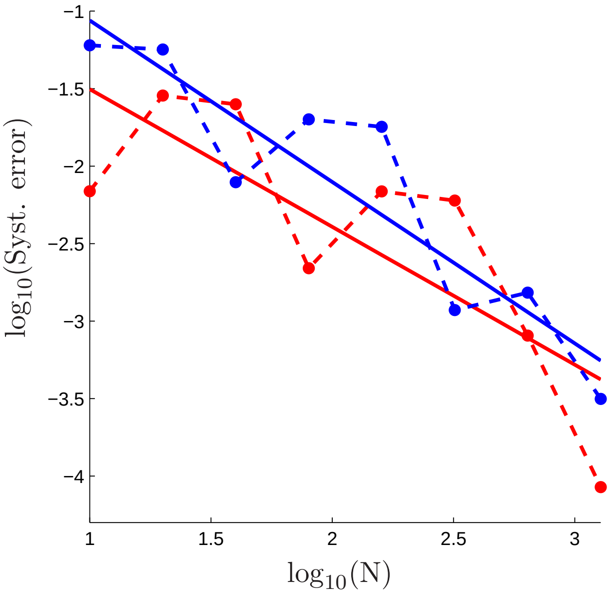

FIGURE 17. The systematic error in three dimensions for f as in (4.29) and $z = 1/2$ (red), rate 0.9 and prefactor 0.2, or $z = 1/4$ (blue), rate 1.0 and prefactor 1.0.

decay rates due to specific symmetries of the environment). We hope this contribution will help mathematicians identify challenging conjectures, and help practitioners make mathematically-based choices on the method to use in more concrete cases.

We have only considered discrete elliptic equations. The discrete case has the advantage of being numerically inexpensive to simulate compared to the case of continuum linear elliptic equations (for which we have to appeal to approximation methods such as the finite element, finite difference or finite volume methods). The extension of the results of this paper to the continuum case is currently under investigation, and [GO11, GO12] have already been extended to the continuum case [GO14a, GO14b]. In the continuous setting, the analog of the RWRE is a diffusion process. The extension of the results presented here to this setting is yet to be done. We hope to address these issues in future works.

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A.-C. Egloffe, Laboratoire MAP5, Université Paris Descartes, France
E-mail address: `anne-claire.egloffe@parisdescartes.fr`

A. Gloria, Université Libre de Bruxelles (ULB), Brussels, Belgium, and Project-team MEPHYSTO, INRIA Lille - Nord Europe, Villeneuve d'Ascq, France
E-mail address: agloria@ulb.ac.be

J.-C. Mourrat, Unité de mathématiques pures et appliquées - UMR 5669 - UMPA, Ecole Normale Supérieure de Lyon, France
E-mail address: jean-christophe.mourrat@ens-lyon.fr

T. N. Nguyen, Faculty of Mathematics - Statistics, Ton Duc Thang University, Vietnam
E-mail address: ntnhan@itam.tdt.edu.vn