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Symmetric Simple Exclusion Process: Regularity of the Self-Diffusion Coefficient

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Dedicated to Joel Lebowitz on his seventieth birthday

Abstract: We prove that the self-diffusion coefficient of a tagged particle in the symmetric exclusion process in Z^d, which is in equilibrium at density α, is of class C^∞ as a function of α in the closed interval [0, 1]. The proof provides also a recursive method to compute the Taylor expansion at the boundaries.

1. Introduction

In the course of the study of macroscopic behavior of large particle systems, effective diffusion coefficients which are functions of the parameters (associated to the conserved quantities) that define the equilibrium measures of the system often appear. These diffusion coefficients are usually expressed in terms of integrals of time correlations functions (Green–Kubo formulas), or through (infinite dimensional) variational formulas. They also appear as coefficients in the diffusive equations that govern the non-equilibrium evolution of the conserved quantities of the system. In order to study the existence and regularity of solutions to these equations it is important to establish first the regularity of these diffusion coefficients as functions of the parameters.

In this article we develop a method for proving smooth dependence, on the density, of the self diffusion coefficient of a tagged or tracer particle in symmetric simple exclusion particle systems that are in equilibrium. It is based on the duality properties of the symmetric simple exclusion process. This method, with modifications, can also be applied to study the smooth dependence on the density of other diffusion coefficients that arise in the study of more general simple exclusion processes. But this will be taken up elsewhere.

The paper is organized along the following lines. In Sect. 2 we introduce the notation and state the main theorem. In Sect. 3 we describe the generalized duality and discuss

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several operators and norms that appear in the dual representation. Section 4 is devoted to some key estimates that are used in Sect. 5 to prove the main result on the smoothness of the self diffusion coefficient of the tagged particle in the case of the symmetric simple exclusion process. At the end, in Remark 5.3, we expose a recursive method to compute the Taylor expansion at the boundaries.

Very few results exist at the present time about the regularity of diffusion coefficients. Continuous dependence on the density has been established in different contexts (cf. [2]). Generally proving continuity does not seem to be considerably harder than establishing the existence of a diffusion coefficient. In [6], Lipschitz continuity of the selfdiffusion coefficient for the tagged particle in the symmetric simple exclusion is proved in dimensions $d \geq 3$.

2. Notation and Results

Let us fix a symmetric finite-range probability distribution $p(\cdot)$ on $\mathbb{Z}^d$. Consider the symmetric simple exclusion process associated with p. We assume, without loss of generality, that the subgroup generated by the support of p is all of $\mathbb{Z}^d$. In addition we assume that we are not dealing with the trivial situation of $d = 1$ and $p(\pm 1) = \frac{1}{2}$, i.e. the one dimensional nearest neighbor case where the self diffusion coefficient is identically zero.

The simple exclusion process is the Markov process on $\mathcal{X} = \{0, 1\}^{\mathbb{Z}^d}$ whose generator L acts on cylinder functions f as

$$\begin{aligned} (Lf)(\eta) &= \sum_{x,y \in \mathbb{Z}^d} p(y-x)\eta(x)[1-\eta(y)][f(\sigma^{x,y}\eta) - f(\eta)] \\ &= \frac{1}{2} \sum_{x,y \in \mathbb{Z}^d} p(y-x)[f(\sigma^{x,y}\eta) - f(\eta)]. \end{aligned} \tag{2.1}$$

Here and below the configurations of $\mathcal{X}$ are denoted by Greek letters. In particular, for x in $\mathbb{Z}^d$, $\eta(x)$ is equal to 1 if the site x is occupied in the configuration η and is equal to 0 if it is not. Moreover, for a configuration η and x, y in $\mathbb{Z}^d$, $\sigma^{x,y}\eta$ is the configuration obtained from η by exchanging the occupation variables $\eta(x), \eta(y)$:

$$(\sigma^{x,y}\eta)(z) = \begin{cases} \eta(y) & \text{if } z = x, \\ \eta(x) & \text{if } z = y, \\ \eta(z) & \text{otherwise.} \end{cases} \tag{2.2}$$

Fix $0 \leq \alpha \leq 1$ and denote by μ_α the Bernoulli product measure on $\mathcal{X}$. This is the probability measure on $\mathcal{X}$ obtained by placing a particle with probability α at each site x, independently from the other sites. It easy to check that the one-parameter family of probability measures $\{\mu_\alpha,\ 0 \leq \alpha \leq 1\}$ are stationary, reversible and ergodic for the Markov process with generator L.

We examine in this article the evolution of a single tagged particle in the symmetric simple exclusion process. Let η be an initial configuration with a particle at the origin, i.e. with $\eta(0) = 1$. Tag this particle and denote by η_t (resp. X_t) the state of the process (resp. the position of the tagged particle) at time t. We shall refer to η_t as the environment. Let ξ_t be the state of the environment as seen from the tagged particle: $\xi_t = \theta_{X_t}\eta_t$. Here, for x in $\mathbb{Z}^d$ and a configuration η, θ_x stands for the translation of η by x, i.e.

$(\theta_x\eta)(y) = \eta(x+y)$. Notice that the origin is always occupied (by the tagged particle) for the environment as seen from the tagged particle. For this reason, we shall consider the process ξ_t as taking values in $\{0,1\}^{\mathbb{Z}^d_*}$, where $\mathbb{Z}^d_* = \mathbb{Z}^d\backslash\{0\}$.

Whereas X_t is not a Markov process due to the presence of the environment, (X_t, ξ_t) and ξ_t are. A simple computation shows that the generator $\mathcal{L}$ of the Markov process ξ_t is given by $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_\tau$, where

$$\begin{aligned}(\mathcal{L}_0 f)(\xi) &= \sum_{x,y\in\mathbb{Z}^d_*} p(y-x)\xi(x)[1-\xi(y)][f(\sigma^{x,y}\xi) - f(\xi)],\\ &= \frac{1}{2}\sum_{x,y\in\mathbb{Z}^d_*} p(y-x)[f(\sigma^{x,y}\xi) - f(\xi)],\\ (\mathcal{L}_\tau f)(\xi) &= \sum_{z\in\mathbb{Z}^d_*} p(z)[1-\xi(z)][f(\tau_z\xi) - f(\xi)].\end{aligned} \tag{2.3}$$

The first part of the generator takes into account the jumps in the environment, while the second one corresponds to jumps of the tagged particle. In the above formula, $\tau_z\xi$ stands for the configuration where the tagged particle, sitting at the origin, is first transferred to the (empty) site z and then the entire environment is translated by $-z$: for all y in $\mathbb{Z}^d_*$,

$$(\tau_z\xi)(y) = \begin{cases}\xi(z) & \text{if } y = -z,\\ \xi(y+z) & \text{for } y \neq -z.\end{cases}$$

For $0 \le \alpha \le 1$, denote by μ_α the Bernoulli product measure on $\mathcal{X}_* = \{0,1\}^{\mathbb{Z}^d_*}$. A simple computation shows that μ_α is a reversible and ergodic stationary measure for the Markov process ξ_t.

In this context Kipnis and Varadhan ([1]) proved a central limit theorem for the position of the tagged particle starting with an initial environment chosen randomly from the equilibrium μ_α. They showed that $\varepsilon X_{t\varepsilon^{-2}}$ converges, as $\varepsilon \downarrow 0$, to a Brownian motion with diffusion coefficient $D(\alpha)$ which we will describe in more detail in the next section.

This result has been generalized by Varadhan ([6]) to the asymmetric case with 0-mean ($\sum_y yp(y) = 0$). More recently, for the general asymmetric case in dimension $d \ge 3$, if $\sum_y yp(y) = m \neq 0$, in Sethuraman-Varadhan-Yau ([5]) it is proved that $\varepsilon[X_{t\varepsilon^{-2}} - mt(1-\alpha)\varepsilon^{-2}]$ converges, as $\varepsilon \downarrow 0$, to a Brownian motion with another diffusion coefficient.

In this article we limit ourselves to the symmetric case and study the regularity properties of $D(\alpha)$ as a function of α. The main result is

Theorem 2.1. *The self-diffusion coefficient $D(\alpha)$, as a function of α, is of class C^∞ in the closed interval* $[0,1]$.

3. Generalized Duality

The proof of Theorem 2.1 relies on the duality properties of the symmetric exclusion process that we will now describe.

We have the Hilbert space $L_2(\mu_\alpha)$ with its natural inner product $\langle\cdot,\cdot\rangle_\alpha$. The operator $\mathcal{L}$ is self adjoint and the natural Dirichlet inner products will be denoted by

$$\langle f, g\rangle_{1,\alpha} = \langle -\mathcal{L} f, g\rangle_\alpha \,,$$
$$\langle f, g\rangle_{1,env,\alpha} = \langle -\mathcal{L}_0 f, g\rangle_\alpha \,.$$

The dual norms $\|f\|_{-1,\alpha}$ and $\|f\|_{-1,env,\alpha}$ are defined by

$$\|f\|^2_{-1,\alpha} = \sup_g \Big\{ 2\,\langle f, g\rangle - \langle g, g\rangle_{1,\alpha} \Big\},$$
$$\|f\|^2_{-1,env,\alpha} = \sup_g \Big\{ 2\,\langle f, g\rangle - \langle g, g\rangle_{1,env,\alpha} \Big\}.$$

For each $n \geq 0$, denote by $\mathcal{E}_{*,n}$ the subsets of $\mathbb{Z}^d_*$ with n points and let $\mathcal{E}_* = \cup_{n\geq 0}\mathcal{E}_{*,n}$ be the class of all finite subsets of $\mathbb{Z}^d_*$. Let us consider an abstract Hilbert space $\mathfrak{H}$ with a complete orthonormal basis consisting of $\{\mathfrak{e}_A : A \in \mathcal{E}_*\}$. The space $\mathfrak{H}$ can be viewed as the space of square summable maps $\mathfrak{f}$ of $\mathcal{E}_* \to \mathbb{R}$. In a natural way $\mathfrak{H} = \oplus_{n\geq 0}\mathfrak{G}_n$, where $\mathfrak{G}_n$ is spanned by $\{\mathfrak{e}_A : A \in \mathcal{E}_{*,n}\}$. For each A in $\mathcal{E}_*$, let the local function in $L_2(\mu_\alpha)$ be defined by

$$\Psi_A = \Psi_A(\alpha, \xi) = \prod_{x\in A} \frac{\xi(x) - \alpha}{\sqrt{\chi(\alpha)}},$$

where $\chi(\alpha) = \alpha(1-\alpha)$. By convention, $\Psi_\phi = 1$. It is easy to check that $\{\Psi_A,\ A \in \mathcal{E}_*\}$ is an orthonormal basis of $L^2(\mu_\alpha)$. For each $n \geq 0$, denote by $\mathcal{G}_n$ the subspace of $L^2(\mu_\alpha)$ generated by $\{\Psi_A,\ A \in \mathcal{E}_{*,n}\}$, so that $L^2(\mu_\alpha) = \oplus_{n\geq 0}\mathcal{G}_n$. Functions of $\mathcal{G}_n$ are said to have degree n. The main property of the symmetric simple exclusion process that will be used here is that part of the generator, i.e. $\mathcal{L}_0$, preserves the degree of the functions.

Consider a local function f. Since $\{\Psi_A : A \in \mathcal{E}_*\}$ is a basis of $L^2(\mu_\alpha)$, we may write

$$f = \sum_{n\geq 0} \sum_{A\in\mathcal{E}_{*,n}} \mathfrak{f}(A)\Psi_A = \sum_{n\geq 0} \pi_n f.$$

Here we have denoted by π_n the orthogonal projection onto $\mathcal{G}_n$. Notice that the coefficients $\mathfrak{f}(A)$ depend not only on f but also on the density α: $\mathfrak{f}(A) = \mathfrak{f}(A, \alpha)$. Since f is a local function, $\mathfrak{f}\colon \mathcal{E}_* \to \mathbb{R}$ has finite support. In other words we have a unitary isomorphism, $f \sim \sum \mathfrak{f}(A)\mathfrak{e}_A$ between $L_2(\mu_\alpha)$ and $\mathfrak{H}$ that takes local functions in $L_2(\mu_\alpha)$ onto finite linear combinations of the basis elements. Of course this establishe also an isomorphism between $\mathcal{G}_n$ and $\mathfrak{G}_n$. We now conclude this section by expressing the operators $\mathcal{L}$ and $\mathcal{L}_0$ as well as their Dirichlet forms, through this isomorphism, in the basis $\{\mathfrak{e}_A\}$ of $\mathfrak{H}$. To begin with, because the isomorphism is unitary, we have

$$\langle f, g\rangle_\alpha = \langle \mathfrak{f}, \mathfrak{g}\rangle = \sum_{A\in\mathcal{E}_*} \mathfrak{f}(A)\mathfrak{g}(A),$$

where

$$f \sim \sum \mathfrak{f}(A)\mathfrak{e}_A \quad \text{and} \quad g \sim \sum \mathfrak{g}(A)\mathfrak{e}_A.$$

The norm in $\mathfrak{H}$ will be denoted by $\|\mathfrak{f}\|_0$.

For a subset A of $\mathbb{Z}^d_*$ and x, y in $\mathbb{Z}^d_*$, denote by $A_{x,y}$, $S_y A$ the sets defined by

$$A_{x,y} = \begin{cases} (A\backslash\{x\}) \cup \{y\} & \text{if } x \in A,\ y \notin A, \\ (A\backslash\{y\}) \cup \{x\} & \text{if } y \in A,\ x \notin A, \\ A & \text{otherwise;} \end{cases}$$
$$S_z A = \begin{cases} A - z & \text{if } z \notin A, \\ ((A\backslash\{z\}) - z) \cup \{-z\} & \text{if } z \in A. \end{cases} \tag{3.1}$$

In this formula, $B + z$ is the set $\{x + z;\ x \in B\}$. Therefore, to obtain $S_z A$ from A in the case where z belongs to A, we first remove z to get a set not containing z, then translate $A\backslash\{z\}$ by $-z$ and finally add the site $-z$.

Recall the definition of the generators $\mathcal{L}_0$, $\mathcal{L}_\tau$ given in (2.3). A simple computation shows that

$$(\mathcal{L}_0 f) \sim \sum_{A\in\mathcal{E}_*} (\mathfrak{L}_0\mathfrak{f})(A)\mathfrak{e}_A, \quad (\mathcal{L}_\tau f) \ \sim \ \sum_{A\in\mathcal{E}_*} (\mathfrak{L}_{\tau,\alpha}\mathfrak{f})(A)\mathfrak{e}_A,$$

where

$$(\mathfrak{L}_0\mathfrak{f})(A) = \frac{1}{2} \sum_{x,y\in\mathbb{Z}^d_*} p(y-x)[\mathfrak{f}(A_{x,y}) - \mathfrak{f}(A)] \tag{3.2}$$

and $\mathfrak{L}_{\tau,\alpha}$ is an operator which can be decomposed as

$$\mathfrak{L}_{\tau,\alpha} = \alpha\mathfrak{L}^1_\tau + (1-\alpha)\mathfrak{L}^2_\tau + \sqrt{\chi(\alpha)}(\mathfrak{L}^+_\tau + \mathfrak{L}^-_\tau),$$

where

$$\begin{aligned} (\mathfrak{L}^1_\tau\mathfrak{f})(A) &= \sum_{y\in A} p(y)[\mathfrak{f}(S_y A) - \mathfrak{f}(A)], \\ (\mathfrak{L}^2_\tau\mathfrak{f})(A) &= \sum_{y\notin A} p(y)[\mathfrak{f}(S_y A) - \mathfrak{f}(A)], \\ (\mathfrak{L}^+_\tau\mathfrak{f})(A) &= \sum_{y\in A} p(y)[\mathfrak{f}(A\backslash\{y\}) - \mathfrak{f}(S_y A\backslash\{-y\})], \\ (\mathfrak{L}^-_\tau\mathfrak{f})(A) &= \sum_{y\notin A} p(y)[\mathfrak{f}(A\cup\{y\}) - \mathfrak{f}(S_y A\cup\{-y\})]. \end{aligned} \tag{3.3}$$

Notice that $\mathcal{L}$ on $L_2(\mu_\alpha)$ is represented on $\mathfrak{H}$ by $\mathfrak{L}_\alpha = \mathfrak{L}_0 + \mathfrak{L}_{\tau,\alpha}$:

$$\mathfrak{L}_\alpha = \mathfrak{L}_0 + \alpha\mathfrak{L}^1_\tau + (1-\alpha)\mathfrak{L}^2_\tau + \sqrt{\chi(\alpha)}[\mathfrak{L}^+_\tau + \mathfrak{L}^-_\tau]. \tag{3.4}$$

We mentioned earlier that the main property to be exploited here is that the generator of the symmetric exclusion process preserves the degree of local functions. It is easy to check that the operators $\mathfrak{L}_0$, $\mathfrak{L}^1_\tau$, $\mathfrak{L}^2_\tau$ preserve the degree of a function, i.e. they map $\mathfrak{G}_n$ into itself. Moreover, $\mathfrak{L}^+_\tau$ increases the degree of a function by one while $\mathfrak{L}^-_\tau$ decreases it by one.

For a function $\mathfrak{f}\colon \mathcal{E}_* \to \mathbb{R}$ and $n \geq 0$, denote by $\pi_n\mathfrak{f}$ or by $\mathfrak{f}_n$ its restriction to $\mathcal{E}_{n,*}$: $(\pi_n\mathfrak{f})(A) = \mathfrak{f}(A)\mathbf{1}\{A \in \mathcal{E}_n\}$.

For local functions $f, g\colon \mathcal{X}_* \to \mathbb{R}$, a long but elementary computation shows that, if we define

$$
\begin{aligned}
2\,\langle \mathfrak{f}, \mathfrak{g}\rangle_{1,\alpha} &= \sum_{x,y\in\mathbb{Z}^d_*}\sum_{A\in\mathcal{E}} p(y-x)[\mathfrak{f}(A_{x,y})-\mathfrak{f}(A)][\mathfrak{g}(A_{x,y})-\mathfrak{g}(A)]\\
&+\sum_{y\in\mathbb{Z}^d_*}\sum_{A\in\mathcal{E}} p(y)r_y(A)[\mathfrak{f}(S_yA)-\mathfrak{f}(A)][\mathfrak{g}(S_yA)-\mathfrak{g}(A)] \qquad (3.5)\\
&-\sqrt{\chi(\alpha)}\sum_{y\in\mathbb{Z}^d_*}\sum_{\substack{A\in\mathcal{E}\\ y\notin A}} p(y)[\mathfrak{f}(S_yA)-\mathfrak{f}(A)][\mathfrak{g}(S_y[A\cup\{y\}])-\mathfrak{g}([A\cup\{y\}])]\\
&-\sqrt{\chi(\alpha)}\sum_{y\in\mathbb{Z}^d_*}\sum_{\substack{A\in\mathcal{E}\\ y\notin A}} p(y)[\mathfrak{f}(S_y[A\cup\{y\}])-\mathfrak{f}([A\cup\{y\}])][\mathfrak{g}(S_yA)-\mathfrak{g}(A)].
\end{aligned}
$$

with $r_y(A)$ is equal to α if y belongs to A and is equal to $1-\alpha$ if y does not belong to A, then

$$\langle f, g\rangle_{1,\alpha} = \langle \mathfrak{f}, \mathfrak{g}\rangle_{1,\alpha}$$

Notice that the last three terms can be recombined to give a positive expression when $\mathfrak{f} = \mathfrak{g}$. The corresponding norm will be denoted by $\|\mathfrak{f}\|_{1,\alpha}$ which of course is equal to $\|f\|_{1,\alpha}$. By completing the space of finitely supported functions with this norm we obtain the Dirichlet space $\mathfrak{H}_1$.

Let $\mathfrak{H}_{-1}$ be the dual of $\mathfrak{H}_1$ with respect to the standard inner product on $\mathfrak{H}$. This is the Hilbert space generated by finitely supported functions and the norm $\|\cdot\|_{-1,\alpha}$ defined by

$$\|\mathfrak{f}\|^2_{-1,\alpha} = \sup_{\mathfrak{g}}\Big\{2\,\langle \mathfrak{f}, \mathfrak{g}\rangle - \langle \mathfrak{g}, \mathfrak{g}\rangle_{1,\alpha}\Big\},$$

where the supremum is carried over all finitely supported functions $\mathfrak{g}$. It follows from the isomorphism that $\|f\|_{-1,\alpha} = \|\mathfrak{f}\|_{-1,\alpha}$.

The Dirichlet form corresponding to $\mathcal{L}_0$ is much simpler to calculate in the $\mathfrak{H}$ representation. Denote by $\|\cdot\|_{1,env}$ and $\|\cdot\|_{-1,env}$ respectively the Dirichlet norm and its dual associated to the generator $\mathfrak{L}_0$:

$$
\begin{aligned}
\|\mathfrak{g}\|^2_{1,env} &= \langle \mathfrak{g}, (-\mathfrak{L}_0)\mathfrak{g}\rangle\\
&= \frac{1}{2}\sum_{x,y\in\mathbb{Z}^d_*}\sum_{A\in\mathcal{E}} p(y-x)[\mathfrak{g}(A_{x,y})-\mathfrak{g}(A)]^2\\
&= \sum_{n\ge 0}\|\pi_n\mathfrak{g}\|^2_{1,env}
\end{aligned}
$$

and

$$
\begin{aligned}
\|\mathfrak{g}\|^2_{-1,env} &= \sup_{\mathfrak{f}}\Big\{2\,\langle \mathfrak{f}, \mathfrak{g}\rangle - \langle \mathfrak{f}, (-\mathfrak{L}_0)\mathfrak{f}\rangle\Big\}\\
&= \sum_{n\ge 0}\|\pi_n\mathfrak{g}\|^2_{-1,env},
\end{aligned}
\qquad (3.6)
$$

where the supremum is carried over all finitely supported functions. In contrast to the norms $\|\cdot\|_{1,\alpha}$, $\|\cdot\|_{-1,\alpha}$, the norms $\|\cdot\|_{1,env}$, $\|\cdot\|_{-1,env}$ do not depend explicitly on the parameter α. Moreover, since $\langle \mathfrak{f}, (-\mathfrak{L}_0)\mathfrak{f}\rangle \leq \langle \mathfrak{f}, (-\mathfrak{L}_\alpha)\mathfrak{f}\rangle$, it follows that $\|\mathfrak{g}\|_{1,env} \leq \|\mathfrak{g}\|_{1,\alpha}$ and $\|\mathfrak{g}\|_{-1,\alpha} \leq \|\mathfrak{g}\|_{-1,env}$. In Lemma 4.4, we estimate $\|\mathfrak{g}\|_{1,\alpha}$ and $\|\mathfrak{g}\|_{-1,env}$ in terms of $\|\mathfrak{g}\|_{1,env}$ and $\|\mathfrak{g}\|_{-1,\alpha}$, respectively.

Finally, for any $k \geq 0$, let us define

$$\begin{aligned} |||\mathfrak{f}|||_{0,k}^2 &= \sum_{n\geq 0} n^{2k}\|\pi_n\mathfrak{f}\|_0^2, \quad |||\mathfrak{f}|||_{1,k}^2 = \sum_{n\geq 0} n^{2k}\|\pi_n\mathfrak{f}\|_{1,env}^2, \\ |||\mathfrak{f}|||_{-1,k}^2 &= \sum_{n\geq 0} n^{2k}\|\pi_n\mathfrak{f}\|_{-1,env}^2. \end{aligned} \tag{3.7}$$

If T is the operator that acts as scalar multiplication by n on the space $\mathfrak{G}_n$ of degree n, these are the quadratic forms $\|T^k\mathfrak{f}\|^2$, $< T^k\mathfrak{f}, (-\mathfrak{L}_0)T^k\mathfrak{f} >$ and $< T^k\mathfrak{f}, (-\mathfrak{L}_0)^{-1}T^k\mathfrak{f} >$ respectively. Note that $\mathfrak{L}_0$ commutes with T. The completion under these norms will be denoted by $\mathfrak{H}_{0,k}$, $\mathfrak{H}_{1,k}$ and $\mathfrak{H}_{-1,k}$ respectively.

4. Some Estimates

Since $\mathfrak{L}_\alpha$ is self adjoint, for the solution $\mathfrak{u}_\lambda$ of the resolvent equation

$$\lambda\mathfrak{u}_\lambda - \mathfrak{L}_\alpha\mathfrak{u}_\lambda = \mathfrak{f}, \tag{4.1}$$

we have the basic estimate

$$\|\mathfrak{u}_\lambda\|_{1,\alpha} \leq \|\mathfrak{f}\|_{-1,\alpha}$$

that implies

$$\|\mathfrak{u}_\lambda\|_{1,env} \leq \|\mathfrak{f}\|_{-1,env}$$

or

$$|||\mathfrak{u}_\lambda|||_{1,0} \leq |||\mathfrak{f}|||_{-1,0}.$$

The following regularity result follows from Eq. (5.5) of [4].

Lemma 4.1. *Let $k \geq 1$ be given. Let $\mathfrak{f}$ be a function such that $|||\mathfrak{f}|||_{-1,k} < \infty$. For $\lambda > 0$, let $\mathfrak{u}_\lambda$ be the solution of the resolvent equation* (4.1). *Then,*

$$|||\mathfrak{u}_\lambda|||_{1,k} \leq C(k)|||\mathfrak{f}|||_{-1,k} \tag{4.2}$$

for a finite constant $C(k)$ independent of α and λ.

In fact the proof of (4.2) given in [4] extends immediately to non-local $\mathfrak{f}$.

We now state some bounds on the restrictions of $\mathfrak{L}_\tau^1$, $\mathfrak{L}_\tau^2$, $\mathfrak{L}_\tau^+$ and $\mathfrak{L}_\tau^2$ on $\mathfrak{G}_n$. These bounds will grow linearly with n. Notice that $\mathfrak{L}_\tau^j$, $j = 1, 2$ are symmetric operators, while $\mathfrak{L}_\tau^+$ is the adjoint of $\mathfrak{L}_\tau^-$:

$$\left\langle \mathfrak{L}_\tau^+\mathfrak{f}, \mathfrak{g}\right\rangle = \left\langle \mathfrak{f}, \mathfrak{L}_\tau^-\mathfrak{g}\right\rangle, \quad \left\langle \mathfrak{L}_\tau^j\mathfrak{f}, \mathfrak{g}\right\rangle = \left\langle \mathfrak{f}, \mathfrak{L}_\tau^j\mathfrak{g}\right\rangle$$

for $j = 1, 2$ and $\mathfrak{f}, \mathfrak{g}$ in $L^2(\mathcal{E}_*)$. Moreover,

$$\begin{aligned} \left\langle \mathfrak{L}_\tau^1\mathfrak{f}, \mathfrak{f}\right\rangle &= (1/2) \sum_{A\in\mathcal{E}_*} \sum_{y\in A} p(y)[\mathfrak{f}(S_yA) - \mathfrak{f}(A)]^2, \\ \left\langle \mathfrak{L}_\tau^2\mathfrak{f}, \mathfrak{f}\right\rangle &= (1/2) \sum_{A\in\mathcal{E}_*} \sum_{y\notin A} p(y)[\mathfrak{f}(S_yA) - \mathfrak{f}(A)]^2. \end{aligned}$$

Lemma 4.2. *There exists a finite constant C_0 depending only on the transition probability p such that*

$$\left\langle (-\mathfrak{L}_\tau^j)\mathfrak{f}, \mathfrak{f} \right\rangle \le; C_0 n \left\langle (-\mathfrak{L}_0)\mathfrak{f}, \mathfrak{f} \right\rangle \tag{4.3}$$

for $j = 1, 2$, all $n \ge 1$ and all $\mathfrak{f}$ in $\mathfrak{H}_n$. Moreover

$$\left\langle (-\mathfrak{L}_\tau^\pm)\mathfrak{f}, \mathfrak{g} \right\rangle^2 \le C_0^2 n^2 \left\langle (-\mathfrak{L}_0)\mathfrak{f}, \mathfrak{f} \right\rangle \left\langle (-\mathfrak{L}_0)\mathfrak{g}, \mathfrak{g} \right\rangle \tag{4.4}$$

for all $n \ge 1$ and all $\mathfrak{f}$ in $\mathfrak{G}_n$, $\mathfrak{g}$ in $\mathfrak{G}_{n\pm 1}$. On the other hand for $j = 1, 2$,

$$\|\mathfrak{L}_\tau^j \mathfrak{f}\|_0^2 \le 4\|\mathfrak{f}\|_0^2 \quad \text{and} \quad \|\mathfrak{L}_\tau^\pm \mathfrak{f}\|_0^2 \le 4\|\mathfrak{f}\|_0^2 \tag{4.5}$$

for all $\mathfrak{f}$ in $\mathfrak{H}$.

Proof. The first estimate (4.3) follows immediately from Lemma 5.1 in [4].

We first prove that for all $\mathfrak{f}$, $\mathfrak{g}$ in $L^2(\mathcal{E}_*)$,

$$\left\langle \mathfrak{L}_\tau^\pm \mathfrak{f}, \mathfrak{g} \right\rangle^2 \le \left\langle (-\mathfrak{L}_\tau^1)\mathfrak{f}, \mathfrak{f} \right\rangle \left\langle (-\mathfrak{L}_\tau^2)\mathfrak{g}, \mathfrak{g} \right\rangle. \tag{4.6}$$

Fix $\mathfrak{f}$, $\mathfrak{g}$ in $L^2(\mathcal{E}_*)$. By the explicit formula for $\mathfrak{L}_\tau^+$, we have that

$$\left\langle (-\mathfrak{L}_\tau^+)\mathfrak{f}, \mathfrak{g} \right\rangle = \sum_y p(y) \sum_{A \ni y} \mathfrak{g}(A) \left\{ \mathfrak{f}(S_y A \backslash \{-y\}) - \mathfrak{f}(A \backslash \{y\}) \right\}.$$

Rewrite this expression as twice one half of it. In one of the pieces, we perform the change of variables $B = S_y A$, $z = -y$ to obtain that it is equal to

$$-(1/2) \sum_y p(y) \sum_{A \ni y} \mathfrak{g}(S_y A) \left\{ \mathfrak{f}(S_y A \backslash \{-y\}) - \mathfrak{f}(A \backslash \{y\}) \right\}.$$

Here we used the fact that $p(\cdot)$ is symmetric. Adding the two expressions we get that $\left\langle (-\mathfrak{L}_\tau^+)\mathfrak{f}, \mathfrak{g} \right\rangle$ is equal to

$$-(1/2) \sum_y p(y) \sum_{A \ni y} \left\{ \mathfrak{g}(S_y A) - \mathfrak{g}(A) \right\} \left\{ \mathfrak{f}(S_y (A \backslash \{y\})) - \mathfrak{f}(A \backslash \{y\}) \right\}.$$

By Schwarz's inequality, this expression is bounded above by

$$\frac{1}{4\beta} \sum_y p(y) \sum_{A \ni y} \left\{ \mathfrak{g}(S_y A) - \mathfrak{g}(A) \right\}^2 + \frac{\beta}{4} \sum_y p(y) \sum_{A \ni y} \left\{ \mathfrak{f}(S_y A \backslash \{-y\}) - \mathfrak{f}(A \backslash \{y\}) \right\}^2$$

for all $\beta > 0$. By the identities presented just before the statement of the lemma, the first term is $(1/2\beta) \left\langle (-\mathfrak{L}_\tau^1)\mathfrak{g}, \mathfrak{g} \right\rangle$. A change of variables $B = A - \{y\}$ shows that the second is bounded by $(\beta/2) \left\langle (-\mathfrak{L}_\tau^2)\mathfrak{f}, \mathfrak{f} \right\rangle$. Minimizing over β, we conclude the proof of (4.6).

We may now prove the second estimate of the lemma. Fix $n \geq 1$, and functions $\mathfrak{f}$ and $\mathfrak{g}$ of degree n and $n+1$, respectively. By (4.6), $\left\langle \mathfrak{L}_\tau^+ \mathfrak{f}, \mathfrak{g} \right\rangle^2$ is bounded above by $\left\langle (-\mathfrak{L}_\tau^1)\mathfrak{f}, \mathfrak{f} \right\rangle \left\langle (-\mathfrak{L}_\tau^2)\mathfrak{g}, \mathfrak{g} \right\rangle$. By the first part of the lemma, this product is bounded by

$$C_0^2 n^2 \left\langle (-\mathfrak{L}_0)\mathfrak{f}, \mathfrak{f} \right\rangle \left\langle (-\mathfrak{L}_0)\mathfrak{g}, \mathfrak{g} \right\rangle$$

This proves (4.4) for $\mathfrak{L}_\tau^+$. The proof for $\mathfrak{L}_\tau^-$ is similar.

The last estimate (4.5) is elementary and follows from Schwarz's inequality and the explicit formulas for the operators $\mathfrak{L}_\tau^1$, $\mathfrak{L}_\tau^2$, $\mathfrak{L}_\tau^+$, and $\mathfrak{L}_\tau^-$. □

Lemma 4.3. *For every $k \geq 0$, there exists a finite constant C_k such that for $j = 1, 2, +, -$,*

$$|||\mathfrak{L}_\tau^j \mathfrak{f}|||_{-1,k} \leq C_k |||\mathfrak{f}|||_{1,k+1},$$

so that $\mathfrak{L}_\tau^j$ maps $\mathfrak{H}_{1,k+1}$ boundedly into $\mathfrak{H}_{-1,k}$

Proof. Follows immediately from the preceding lemma. □

Lemma 4.4. *There exists a finite constant C_0 such that for all $n \geq 1$,*

$$\|\mathfrak{f}\|_{1,\alpha} \leq C_0 n \|\mathfrak{f}\|_{1,\text{env}}, \quad \|\mathfrak{f}\|_{-1,\text{env}} \leq C_0 n \|\mathfrak{f}\|_{-1,\alpha}$$

for all α in $[0, 1]$, and all $\mathfrak{f}$ in $\mathfrak{G}_n$.

Proof. Fix $n \geq 1$ and $\mathfrak{f}$ in $\mathfrak{G}_n$. By (3.5) and Schwarz's inequality, $< \mathfrak{f}, \mathfrak{f} >_{1,\alpha}$ is bounded above by

$$\|\mathfrak{f}\|_{1,\text{env}}^2 + 2 \sum_{A \in \mathcal{E}_*} \sum_{y \in \mathbb{Z}_*^d} p(y)[\mathfrak{f}(S_y A) - \mathfrak{f}(A)]^2 \\ + \sum_{A \in \mathcal{E}_*} \sum_{y \notin A} p(y)[\mathfrak{f}(S_y[A \cup \{y\}]) - \mathfrak{f}([A \cup \{y\}])]^2$$

because $|r_y(A)| \leq 1$ and $\chi(\alpha) \leq 1$. Since $\mathfrak{f}$ belongs to $\mathfrak{G}_n$, we may restrict the second sum to sets A in $\mathcal{E}_{n,*}$. A change of variables permits us to estimate the third sum by the second one. In conclusion,

$$\langle \mathfrak{f}, \mathfrak{f} \rangle_{1,\alpha} \leq \|\mathfrak{f}\|_{1,\text{env}}^2 + 3 \sum_{A \in \mathcal{E}_{*,n}} \sum_{y \in \mathbb{Z}_*^d} p(y)[\mathfrak{f}(S_y A) - \mathfrak{f}(A)]^2.$$

By Lemma 4.2, the second term on the right-hand side is less than or equal to $C_0 n \|\mathfrak{f}\|_{1,\text{env}}^2$ because $\mathfrak{f}$ belongs to $\mathfrak{G}_n$. The second estimate of the lemma is obtained by duality. □

5. The Self-Diffusion Coefficient

By [1], the self–diffusion coefficient $D(\alpha)$ in the direction v is given by the variational formula :

$$v \cdot D(\alpha)v = \inf_f \Big\{ \sum_{z\in\mathbb{Z}^d_*} p(z)E_{\mu_\alpha}\Big[[1-\xi(z)]\{v\cdot z - [f(\tau_z\xi) - f(\xi)]\}^2\Big] + \sum_{x,y\in\mathbb{Z}^d_*} p(x-y)E_{\mu_\alpha}\Big[\xi(x)[1-\xi(y)]\{f(\sigma^{x,y}\xi) - f(\xi)\}^2\Big]\Big\},$$

where the infimum is carried over all cylinder functions f. A simple computation shows that

$$v \cdot D(\alpha)v = (1-\alpha)\sum_{z\in\mathbb{Z}^d_*}(z\cdot v)^2 p(z) - \alpha(1-\alpha)\|f_v\|^2_{-1,\alpha} \tag{5.1}$$

for each v in $\mathbb{R}^d$. Here f_v is the cylinder function given by

$$f_v(\xi) = \frac{1}{\sqrt{\alpha(1-\alpha)}}\sum_{y\in\mathbb{Z}^d_*} p(y)(y\cdot v)[1-\xi(y)] = \frac{1}{\sqrt{\alpha(1-\alpha)}}\sum_{y\in\mathbb{Z}^d_*} p(y)(y\cdot v)[\alpha-\xi(y)]$$

because p has mean zero. With the notation introduced in the previous section, we may write f_v as

$$f_v(\xi) = -\sum_{y\in\mathbb{Z}^d_*}(y\cdot v)p(y)\Psi_y,$$

where $\Psi_z = \Psi_{\{z\}}$ for z in $\mathbb{Z}^d_*$.

We are now in a position to state the main result of this section. Theorem 2.1 follows from this result in view of formula (5.1).

Theorem 5.1. *As a function of* α, $\|f_v\|^2_{-1,\alpha}$ *is of class* C^∞ *on* $[0, 1]$.

The proof is based on the lemmas at the end of the previous section. To explain the strategy of the proof we introduce the resolvent equation associated to f_v: for $\lambda > 0$, denote by u_λ the solution of the resolvent equation:

$$\lambda u_\lambda - \mathcal{L}u_\lambda \ = \ f_v.$$

We will use the dual representation and carry out the estimates in $\mathfrak{H}$. Let $u_\lambda \sim \mathfrak{u}_\lambda$ through the unitary isomorphism. Of course $\mathfrak{u}_\lambda = \mathfrak{u}_\lambda(\alpha)$ depends on α,

$$f_v \sim \mathfrak{f}_v = -\sum_{z\in\mathcal{E}_*}(z\cdot v)p(z)\mathfrak{e}_{\{z\}}$$

is independent of α and is actually in $\mathfrak{H}_{-1}$. We have

$$\lambda\mathfrak{u}_\lambda(\alpha) - \mathfrak{L}_\alpha\mathfrak{u}_\lambda = \mathfrak{f}_v. \tag{5.2}$$

It follows from [1] that

$$\begin{aligned}\|f_v\|^2_{-1,\alpha} &= \lim_{\lambda\to 0}\langle f_v, u_\lambda\rangle_\alpha = -\lim_{\lambda\to 0}\sum_{z\in\mathbb{Z}^d_*}(z\cdot v)p(z)\mathfrak{u}_\lambda(\{z\},\alpha)\\ &= \lim_{\lambda\to 0}\ \frac{1}{2}\sum_{z\in\mathbb{Z}^d_*}(z\cdot v)p(z)\left[\mathfrak{u}_\lambda(\{-z\},\alpha)-\mathfrak{u}_\lambda(\{z\},\alpha)\right]\end{aligned} \tag{5.3}$$

because $p(\cdot)$ is symmetric. In view of this identity, to prove Theorem 5.1 we just need to show that there exists a subsequence $\lambda_k \downarrow 0$ such that, for each z with $p(z) > 0$, $\{\mathfrak{u}_{\lambda_k}(\alpha,\{z\}) - \mathfrak{u}_{\lambda_k}(\alpha,\{-z\}),\ k \geq 1\}$ converges uniformly in α to a smooth function. To prove the existence of such a subsequence, it is enough to show that the functions $\{\mathfrak{u}_\lambda(\alpha,\{z\})\}$ are smooth for each $\lambda > 0$ and, for each z and $j \geq 0$, to obtain the uniform bounds

$$\sup_{0<\lambda\leq 1}\ \sup_{0\leq\alpha\leq 1}\ |\mathfrak{u}^{(j)}_\lambda(\alpha,\{-z\}) - \mathfrak{u}^{(j)}_\lambda(\alpha,\{z\})| < \infty. \tag{5.4}$$

Here $\mathfrak{u}^{(j)}_\lambda$ stands for the j^{th} derivative of $\mathfrak{u}_\lambda$ with respect to the density α.

By Schwarz's inequality,

$$\left(\sum_z p(z)|\mathfrak{u}^{(j)}_\lambda(\alpha,\{-z\}) - \mathfrak{u}^{(j)}_\lambda(\alpha,\{z\})|\right)^2 \leq \sum_z p(z)[\mathfrak{u}^{(j)}_\lambda(\alpha,\{-z\}) - \mathfrak{u}^{(j)}_\lambda(\alpha,\{z\})]^2.$$

Since the support of p generates $\mathbb{Z}^d$, and we can exclude the one dimensional nearest neighbor case, there exists a path $z_0 = -z, z_1, \ldots, z_n = z$, avoiding 0, such that $p(z_{i+1} - z_i) > 0$ for $0 \leq i < n$. Rewriting the difference $\mathfrak{u}^{(j)}_\lambda(\alpha,\{-z\}) - \mathfrak{u}^{(j)}_\lambda(\alpha,\{z\})$ as $\sum_{0\leq i<n}\mathfrak{u}^{(j)}_\lambda(\alpha,\{z_{i+1}\}) - \mathfrak{u}^{(j)}_\lambda(\alpha,\{z_i\})$ and applying Schwarz's inequality, we prove that the previous expression is bounded above by

$$C_0\|\pi_1\mathfrak{u}^{(j)}_\lambda\|^2_{1,env} \leq C_0|||\mathfrak{u}^{(j)}_\lambda|||^2_{1,0}. \tag{5.5}$$

By (5.5), in order to prove (5.4) it is enough to obtain for each $j \geq 0$, the bound

$$\sup_{0<\lambda\leq 1}\ \sup_{0\leq\alpha\leq 1}\ |||\mathfrak{u}^{(j)}_\lambda|||_{1,0} < \infty.$$

Notice that the coefficients of $\mathfrak{L}_\alpha$ are not smooth at the boundary of [0, 1]. For this reason, we reparametrize the family of equations by $\alpha = \sin^2 t$, $t \in [0, \pi/2]$ to get

$$\mathfrak{L}(t) = \mathfrak{L}_0 + (\sin^2 t)\ \mathfrak{L}^1_\tau + (\cos^2 t)\ \mathfrak{L}^2_\tau + (\sin t\cos t)\ \left[\mathfrak{L}^+_\tau + \mathfrak{L}^-_\tau\right]$$

and consider the resolvent equation

$$\lambda\mathfrak{v}_\lambda(t) - \mathfrak{L}(t)\mathfrak{v}_\lambda(t) = \mathfrak{f}_v.$$

Since $\mathfrak{f}_v$ does not depend on α we have $\mathfrak{u}_\lambda(\alpha(t)) = \mathfrak{v}_\lambda(t)$. To prove that the sequences $\{\mathfrak{u}^{(j)}_\lambda(A,\alpha),\ \lambda > 0\}$, $j \geq 0$, are uniformly bounded in the $|||\cdot|||_{1,0}$ norm, we first prove such a statement for the sequences $\{\mathfrak{v}_\lambda^{(j)}(A,t),\ \lambda > 0\}$, $j \geq 0$. From this result and the relation between $\mathfrak{u}_\lambda$ and $\mathfrak{v}_\lambda$, t and α, we deduce boundedness in $\|\!|\cdot|\!\|_{1,0}$ norm of $\{\mathfrak{u}_\lambda^{(j)}(A,\alpha),\ \lambda > 0\}$ in the interior of the domain. An extra argument, presented at the end of the proof, extends the smoothness up to the boundary.

We start by observing that the function $\mathfrak{f}$ has finite $\mathfrak{H}_{-1,k}$ norm for all $k \geq 0$, i.e. there exists a finite constant C_0 such that

$$\|\!|\mathfrak{f}_v|\!\|_{-1,k} \leq C_0 \tag{5.6}$$

for all $k \geq 0$. The proof of this claim is elementary. Since $\mathfrak{f}_v$ has degree 1, $\|\!|\mathfrak{f}_v|\!\|_{-1,k} = \|\!|\mathfrak{f}_v|\!\|_{-1,0} = \|\mathfrak{f}_v\|_{-1,env}$ is finite as soon as $\|\mathfrak{f}\|_{-1,env}$ is finite. To prove that $\|\mathfrak{f}_v\|_{-1,env}$ is finite, recall the variational formula (3.6) for the $\|\cdot\|_{-1,env}$ norm and fix a finite supported function $\mathfrak{g}$. Since $\mathfrak{L}_0$ does not change the degree of a function and since $\mathfrak{f}_v$ has degree one, we may assume that $\mathfrak{g}$ has degree one. Since p is symmetric,

$$\langle \mathfrak{f}, \mathfrak{g}\rangle = \frac{1}{2}\sum_z p(z)(z\cdot v)[\mathfrak{g}(\{-z\}) - \mathfrak{g}(\{z\})].$$

By Schwarz's inequality, the square of this expression is bounded by

$$\frac{1}{4}\sum_z p(z)|(z\cdot v)|^2 \sum_z p(z)[\mathfrak{g}(\{-z\}) - \mathfrak{g}(\{z\})]^2.$$

Now we proceed as for the bound (5.5): there exists a path $z_0 = -z, z_1, \dots, z_n = z$, avoiding 0, such that $p(z_{i+1} - z_i) > 0$ for $0 \leq i < n$. Rewriting the difference $\mathfrak{g}(\{-z\}) - \mathfrak{g}(\{z\})$ as $\sum_{0\leq i<n} \mathfrak{g}(\{z_{i+1}\}) - \mathfrak{g}(\{z_i\})$ and applying Schwarz's inequality, we prove that the previous expression is bounded above by $C_0 < \mathfrak{g}, (-\mathfrak{L}_0\mathfrak{g}) >$, which proves the claim (5.6) in view of the variational formula (3.6) for the $\|\cdot\|_{-1,env}$ norm.

We now start our way through the proof that $\mathfrak{v}_\lambda$ is a sequence of smooth functions with bounded derivatives. Lemma 4.1 applied to $\mathfrak{f}$ shows that

$$\sup_{0<\lambda\leq 1}\ \sup_{0\leq t\leq \pi/2} \|\!|\mathfrak{v}_\lambda(t)|\!\|_{1,k}$$

is finite for all $k \geq 1$.

We now turn to the proof of the differentiability of $\mathfrak{v}_\lambda(\cdot)$. We say that a function $\mathfrak{g}(t)$ with values in $\mathfrak{H}$ is differentiable at t if $\gamma^{-1}[\mathfrak{g}(t+\gamma) - \mathfrak{g}(t)]$ converges, as $\gamma \downarrow 0$, strongly in $\mathfrak{H}$ to some function that we denote by $\mathfrak{g}'$. Notice that differentiating formally $\mathfrak{L}(t)$ in t we get the operator

$$\mathfrak{L}'(t) = (2\sin t\cos t)\ (\mathfrak{L}_\tau^1 - \mathfrak{L}_\tau^2) + (\cos^2 t - \sin^2 t)\ \left[\mathfrak{L}_\tau^- + \mathfrak{L}_\tau^+\right].$$

Lemma 5.2. *Suppose that* $\mathfrak{f}(t)$ *is a differentiable function of* t. *Let* $\mathfrak{u}_\lambda$ *be the solution of the resolvent equation*

$$\lambda\mathfrak{u}_\lambda(t) - \mathfrak{L}(t)\mathfrak{u}_\lambda(t) = \mathfrak{f}(t).$$

Then, $\mathfrak{u}_\lambda(t)$ *is differentiable and its derivative is the solution* $\mathfrak{u}_\lambda'(t)$ *of*

$$\lambda\mathfrak{u}_\lambda' - \mathfrak{L}(t)\mathfrak{u}_\lambda' = \mathfrak{f}'(t) + \mathfrak{L}'(t)\,\mathfrak{u}_\lambda. \tag{5.7}$$

Proof. The proof of the differentiability of $\mathfrak{u}_\lambda(t)$ is standard; all we need to control is that $\mathfrak{L}'(t)\mathfrak{u}_\lambda(t)$ is in $\mathfrak{H}$, which follows from (4.5) of Lemma 4.2 and the boundedness of the coefficients of $\mathfrak{L}'(t)$. □

The previous lemma applied to $\mathfrak{f} = \mathfrak{f}_v$ shows that the family of functions $\mathfrak{u}_\lambda$ is differentiable for each fixed λ and that the derivative $\mathfrak{u}'_\lambda$ satisfies some resolvent-type equation.

Proof of Theorem 5.1. We first show that $\{\mathfrak{u}_\lambda(t),\ \lambda > 0\}$ is a family of smooth functions whose derivatives satisfy for each $k \geq 0$,

$$\sup_{0<\lambda\leq 1}\ \sup_{0\leq t\leq \frac{\pi}{2}} \|\!|\mathfrak{u}'_\lambda(t)\|\!|_{1,k} < \infty. \tag{5.8}$$

By (5.6) $\|\!|\mathfrak{f}\|\!|_{-1,k}$ is bounded uniformly in t. Hence, by Lemma 4.1, $\|\!|\mathfrak{u}_\lambda\|\!|_{1,k}$ is bounded, uniformly in λ and t. Since $\mathfrak{f}$ does not depend on t, by Lemma 5.2, $\mathfrak{u}_\lambda$ is differentiable and its derivative $\mathfrak{u}'_\lambda$ satisfies

$$\lambda\mathfrak{u}'_\lambda\ -\ \mathfrak{L}(t)\mathfrak{u}'_\lambda = \mathfrak{L}'(t)\,\mathfrak{u}_\lambda .$$

By Lemma 4.3 and the explicit form of the operator $\mathfrak{L}(t)$,

$$\|\!|\mathfrak{L}'(t)\,\mathfrak{u}_\lambda\|\!|_{-1,k} \leq 2 \sum_{j=1,2,+,-} \|\!|\mathfrak{L}^j(t)\,\mathfrak{u}_\lambda\|\!|_{-1,k} \leq 8C_k\|\!|u_\lambda\|\!|_{1,k+1}$$

then by Lemma 4.1 $\|\!|\mathfrak{L}'(t)\,\mathfrak{u}_\lambda\|\!|_{-1,k}$ is bounded for each $k \geq 1$, uniformly in λ and t. We may therefore apply again Lemma 4.1 to show that $\|\!|\mathfrak{u}'_\lambda(t)\|\!|_{1,k}$ is uniformly bounded in (t, λ) for all $k \geq 1$.

To iterate the argument, we just need to prove by induction the existence of constants $\{a_{n,i},\ n \geq 1, 0 \leq i < n\}$ such that

$$\lambda\mathfrak{u}^{(j)}_\lambda\ -\ \mathfrak{L}(t)\mathfrak{u}^{(j)}_\lambda = \sum_{i=0}^{j-1} a_{j,i}\,\mathfrak{L}^{(j-i)}(t)\,\mathfrak{u}^{(i)}_\lambda, \tag{5.9}$$

where $\mathfrak{u}^{(i)}_\lambda$, $\mathfrak{L}^{(i)}(t)$ stands for the i^{th} derivative of $\mathfrak{u}_\lambda(t)$, $\mathfrak{L}(t)$. This is elementary and left to the reader.

The previous argument shows that $\mathfrak{u}_\lambda(t)$ is a sequence of smooth functions on $[0, 1]$ with their derivatives having the uniform bounds

$$\sup_{0<\lambda\leq 1}\ \sup_{0\leq t\leq \pi/2} \|\!|\mathfrak{u}^{(j)}_\lambda(t)\|\!|_{1,k} < \infty$$

for each $j \geq 0$. We have seen just after (5.3) that these uniform estimates guarantee the smoothness of $\|\mathfrak{f}\|_{-1,\alpha(t)}$ as a function of t defined in $[0, \pi/2]$. Since $\alpha = \sin^2 t$, this translates immediately into smoothness in α for $\alpha \in (0, 1)$. Regularity at the boundary requires the following extra argument.

We claim that the odd derivatives of $< \mathfrak{f}, \mathfrak{u}_\lambda(t) >$ vanish at $t = 0$ and $\pi/2$. We consider the case $t = 0$, the other being similar. To keep notation simple, let $U_\lambda(t) =< \mathfrak{f}, \mathfrak{u}_\lambda(t) >$. Since $\mathfrak{f}$ does not depend on α, for $j \geq 0$, $U^{(j)}_\lambda(0) = < \mathfrak{f}, \mathfrak{u}^{(j)}_\lambda(0) >$. Since $\mathfrak{f}$ is a function of degree 1, to prove that the odd derivatives of $U_\lambda(t)$ vanish at 0, it is enough to prove that $\mathfrak{u}^{(2j+1)}_\lambda(0)$ is a function of even degree. We prove this statement by induction on j.

Observe that $\mathfrak{L}(0) = \mathfrak{L}_0 + \mathfrak{L}_\tau^2$, which are operators that preserve the degree of a function. On the other hand, since $\sin^2 t$, $\cos^2 t$ are even functions and since $\sin t \cos t$ is an odd function, there exist constants a_j, b_j, c_j such that

$$\mathfrak{L}^{(2j)}(0) = a_j \mathfrak{L}_\tau^1 + b_j \mathfrak{L}_\tau^2, \quad \mathfrak{L}^{(2j+1)}(0) = c_j[\mathfrak{L}_\tau^+ + \mathfrak{L}_\tau^-]$$

for $j \geq 0$. In particular, while $\mathfrak{L}^{(2j)}(0)$ preserves the degree of a function, $\mathfrak{L}^{(2j+1)}(0)$ changes it by one.

To prove that $\mathfrak{u}_\lambda^{(2j+1)}(0)$ (resp. $\mathfrak{u}_\lambda^{(2j)}(0)$), $j \geq 0$, are functions of even (resp. odd) degree, notice first that $\mathfrak{u}_\lambda(0)$ is the solution of

$$[\lambda - (\mathfrak{L}_0 + \mathfrak{L}_\tau^2)]\mathfrak{u}_\lambda(0) = \mathfrak{f}.$$

Since $\mathfrak{f}$ is a function of degree 1, $\mathfrak{u}_\lambda(0)$ is also of degree 1. This proves the claim for $j = 0$. It is easy to conclude the proof by induction using formula (5.9) and the fact that $\mathfrak{L}^{(2j)}(0)$ preserves the degree, while $\mathfrak{L}^{(2j+1)}(0)$ changes it by one.

Since $\mathfrak{u}_\lambda^{(2j+1)}(0)$ are functions of even degree, $U_\lambda^{(2j+1)}(0) =< \mathfrak{f}, \mathfrak{u}_\lambda^{(2j+1)}(0) >$ vanishes because $\mathfrak{f}$ has degree one. Since we proved uniform convergence of a subsequence $\mathfrak{u}_{\lambda_k}(t)$ and its derivatives, the limit $U(t) = \|\mathfrak{f}\|_{-1,\alpha(t)}^2$ of $U_\lambda(\cdot)$ inherits these properties. In particular, $U^{2j+1}(0) = 0$. Elementary analytic considerations show that $U(t)$ is in fact a smooth function of t^2 and hence of $\sin^2 t = \alpha$. $\square$

Remark 5.3. The proof of the smoothness at the boundary provides a recursive method to compute the Taylor expansion at the origin of the diffusion coefficient. Recall that $U(t) = \|\mathfrak{f}\|_{-1,\alpha(t)}$. By Theorem 5.1, $U(0) = \lim_{\lambda\to 0} < \mathfrak{f}, \mathfrak{u}_\lambda(0) >= < \mathfrak{f}, \mathfrak{u}(0) >$, where $\mathfrak{u}(0)$ is the solution of

$$-[\mathfrak{L}_0 + \mathfrak{L}_\tau^2]\, \mathfrak{u}(0) = \mathfrak{f}. \tag{5.10}$$

Since $\mathfrak{f}$ has degree one and since $\mathfrak{L}_0$, $\mathfrak{L}_\tau^2$ preserve the degree, this equation can be solved in $\mathfrak{H}_1$. In this space both $\mathfrak{L}_0$, $\mathfrak{L}_\tau^2$ are essentially Laplace operators and this equation may be solved. Knowing $\mathfrak{u}(0)$, we may examine the equation

$$-[\mathfrak{L}_0 + \mathfrak{L}_\tau^2]\, \mathfrak{u}^{(1)}(0) = \mathfrak{L}^{(1)}(0)\mathfrak{u}(0).$$

As noticed earlier, the right hand side is a function of degree 0 and 2 so that $\mathfrak{u}^{(1)}(0)$ has this property. By induction we may obtain $\mathfrak{u}^{(j)}(0)$ for all $j \geq 1$ by inverting an operator which is essentially a Laplacian. This permits us to compute the Taylor expansion of U around the origin because $U^{(j)}(0) =< \mathfrak{f}, \mathfrak{u}^{(j)}(0) >$. In particular, from (5.1),

$$v \cdot D(\alpha)v = (1-\alpha) \sum_{z\in\mathbb{Z}_*^d} (z \cdot v)^2 p(z) - \alpha(1-\alpha) < \mathfrak{u}(0), \mathfrak{f}_v > \; + O(\alpha^2)$$

includes the first order correction, where $\mathfrak{u}(0)$ is the solution of (5.10).

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