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SOME PROPERTIES OF THE DIFFUSION COEFFICIENT FOR ASYMMETRIC SIMPLE EXCLUSION PROCESSES

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The hydrodynamical limit of asymmetric simple exclusion processes is given by an inviscid Burgers equation and its next-order correction is given by the viscous Burgers equation. The diffusivity can be characterized by an abstract formulation in a Hilbert space with the inverse of the diffusivity characterized by a variational formula. Alternatively, it can be described by the Green–Kubo formula. We give arguments that these two formulations are equivalent. We also derive two other variational formulas, one for the inverse of the diffusivity and one for the diffusivity itself, characterizing diffusivity as a supremum and as an infimum. These two formulas also provide an analytic criterion for deciding whether the diffusivity as defined by the linear response theory is symmetric. Furthermore, we prove the continuity of the diffusivity and a few other relations concerning diffusivity and solutions of the Euler–Lagrange equations of these variational problems.

1. Introduction. The diffusion coefficient of driven lattice gases has long been characterized by the Green–Kubo formula and discussed in great detail in many articles; see [10], [5] and [3] for references. The Green–Kubo formula contains the time integral of current–current correlation functions which is finite only if the current–current correlation functions decay sufficiently fast. For reversible lattice gases, the Green–Kubo formula is proved to be finite in [10]. Even with this result, the current–current correlation functions are still very hard to work with analytically. Recently in [11] a variational formulation of diffusivity was presented which is always well defined and finite. It avoids the current–current correlation functions and, being a variational formulation, it provides an excellent starting point for a rigorous analysis of diffusivity. This formulation was initially given for Ginzburg–Landau dynamics but can be extended handily to lattice gases with reversible dynamics (cf. [8] and [10]). It is similar to the homogenization formula for diffusivity in a random medium except that the setting is now infinite dimensional. This formula is shown in [10] to be equivalent to the Green–Kubo formula for reversible lattice gas dynamics (this argument is rigorous for the symmetric exclusion process).

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The first question encountered for nonreversible dynamics is that models with known invariant measures are very limited. We shall restrict ourselves in this article to simple exclusion processes on the lattice except in Section 2, where general results on particle systems are considered.

Simple exclusion processes are Markov processes on $\{0,1\}^{\mathbb{Z}^d}$ whose generator L acts on cylinder functions as

$$(1.1)\qquad (Lf)(\eta) = \sum_{x,y} p(x,y)\eta(x)[1-\eta(y)][f(\eta^{x,y})-f(\eta)].$$

Here η denotes a configuration of $\{0,1\}^{\mathbb{Z}^d}$ so that $\eta(x)$ is equal to 1 if site x is occupied and is equal to 0 otherwise; $\eta^{x,y}$ stands for the configuration obtained from η by letting one particle jump from x to y:

$$\eta^{x,y}(z) = \begin{cases} \eta(z), & \text{if } z \neq x, y, \\ \eta(x) - 1, & \text{if } z = x, \\ \eta(y) + 1, & \text{if } z = y. \end{cases}$$

Moreover, $p(x,y) = p(y-x)$ is a positive finite range function on $\mathbb{Z}^d$ such that

$$\sum_x p(x) = d$$

and

$$p(z) = 0 \quad \text{if } |z| \geq R \text{ for some } R \in \mathbb{N}.$$

Most of the time, to keep the notation simple, we shall restrict ourselves to nearest-neighbor simple exclusion processes: $p(z) = 0$ unless $|z| = 1$ and $p(e_i) + p(-e_i) = 1$, where e_i denotes the ith element of the canonical basis of $\mathbb{R}^d$.

For each ρ in $[0,1]$, denote by ν_ρ the Bernoulli product measure on $\{0,1\}^{\mathbb{Z}^d}$ with density ρ. These measures are invariant for simple exclusion processes. Hereafter $\langle \cdot \rangle_\rho$ denotes expectation with respect to ν_ρ. Moreover, for two cylinder functions f, g and a density ρ, denote by $\langle f; g\rangle_\rho$ the covariance of f and g with respect to ν_ρ:

$$\langle f; g\rangle_\rho = \langle fg\rangle_\rho - \langle f\rangle_\rho \langle g\rangle_\rho.$$

Let χ be the compressibility given by

$$\chi = \chi(\rho) = \sum_x \langle \eta_x; \eta_0\rangle_\rho.$$

In our setting, $\chi(\rho) = \rho(1-\rho)$.

The asymmetric simple exclusion process is the most simple example of a driven diffusive lattice gas. Under hyperbolic scaling of space and time, Rezakhanlou proved that the empirical density of particles converges to the entropic solution of the Burgers equation (cf. [9]):

$$(1.2)\qquad \partial_t \rho + \gamma \cdot \nabla(\rho(1-\rho)) = 0 \quad \text{where } \gamma = \sum_z z p(z).$$

The convergence is intended here as a law of large numbers.

In [7] we proved the so-called *Navier–Stokes corrections* to this hydrodynamic limit (cf. [10] and [3]). That is, the first-order corrections to this limit are given by the solution of a viscous Burgers equation

$$\partial_t \rho + \gamma \cdot \nabla(\rho(1-\rho)) = N^{-1} \sum_{i,j} \partial_{u_i}\Big(a^{i,j}(\rho)\, \partial_{u_j} \rho \Big). \tag{1.3}$$

This correction is obtained only in the smooth regime of (1.2) and in a certain weak sense (cf. [7] for a precise formulation). Furthermore, the diffusion coefficient can be characterized as in [2].

For a configuration η and a density ρ, denote respectively by P_η and P_ρ the probability on the path space $D([0,T],\{0,1\}^{\mathbb{Z}^d})$ corresponding to the Markov process with generator L starting from η, ν_ρ. Expectations with respect to P_η or P_ρ are respectively denoted by E_η and E_ρ. Thus $E_\rho[\{\eta_t(x) - \eta_0(x)\}\eta_0(0)]$ stands for the time-dependent correlation functions of a general driven diffusive system in equilibrium with density ρ. Suppose these correlation functions are (noncentered) Gaussian. Then one obtains the diffusion coefficient (the bulk diffusion coefficient) as the following limit:

$$\begin{aligned} D^{(1)}_{i,j}(\rho) = \lim_{t\to\infty} \frac{1}{t}\frac{1}{2\chi}\Big\{ \sum_{x\in\mathbb{Z}^d} x_i x_j E_\rho\big[\{\eta_t(x) - \eta_0(x)\}\eta_0(0)\big] \\ - \chi(v_i t)(v_j t)\Big\}, \end{aligned} \tag{1.4}$$

where η in $\mathbb{R}^d$ is the velocity defined by

$$vt = \frac{1}{\chi} \sum_{x\in\mathbb{Z}^d} x E_\rho\big[\{\eta_t(x) - \eta_0(x)\}\eta_0(0)\big]. \tag{1.5}$$

The velocity can be explicitly computed (cf. [10]):

$$v = (1-2\rho)\gamma. \tag{1.6}$$

We shall take (1.4) and (1.5) as the first definition of the diffusion coefficient in this article, hence the superscript 1. From (1.4), $D^{(1)}$ is automatically symmetric. Note that, in principle, (1.4) may not be finite. In the special case of simple exclusion processes, a simple coupling argument involving a second-class particle shows that the expectation decays as $\exp\{-c|x|/t\}$ and therefore that the sum is finite for each fixed t.

Another definition of the diffusion coefficient is through the linear response theory. To fix ideas, consider the nearest-neighbor simple exclusion process. Denote the instantaneous current (i.e., the difference between the rate at which a particle jumps from x to $x+e_i$ and the rate at which a particle jumps from $x+e_i$ to x) by $W_{x,x+e_i}$:

$$W_{x,x+e_i} = p(e_i)\eta(x)[1-\eta(x+e_i)] - p(-e_i)\eta(x+e_i)[1-\eta(x)] \tag{1.7}$$

so that

$$L\eta(0) = \sum_i \{W_{-e_i,0} - W_{0,e_i}\}.$$

Let $w_i(\rho, \eta) = w_i(\eta)$, $1 \le i \le d$, denote the normalized current in the ith direction:

$$w_i(\eta) = W_{0,e_i} - \langle W_{0,e_i}\rangle_\rho - \frac{d}{d\theta}\langle W_{0,e_i}\rangle_\theta\Big|_{\theta=p}(\eta(0)-\rho). \tag{1.8}$$

Similarly, we can define the current $W^*_{x,x+e_i}$ of the reversed process characterized by the generator L^* which is the formal adjoint of L with respect to ν_ρ, or the generator of the reversed dynamics. The generator L^* is given explicitly by

$$(L^*f)(\eta) = \sum_{x,y}\check{p}(x,y)\eta(x)[1-\eta(y)][f(\eta^{x,y})-f(\eta)],$$

where $\check{p}(x,y) = p(y,x)$ and the current $W^*_{x,x+e_i}$ is given by

$$W^*_{x,x+e_i} = \check{p}(e_i)\eta(x)[1-\eta(x+e_i)] - \check{p}(-e_i)\eta(x+e_i)[1-\eta(x)].$$

Similarly, $w^*_i(\rho,\eta) = w^*_i(\eta)$ is defined by

$$w^*_i = W^*_{0,e_i} - \langle W^*_{0,e_i}\rangle_\rho - \frac{d}{D\theta}\langle W^*_{0,e_i}\rangle_\theta\Big|_{\theta=\rho}(\eta(0)-\rho). \tag{1.9}$$

Then the diffusion coefficient, $D^{(2)}(\rho) = (D^{(2)}_{i,j}(\rho))_{1\le i,j\le d}$, obtained through the linear response theory is given by the Green–Kubo formula as [3]

$$\begin{aligned} D^{(2)}_{i,j}(\rho) = \frac{1}{\chi(\rho)}\bigg\{&-\frac{1}{2}\delta_{i,j}\Big\langle[\eta(e_i)-\eta(0)]W_{0,e_i}\Big\rangle_\rho \\ &-\int_0^\infty dt\sum_x\langle w_i(\eta); e^{tL^*}\tau_x w^*_j(\eta)\rangle_\rho\bigg\}. \end{aligned} \tag{1.10}$$

In this formula and below $\delta_{i,j}$ (or $\delta_{x,y}$) stands for the Kronecker delta and is equal to 1 if $i=j$ and 0 otherwise. Moreover, e^{tL} (e^{tL^*}) represents the semigroup of the Markov process withe generator L (L^*). Unlike in the reversible case, there is no argument suggesting that the time integration in the Green–Kubo formula (1.10) is finite.

Finally, one can define the diffusion coefficient via the formal equation

$$w_i = \sum_j a^{i,j}(\rho)\nabla_{e_j}\eta(0) + Lh_i, \tag{1.11}$$

where h_i is some function of the configuration, L is the generator of the dynamics and $\nabla_{e_j}\eta(0)$ is the gradient $\eta(e_j) - \eta(0)$ for $1 \le j \le d$. The density dependence of the diffusion coefficient indicates that (1.11) should be understood with respect to the invariant measure ν_ρ. The diffusivity a is the proportionality constant such that $w_i - \sum_j a^{i,j}\nabla_{e_j}\eta(0)$ can be inverted by the generator of the dynamics. We stress that this formulation is formal because in (1.11) the generator L is acting on an infinite-dimensional space which we do not even specify here. The precise meaning of (1.11) will be given in Section 5, following [11], [13] and [2]. We shall take (1.11) as the definition of diffusivity.

The diffusivities as defined by (1.10) and (1.11) might not be symmetric. For the bulk diffusion coefficient appearing in (1.2), only the symmetric part of the diffusion coefficient is relevant. The relations between various definitions and properties of the diffusion coefficients are the main subject of this article.

As remarked previously, $D^{(2)}$ is not well defined due to the possible divergence of the time integration. We have no solution to this problem. With a heuristic argument at one step of our derivation, in Section 2 we shall "prove" that $D^{(2)} = a$. Also, assuming $D^{(2)}$ to be finite, we shall prove that $D^{(1)} = (D^{(2)})^s$, the symmetric part of $D^{(2)}$. This has already been proved in [10] for the reversible case and in [3] for the general case. Our proof is based entirely on Itô's formula. This is the content of Section 2. The argument presented there holds for a larger class of processes.

We do not prove directly any relation between $D^{(1)}$ and a although such a relation can be obtained through $D^{(2)}$. Another insight on the relation between $D^{(1)}$ and a is obtained through the scaling limit. If the scaling limit of the fluctuation of the density field is proved to be Gaussian with diffusion coefficient a, then $D^{(1)} = a$. Though it is believed that the equilibrium fluctuation theory can be obtained without difficulty once the hydrodynamic is obtained ([2] and [7]), it has not been carried out explicitly.

The definition of the diffusion coefficient through (1.11) in particle systems is given in [11], where a variational formula is provided for a reversible system. The rigorous meaning of (1.11) for a nonreversible system is given in [13] for simple exclusion processes with mean-zero conditions, that is, for processes whose transition probabilities appearing in (1.1) satisfy

$$\sum_z zp(z) = 0.$$

The mean-zero conditions are later removed in [2] for dimension $d \geq 3$ and hence drifts are allowed in the hydrodynamic equation in the *incompressible limit*. For $d \leq 2$ one conjectures that the dynamics are not diffusive if the mean-zero conditions are violated. In both articles, variational formulas of diffusivity are also given via a min–max principle.

Strictly speaking, the variational formulation of [2] is a formula for $(a^{-1})^s$ and not for $a^s = D^{(1)}$, which is the bulk diffusivity appearing in the hydrodynamic equation. For models with symmetry such that $a = a^s$, this provides a variational formula for the bulk diffusivity. In this paper, we shall give variational formulas for $(a^s)^{-1}$ as well as $(a^{-1})^s$. The formula for $(a^{-1})^s$ is related to [2] but formulated in a clearer manner (cf. also [1]). The diffusion coefficient is symmetric if and only if $(a^{-1})^s = (a^s)^{-1}$. Hence these two formulas provide at least a numerical way to check the symmetry of a. Unfortunately, we are not able to prove that $(a^{-1})^s \neq (a^s)^{-1}$ for any choice of $p(z)$.

The diffusion coefficient defined by (1.11) is believed to be a smooth function of the density. We are far from proving this property. The best we can achieve is a proof of the continuity of the diffusivity. The proof is rather involved due to the infinite dimensionality and nonreversibility of our problem. In the reversible setting, our argument proves that the diffusion coefficient is Lipschitz continuous. This should not be confused with the self-diffusion coefficient, proved to be Lipschitz in [12] for $d \ge 3$. We also obtain two variational formulas for the diffusion coefficient that provide an upper bound and a lower bound for the diffusivity and prove a few technical properties related to the diffusion coefficients, filling the gap left in [7].

2. The Green–Kubo formula. In this section we present a heuristic argument to show that the diffusion coefficient defined in (1.11) is equal to the one given by the Green–Kubo formula (1.10): $a = D^{(2)}$. Furthermore, the bulk diffusion coefficient $D^{(1)}$ is equal to the symmetric part of the Green–Kubo coefficient: $D^{(1)} = (D^{(2)})^s$. To fix ideas, consider a nearest-neighbor asymmetric simple exclusion process on $\mathbb{Z}^d$ and recall all notation introduced in the previous section.

Denote by L^* the adjoint of L in $L^2(\nu_\rho)$ and by L^s the symmetric part of the generator L. In our case L^s corresponds to the generator of a nearest-neighbor symmetric simple exclusion process.

Recall from (1.8) and (1.9) the definition of the normalized current w_i and w_i^*. A simple computation shows that

$$
\begin{aligned}
w_i &= [\rho - p(-e_i)]\, \nabla_{e_i}\eta(0) \\
&\qquad -[p(e_i) - p(-e_i)][\eta(0) - \rho][\eta(e_i) - \rho], \\
w_i^* &= [\rho - p(e_i)]\, \nabla_{e_i}\eta(0) \\
&\qquad +[p(e_i) - p(-e_i)][\eta(0) - \rho][\eta(e_i) - \rho].
\end{aligned}
\tag{2.1}
$$

The static term of the Green–Kubo formula is easy to compute. It is equal to $(1/2)\delta_{i,j}\chi$ so that

$$
\begin{aligned}
D^{(2)}_{i,j} - \frac{1}{2}\delta_{i,j} &= -\frac{1}{\chi}\int_0^\infty dt \sum_x \langle w_i ; e^{tL^*}\tau_x w_j^* \rangle_\rho \\
&= -\frac{1}{\chi}\int_0^\infty dt \sum_x \langle w_j^* ; e^{rL}\tau_x w_i \rangle_\rho .
\end{aligned}
\tag{2.2}
$$

For two cylinder functions f and g, denote by $\langle f, g\rangle_{\rho,0}$ the inner product defined by

$$
\langle f, g\rangle_{\rho,0} = \sum_x \langle f ; \tau_x g\rangle_\rho .
$$

This sum is well defined since all but a finite number of terms vanish. Notice that for this inner product the gradients $\{\nabla_{e_i}\eta(0) = \eta(e_i) - \eta(0),\ 1 \le i \le d\}$ are equal to 0.

Formally, $(-L)^{-1} = \int_0^\infty dt\, e^{tL}$. We may therefore rewrite the right-hand side of (2.2) as

$$-\frac{1}{\chi}\langle w_j^*; (-L)^{-1} w_i\rangle_{\rho,0}.$$

Since, for the inner product $\langle \cdot, \cdot \rangle_{\rho,0}$, the gradients are equivalent to 0, from the explicit formulas (2.1) for w_i and w_j^*, we have that $w_j^* = -w_j$ for this inner product. In particular, the last expression is equal to

$$\frac{1}{\chi}\langle w_j; (-L)^{-1} w_i\rangle_{\rho,0}.$$

Recall the definition of the diffusion coefficient a. It is the unique matrix $a^{i,j}(\rho)$ such that $w_i - \sum_{1\le k\le d} a^{i,j}(\rho)\nabla_{0,e_k}\eta(0)$ belongs to the space $L\mathscr{C} = \{Lg;$ g is a cylinder function$\}$. Denote, in particular, by H_i the cylinder function such that

$$w_i - \sum_{1\le k\le d} a^{i,k}(\rho)\nabla_{0,e_k}\eta(0) = LH_i.$$

Of course, such a function may not exist and we have to interpret the last identity as a proper limit (cf. Lemma 7.3). Since the gradients $\nabla_{0,e_i}\eta(0)$ are equal to 0 for the inner product $\langle \cdot, \cdot \rangle_{\rho,0}$, we have that

$$\left\langle w_j(\eta), (-L)^{-1} w_i\right\rangle_{\rho,0} = \langle -LH_j, H_i\rangle_{\rho,0} = \langle H_j, (-L^*)H_i\rangle_{\rho,0}.$$

In formula (7.2) we prove that

$$\langle -L^* H_i, H_j\rangle_{\rho,0} = \chi\left\{a^{i,j}(\rho) - \tfrac{1}{2}\delta_{i,j}\right\}$$

so that $D^{(2)}_{i,j}(\rho) = a^{i,j}(\rho)$. This shows that the diffusion coefficient a is given by the current–current correlation formula (1.10).

We conclude this section by presenting a heuristic argument to show that the symmetric part of the diffusion coefficient given by the Green–Kubo formula is equal to the bulk diffusion coefficient: $D^{(1)} = (D^{(2)})^s$. We start with a rigorous result relating the bulk diffusion coefficient to the Green–Kubo formula. Recall from the previous section the definition of P_η, P_ρ, E_η and E_ρ. Here P_η^*, P_ρ^*, E_η^* and E_ρ^* are defined in an analogous way with respect to the time-reversed process with generator L^*.

LEMMA 2.1. *For each fixed $t > 0$,*

$$\begin{aligned}\sum_{x\in\mathbb{Z}^d} & x_i x_j E_{\nu_\rho}\left[\{\eta_t(x) - \eta_0(x)\}\eta_0(0)\right]\\ &= -\delta_{i,j} t\left\langle [\eta(e_i) - \eta(0)] W_{0,e_i}\right\rangle_\rho\\ &\quad - \int_0^t ds \int_0^s dr \sum_x \left\langle W_{0,e_i}(\eta); E_\eta^*\left[W^*_{x,x+e_j}(\eta_r)\right]\right\rangle_\rho\\ &\quad - \int_0^t ds \int_0^s dr \sum_x \left\langle W_{0,e_j}(\eta); E_\eta^*\left[W^*_{x,x+e_i}(\eta_r)\right]\right\rangle_\rho.\end{aligned}$$

PROOF. Since ν_ρ is translation invariant, we may rewrite the left-hand side as

$$-\tfrac{1}{2}\sum_{x\in\mathbb{Z}^d} x_i x_j E_{\nu_\rho}\big[\{\eta_t(x)-\eta_0(x)\}\{\eta_t(0)-\eta_0(0)\}\big]. \tag{2.3}$$

Computing the generator applied to $[\eta_t(x)-\eta_0(x)][\eta_t(0)-\eta_0(0)]$, we get that the expectation in the last formula is equal to

$$\begin{aligned}
&\int_0^t ds \sum_{k=1}^d E_{\nu_\rho}\big[[\eta_s(0)-\eta_0(0)]\big[W_{x-e_k,x}(\eta_s)-W_{x,x+e_k}(\eta_s)\big]\big]\\
&\quad+\int_0^t ds \sum_{k=1}^d E_{\nu_\rho}\big[[\eta_s(x)-\eta_0(x)]\big[W_{-e_k,0}(\eta_s)-W_{0,e_k}(\eta_s)\big]\big]\\
&\quad-\int_0^t ds \sum_{k=1}^d \delta_{x,e_k} E_{\eta_\rho}\big[[\eta_s(e_k)-\eta_s(0)]W_{0,e_k}(\eta_s)\big]\\
&\quad-\int_0^t ds \sum_{k=1}^d \delta_{x,-e_k} E_{\nu_\rho}\big[[\eta_s(0)-\eta_s(-e_k)]W_{-e_k,0}(\eta_s)\big].
\end{aligned}$$

Replacing the covariance in (2.3) by this last sum, changing variables and integrating by parts, we obtain that (2.3) is equal to

$$\begin{aligned}
&-\int_0^t ds \sum_x \Big\{x_j E_{\nu_\rho}\big[W_{x,x+e_i}(\eta_s)[\eta_s(0)-\eta_0(0)]\big]\\
&\qquad\qquad+x_i E_{\nu_\rho}\big[W_{x,x+e_j}(\eta_s)[\eta_s(0)-\eta_0(0)]\big]\Big\}\\
&\quad+\delta_{i,j}\int_0^t ds \sum_x E_{\nu_\rho}\big[W_{x,x+e_i}(\eta_s)[\eta_s(0)-\eta_0(0)]\big]\\
&\quad-\delta_{i,j}t\big\langle[\eta(e_i)-\eta(0)]W_{0,e_i}(\eta)\big\rangle_\rho.
\end{aligned} \tag{2.4}$$

Consider the first term in this sum. We have

$$\begin{aligned}
E_{\nu_\rho}\big[W_{x,x+e_i}(\eta_s)[\eta_s(0)-\eta_0(0)]\big] &= E_{\nu_\rho}\big[W_{x,x+e_i}(\eta_s)E^*_{\eta_s}[\eta_0(0)-\eta_s(0)]\big]\\
&=\big\langle W_{0,e_i}(\eta)E^*_\eta[\eta_0(-x)-\eta_s(-x)]\big\rangle_\rho.
\end{aligned}$$

In the last step we used the invariance of ν_ρ and the dynamics translation invariance. Recall that E^* indicates we take expectation with respect to the time-reversed process. Since

$$E^*_\eta[\eta_0(-x)-\eta_s(-x)] = -\sum_{k=1}^d\int_0^s dr\, E^*_\eta\big[W^*_{-x-e_k}(\eta_r)-W^*_{-x,-x+e_k}(\eta_r)\big],$$

after summation by parts the first term in (2.4) can be written as

$$-\int_0^t ds\int_0^s dr\sum_x\big\langle W_{0,e_i}(\eta); E^*_\eta\big[W^*_{x,x+e_k}(\eta_r)\big]\big\rangle_\rho.$$

Proceeding in the same way with the other two terms involving the current, we obtain that (2.4) is equal to

$$-\int_0^t ds \int_0^s dr \sum_x \Big\langle W_{0,e_i}(\eta); E^*_\eta\big[W^*_{x,x+e_j}(\eta_r)\big]\Big\rangle_\rho$$
$$-\int_0^t ds \int_0^s dr \sum_x \Big\langle W_{0,e_j}(\eta); E^*_\eta\big[W^*_{x,x+e_i}(\eta_r)\big]\Big\rangle_\rho$$
$$-\delta_{i,j} t \Big\langle [\eta(e_i) - \eta(0)] W_{0,e_i}(\eta)\Big\rangle_\rho .$$

This concludes the proof of the lemma. □

Recall the definition of the normalized current w_i. We claim that

$$\begin{aligned}&\int_0^t ds \int_0^s dr \sum_x \langle w_i(\eta); e^{rL^*}\tau_x w_j^*(\eta)\rangle_\rho \\ &\quad = \int_0^t ds \int_0^s dr \sum_x \langle W_{0,e_i}(\eta); e^{rL^*}\tau_x W^*_{0,e_j}(\eta)\rangle_\rho + \frac{\chi}{2}(v_i t)(v_j t).\end{aligned} \tag{2.5}$$

From (1.6) and the definition of the current W_{0,e_i} given in (1.7), we have that the ith component of the velocity $v(\rho)$ is equal to the derivative of $\langle W_{0,e_i}\rangle_\theta$ calculated at ρ:

$$v_i(\rho) = \frac{d}{d\theta}\langle W_{0,e_i}\rangle_\theta\Big|_{\theta=p}$$

and

$$v_i^*(\rho) = -\frac{d}{d\theta}\langle W_{0,e_i}\rangle_\theta\Big|_{\theta=\rho}$$

for $1 \le i \le d$. In particular,

$$\begin{aligned} w_i &= W_{0,e_i} - \langle W_{0,e_i}\rangle_\rho - v_i(\rho)[\eta(0) - p],\\ w_i^* &= W^*_{0,e_i} - \langle W^*_{0,e_i}\rangle_\rho + v_i(\rho)[\eta(0) - \rho]\end{aligned}$$

and the left-hand side of (2.5) is equal to

$$\int_0^t ds \int_0^s dr \sum_x \Big\langle W_{0,e_i} - v_i\eta(0); e^{rL^*}\tau_x\big\{W^*_{0,e_j} + v_j\eta(0)\big\}\Big\rangle_\rho . \tag{2.6}$$

We omitted all the constants because we are considering covariances. To prove identity (2.5), we have to compute the four terms in (2.6). The first one is equal to the first term on the right-hand side of (2.5). The second one is

$$\begin{aligned} v_j\int_0^t ds \int_0^s dr \sum_x \langle e^{rL}\tau_x W_{0,e_i}; \eta(0)\rangle_\rho &= v_j \int_0^t ds \sum_x x_i \langle e^{sL}\tau_x \eta(0); \eta(0)\rangle_\rho \\ &= v_j \int_0^t ds \sum_x v_i s\chi = \chi v_i v_j \frac{t^2}{2}.\end{aligned}$$

The first identity follows from Itô's formula. This argument was repeatedly used in the proof of Lemma 2.1. The second equality follows from the definition of the velocity given in (1.5). A similar argument shows that the third term in (2.6) is equal to

$$-v_i \int_0^t ds \int_0^s dr \sum_x \langle \eta(0); e^{rL^*} \tau_x W^*_{0,e_j} \rangle_\rho = -\chi v_i v_j^* \frac{t^2}{2}.$$

Since $v_j^* = -v_j$, this expression is equal to $\chi v_i v_j (t^2/2)$. Finally, the fourth term is

$$-v_i v_j \int_0^t ds \int_0^s dr \sum_x \langle \eta(0); e^{rL^*} \tau_x \eta(0) \rangle_\rho = -v_i v_j \int_0^t ds \int_0^s dr\, \chi$$

because the total number of particles is conserved. This proves (2.5).

Since $p(e_i) + p(-e_i) = 1$, $\langle [\eta(e_i) - \eta(0)] W_{0,e_i} \rangle_\rho = -\chi$. In particular, identity (2.5) and Lemma 2.1 show that the bulk diffusion coefficient $D^{(1)}$ is such that

$$D^{(1)}_{i,j} - \frac{1}{2}\delta_{i,j} = \lim_{t\to\infty} \frac{1}{2t\chi} \left\{ -\int_0^t ds \int_0^s dr \sum_x \langle w_i; e^{rL^*} \tau_x w_j^* \rangle_\rho \right.$$
$$\left. - \int_0^t ds \int_0^s dr \sum_x \langle w_j; e^{rL^*} \tau_x w_i^* \rangle_\rho \right\}.$$

Assume that the time correlations decay fast enough so that the limit as $t \uparrow \infty$ of

$$\int_0^t ds \sum_x \langle w_i; e^{sL^*} \tau_x w_j^* \rangle_\rho$$

exists and is equal to

$$\int_0^\infty ds \sum_x \langle w_i; e^{sL^*} \tau_x w_j^* \rangle_\rho.$$

In particular,

$$D^{(1)}_{i,j} - \frac{1}{2}\delta_{i,j} = \frac{1}{2\chi} \left\{ -\int_0^\infty dt \sum_x \langle w_i; e^{tL^*} \tau_x w_j^* \rangle_\rho - \int_0^\infty dt \sum_x \langle w_j; e^{tL^*} \tau_x w_i^* \rangle_\rho \right\}$$

and this is exactly the symmetrization of the Green–Kubo formula (1.10).

3. The Hilbert space of fluctuations. To keep the notation simple, hereafter for a positive integer K let $\overline{K} = 2K + 1$. Denote by $\mathscr{C}$ the space of cylinder functions. Recall from [7] that for each positive integer K and m in $\{0, 1/(\overline{K}^d), \dots, 1\}$ we denote by Λ_K the cube of length $2K+1$ centered at the origin and by $\nu_{K,m}$ the canonical measure on $\{0,1\}^{\Lambda_K}$ with density m. Let $\mathscr{G}$ be the linear space of cylinder functions that have mean 0 with respect to all canonical measures on a sufficiently large box Λ_K:

(3.1) $$\mathscr{G} = \{ g \in \mathscr{C};\ \nu_{K,m}[g] = 0 \text{ for some } K > 0 \text{ and all } m \}.$$

Moreover, for a density $0 \le m \le 1$, let $\mathcal{G}_m$ be the space of cylinder functions such that

$$\tilde{g}(m) = \nu_m[g] = 0$$

and

$$\partial_\rho \nu_\rho[g]|_{\rho=m} = \tilde{g}'(m) = 0.$$

Note that the second condition is equivalent to requiring that the covariance, with respect to the measure ν_m, of g and the formal sum $\sum_x \eta(x)$ vanishes:

$$\sum_z \langle g(\eta); \eta(z)\rangle_m = \langle g; \eta(0)\rangle_{m,0} = 0.$$

Notice that $\mathcal{G} \subset \mathcal{G}_m$ for all m in $[0,1]$. The following definition is taken from [2].

DEFINITION 3.1. Let g be a cylinder function and denote by $s(g)$ its support

$$s(g) = \min\{\ell \in \mathbb{N}; \operatorname{supp} g \subset \{-\ell, \dots, \ell\}^d\}.$$

For each $\ell \ge s(g)$ and m in $\{0, 1/\bar{\ell}^d, \dots, 1\}$, define the "variance" $V_\ell(g,m)$ of g with respect to $\nu_{\ell,m}$ by

$$(3.2)\qquad \begin{aligned} V_\ell(g,m) = \frac{1}{\overline{\ell(g)}^d}\Bigg\langle &\Bigg[\sum_{|x|\le \ell(g)} (\tau_x g - \tilde{g}_\ell(m))\Bigg] \\ &\times(-L_\ell^s)^{-1}\Bigg[\sum_{|x|\le \ell(g)} (\tau_x g - \tilde{g}_\ell(m))\Bigg]\Bigg\rangle_{\nu_{\ell,m}}. \end{aligned}$$

In this formula $\ell(g)$ denotes the integer $\ell - s(g)$ such that $\sum_{|x|\le \ell(g)} \tau_x g$ is measurable with respect to $\{\eta(x);\ x \in \Lambda_\ell\}$. Moreover, L_ℓ^s is the restriction to Λ_ℓ of the symmetric part of the generator L and $\tilde{g}_\ell(m)$ is the expected value of g with respect to the canonical measure $\nu_{\ell,m}$. Notice that for $g \in \mathcal{G}$ the subtraction in (3.2) is unnecessary.

If $g \in \mathcal{G}_m$ we also define the "variance" of g by

$$\mathbb{V}_m(g) = \limsup_{\ell\to\infty} \nu_m\big[V_\ell\big(g, \eta^\ell(0)\big)\big],$$

where $\eta^\ell(x)$ stands for the empirical density of particles on a box of length $2\ell + 1$ centered at x:

$$\eta^\ell(x) = \frac{1}{\bar{\ell}^d} \sum_{|y-x|\le \ell} \eta(y).$$

For any local function g and any integer $K \ge s(g)$ fixed, define

$$(3.3)\qquad g_{(K)} = \big\{g - \nu_\rho\big[g|\eta^K(0)\big]\big\}.$$

Notice that, for each K, $g_{(K)}$ belongs to $\mathcal{G}$ since it has mean 0 with respect to all canonical measures on boxes of length larger than $\overline{K}$.

The proof of the next result can be found in [8], [11], [4] and [6].

THEOREM 3.2. *For each cylinder function g in $\mathscr{G}$, the finite-volume variance of g converges to the infinite-volume variance*:

$$\mathbb{V}_m(g) = \lim_{\ell\to\infty} \nu_m\big[V_\ell(g, \eta^\ell(0))\big].$$

Furthermore, for each function g in $\mathscr{G}_m$,

$$\begin{aligned}\mathbb{V}_m(g) = \sum_{i=1}^{d} \sup_{\alpha\in\mathbb{R}} &\left\{2\alpha t_i(g) - \frac{\alpha^2}{4}\Big\langle\big(\nabla_{e_i}\eta(0)\big)^2\Big\rangle_m\right\}\\ &+ \sup_{h\in\mathscr{C}}\left\{2\langle g, h\rangle_{m,0} - \frac{1}{4}\sum_{i=1}^{d}\left\langle\Big(\nabla_{e_i}\sum_x \tau_x h\Big)^2\right\rangle_m\right\}.\end{aligned}$$

In this formula, for $1 \le i \le d$, g in $\mathscr{G}_m$ and h in $\mathscr{C}$, $t_i(g)$ and $\langle g, h\rangle_{m,0}$ are given by

$$t_i(g) = \sum_x \langle g, x_i\eta(x)\rangle_m, \qquad \langle g, h\rangle_{m,0} = \sum_x \langle g, \tau_x h\rangle_m$$

and $\langle\,\cdot\,,\cdot\,\rangle_m$ denotes expectation with respect to η_m.

Notice that the first supremum in the above formula can be computed explicitly. The slight difference between this formula for the variance and the one obtained in [2] comes from the fact that their generator is accelerated by 2. It is clear that we may replace $\mathscr{C}$ by $\mathscr{G}_m$ in the second supremum.

In the asymmetric case we are forced to consider cylinder functions that do not have mean 0 with respect to all canonical measures. The normalized currents w_i are examples of such functions. In [7] we proved that, for each function g in $\mathscr{G}_m$, the finite-volume variance of $g_{(K)}$ converges to the infinite-volume variance.

PROPOSITION 3.3. *For each cylinder function g in $\mathscr{G}_m$, the finite-volume variance of $g_{(K)}$ converges to the infinite-volume variance*:

$$\lim_{K\to\infty} \mathbb{V}_m(g_{(K)}) = \mathbb{V}_m(g)$$

uniformly in m.

4. Regularity of variances. In this section we prove that the variance $\mathbb{V}_m(g)$ is Lipschitz continuous as a function of the density m for each cylinder function g in $\mathscr{G}$. We start by introducing some notation.

Fix a cube $\Lambda_\ell = \{-\ell, \dots, \ell\}^d$. For a bond $b = (b_1, b_2)$ in Λ_ℓ, consider the operator T_b that transforms a configuration η to a configuration with the values of the occupation variables $\eta(b_1)$ and $\eta(b_2)$ interchanged:

$$(T_b\eta)(z) = \begin{cases} \eta(z), & \text{if } z \neq b_1, b_2, \\ \eta(b_2), & \text{if } z = b_1, \\ \eta(b_1), & \text{if } z = b_2. \end{cases}$$

For each bond b and each cylinder function u, denote by $\nabla_b u$ the function defined by $(\nabla_b u)(\eta) = u(T_b\eta) - u(\eta)$.

For each $x \in \Lambda_\ell$ denote by $\sigma_x\eta$ the configuration η with the occupation variable at x flipped:

$$\sigma_x\eta(y) = \begin{cases} 1 - \eta(x), & y = x, \\ \eta(y), & y \neq x. \end{cases}$$

Let n be the total number of particles: $n = m\bar{\ell}^d$. To keep the notation simple, in this section we shall denote by $\langle \cdot , \cdot \rangle_{\ell, n}$ the inner product with respect to the measure $\nu_{\bar{\ell}, m}$.

Define the operators $\sigma_{\ell, n}$ and $\sigma^+_{\ell, n}$ on the cylinder functions u by

$$(\sigma^-_{\ell, n}u)(\eta) = \frac{1}{n} \sum_{x \in \Lambda_\ell} u(\sigma_x\eta)\eta_x,$$

$$(\sigma^+_{\ell, n}u)(\eta) = \frac{1}{\bar{\ell}^d - n} \sum_{x \in \Lambda_\ell} u(\sigma_x\eta)(1 - \eta_x).$$

One can check directly that $\sigma^{\pm}_{\ell, n}$ and ∇_b commute:

$$\left[\sigma^{\pm}_{\ell, n}; \nabla_b\right] = 0$$

for any bond $b \in \Lambda_\ell$, where [;] denotes the commutator. Furthermore, for any cylinder functions u and h,

$$\langle u, \sigma^+_{\ell, n}h\rangle_{\ell, n} = \langle h, \sigma^-_{\ell, n+1}u\rangle_{\ell, n+1}. \tag{4.1}$$

In particular, since the total number of particles is equal to n, we have $\sigma^+_{\ell, n}1 = 1$ and

$$\langle u\rangle_{\ell, n} = \langle \sigma^-_{\ell, n+1}u\rangle_{\ell, n+1}.$$

Therefore, since $\sigma^-_{\ell, n}$ and ∇_b commute, by the Schwarz inequality,

$$\begin{aligned} \left\langle\left(\nabla_b(\sigma^-_{\ell, n+1}u)\right)^2\right\rangle_{\ell, n+1} &= \left\langle\left(\sigma^-_{\ell, n+1}\,\nabla_b u\right)^2\right\rangle_{\ell, n+1} \\ &\le \left\langle \sigma^-_{\ell, n+1}(\nabla_b u)^2\right\rangle_{\ell, n+1} = \left\langle(\nabla_b u)^2\right\rangle_{\ell, n}. \end{aligned} \tag{4.2}$$

Moreover, by (4.1) and since $\sigma^-_{\ell, n}$ and ∇_b commute, we also have the identity:

$$\langle \tau_b h, \nabla_b \sigma^-_{\ell, n+1}u\rangle_{\ell, n+1} - \langle \tau_b h, \nabla_b u\rangle_{\ell, n} = \left\langle\left[(\sigma^+_{\ell, n} - 1)\tau_b h\right], \nabla_b u\right\rangle_{\ell, n}. \tag{4.3}$$

LEMMA 4.1 (Integration-by-parts formula for functions in $\mathscr{G}$). *For $1 \le i \le d$, denote by $\mathscr{B}_i$ the set of bonds $b = (b_1, b_2)$ such that $b_2 - b_1 = \pm e_i$. For each function g in $\mathscr{G}$, there exist cylinder functions h_i such that*

$$\sum_{x \in \Lambda_\ell(g)} \langle \tau_x g, u \rangle_{\ell, n} = \tfrac{1}{4} \sum_{i=1}^{d} \sum_{b \in \mathscr{B}_i} \langle \tau_b h_i, \nabla_b u \rangle_{\ell, n}$$

for all positive integers ℓ, $0 \le n \le (2\ell + 1)^d$, and u in $L^2(\nu_{\ell, n/\bar{\ell}^d})$.

PROOF. Since g belongs to $\mathscr{G}$, there exists a positive integer k such that g has mean 0 with respect to all canonical measures $\nu_{k,m}$ for m in $\{0, 1/\bar{k}^d, \dots, 1\}$. In particular, g belongs to the image of L_k^s. Therefore,

$$\sum_{x \in \Lambda_\ell(g)} \langle \tau_x g, u \rangle_{\ell, n} = \sum_x \langle \tau_x L_k^s (L_k^s)^{-1} g, u \rangle_{\ell, n}.$$

Denote by $L_{x+\Lambda_k}^s$ the symmetric part of the generator L restricted to the set $x + \Lambda_k$. Since we have that $\tau_x L_k^s = L_{x+\Lambda_k}^s \tau_x$, the right-hand side is equal to

$$\sum_x \langle L_{x+\Lambda_k}^s \tau_x (L_k^s)^{-1} g, u \rangle_{\ell, n} = \tfrac{1}{4} \sum_x \sum_{b \in x + \Lambda_k} \langle \nabla_b \tau_x (-L_k^s)^{-1} g, \nabla_b u \rangle_{\ell, n}.$$

A standard computation shows that $\nabla_b \tau_x = \tau_x \nabla_{b-x}$ so that the right-hand side is equal to

$$\tfrac{1}{4} \sum_b \left\langle \tau_b \sum_{x;\, b-x \in \Lambda_k} \tau_{x-b} \nabla_{b-x} (-L_k^s)^{-1} g, \nabla_b u \right\rangle_{\ell, n}.$$

Of course, $\sum_{x;\, b-x \in \Lambda_k} \tau_{x-b} \nabla_{b-x} (-L_k^s)^{-1} g$ depends on the bond b only through the direction $b_2 - b_1$. This is shown by a change of variables. To conclude the proof of the lemma, we just have to define h_i, for $1 \le i \le d$, by

$$h_i = \sum_{x;\, b-x \in \Lambda_k} \tau_{x-b} \nabla_{b-x} (-L_k^s)^{-1} g \quad \text{if } b_2 = b_1 \pm e_i. \qquad \square$$

LEMMA 4.2. *For each $g \in \mathscr{G}$, the variance $\mathbb{V}_m(g)$ is Lipschitz continuous in m uniformly on compact sets of* $(0,1)$.

PROOF. Fix a cylinder function g in $\mathscr{G}$. From Definition 3.1 it suffices to prove that $V_\ell(g, m)$ is Lipschitz continuous uniformly in ℓ. By definition,

$$V_\ell(g, m) = \frac{1}{\bar{\ell}^d} \sup_u \left\{ 2 \left\langle \sum_{|x| \le \ell(g)} \tau_x g, u \right\rangle_{\ell, n} - \frac{1}{4} \sum_{b \in \Lambda_\ell} \langle (\nabla b_u)^2 \rangle_{\ell, n} \right\}. \tag{4.4}$$

Here the second summation is carried out over all bounds $b = (b_1, b_2)$ of Λ_ℓ and the supremum is taken over all functions on Λ_ℓ.

By the integration-by-parts formula, the linear term is equal to

$$\tfrac{1}{2} \sum_{i=1}^{d} \sum_{b \in \mathscr{B}_i} \langle \tau_b h_i, \nabla_b u \rangle_{\ell, n} \tag{4.5}$$

for some cylinder functions h_i. By the Schwarz inequality, this expression is bounded above by

$$C(g)\bar{\ell}^d + \tfrac{1}{4}\sum_{b\in\Lambda_\ell}\langle(\nabla_b u)^2\rangle_{\ell,n}$$

for some constant C that depends only on g. In particular, we may restrict the supremum on the right-hand side of (4.4) to functions with global Dirichlet form bounded by $C_1(g)\bar{\ell}^d$.

Fix $1\le i\le d$ and a bond b in $\mathscr{B}_i$. From inequalities (4.2) and (4.3), adding and subtracting $\langle\tau_b h, \nabla_b\sigma^-_{\ell,n+1}u\rangle_{\ell,n+1}$, we obtain

$$\begin{aligned}\tfrac{1}{2}\langle\tau_b h_i,\nabla_b u\rangle_{\ell,n} - \tfrac{1}{4}\langle(\nabla_b u)^2\rangle_{\ell,n} \le{}& \tfrac{1}{2}\langle\tau_b h_i,\nabla_b\sigma^-_{\ell,n+1}u\rangle_{\ell,n+1}\\ &-\tfrac{1}{4}\Big\langle\big[\nabla_b(\sigma^-_{\ell,n+1}u)\big]^2\Big\rangle_{\ell,n+1}\\ &-\tfrac{1}{2}\langle(\sigma^+_{\ell,n}-1)\tau_b h_i,\nabla_b u\rangle_{\ell,n}.\end{aligned}\tag{4.6}$$

Since h_i is a local function,

$$\begin{aligned}\big|(\sigma^+_{\ell,n}-1)\tau_b h_i(\eta)\big| &= \frac{1}{\bar{\ell}^d - n}\sum_x\big|\tau_b h_i(\sigma_x\eta)-\tau_b h_i(\eta)\big|(1-\eta(x))\\ &\le \frac{1}{\bar{\ell}^d}\frac{C_1}{1-m}.\end{aligned}$$

With this upper bound and the elementary inequality $2ab\le a^2+b^2$, we may estimate the last term on the right-hand side of (4.6) as follows:

$$\begin{aligned}&\sum_{b\in\mathscr{B}_i}\Big|\Big\langle(\sigma^+_{\ell,n}-1)\tau_b h_i,\nabla_b u\Big\rangle_{\ell,n}\Big|\\ &\quad\le \frac{A}{2}\bar{\ell}^d\frac{C_3(g)}{(1-m)^2\bar{\ell}^{2d}} + \frac{1}{2A}\sum_{b\in\mathscr{B}_i}\langle(\nabla_b u)^2\rangle_{\ell,n}.\end{aligned}\tag{4.7}$$

Since we consider in the supremum only functions u with global Dirichlet form bounded by $C(g)\ell^d$, optimizing in A, we obtain that the last expression is bounded above by $C_4(g)(1-m)^{-1}$.

In conclusion, in view of (4.5) and estimates (4.6) and (4.7), the right-hand side of (4.4) is bounded above by

$$\begin{aligned}&\frac{1}{\bar{\ell}^d}\sup_u\Bigg\{\sum_{i=1}^d\sum_{b\in\mathscr{B}_i}\frac{1}{2}\langle\tau_b h_i,\nabla_b(\sigma^-_{\ell,n+1}u)\rangle_{\ell,n+1}\\ &\qquad\qquad -\frac{1}{4}\sum_{b\in\Lambda_l}\Big\langle\big(\nabla_b(\sigma^-_{\ell,n+1}u)\big)^2\Big\rangle_{\ell,n+1}\Bigg\} + \frac{C_4(g)}{\bar{\ell}^D(1-m)}\\ &\quad=\frac{1}{\bar{\ell}^d}\sup_u\Bigg\{2\sum_{x\in\Lambda_\ell(g)}\langle\tau_x g,\sigma^-_{\ell,n+1}u\rangle_{\ell,n+1}\\ &\qquad\qquad -\frac{1}{4}\sum_{b\in\Lambda_\ell}\Big\langle\big(\nabla_b(\sigma^-_{\ell,n+1}u)\big)^2\Big\rangle_{\ell,n+1}\Bigg\} + \frac{C_4(g)}{\bar{\ell}^d(1-m)}.\end{aligned}$$

Since the first term in the last expression is, by definition, bounded by $V_{\ell}(g, m + \bar{\ell}^{-d})$, we proved that

$$V_{\ell}(g, m) \le V_{\ell}\left(\frac{g, m+1}{\bar{\ell}^d}\right) + \frac{1}{\bar{\ell}^d}\frac{C_4(g)}{l-m}.$$

From the particle–hole duality,

$$V_{\ell}\left(\frac{g, m+1}{\bar{\ell}^d}\right) \le V_{\ell}(g, m) + \frac{1}{\bar{\ell}^d}\frac{C_4(g)}{1-m}.$$

This proves the Lipschitz continuity. □

Denote by $\mathfrak{F}$ the space of functions $F\colon [0,1] \times \{0,1\}^{\mathbb{Z}^d} \to \mathbb{R}$ such that:

1. For each $\rho \in [0,1]$, $F(\rho, \cdot)$ is a cylinder function with uniform support. That is, there exists a finite set Λ such that for each ρ in $[0,1]$ the support of $F(\rho, \cdot)$ is contained in Λ.
2. For each configuration η, $F(\cdot, \eta)$ is a smooth function.
3. For each density ρ, the cylinder function $F(\rho, \cdot)$ has mean 0 with respect to ν_ρ and the derivative with respect to the parameter θ of the expected value $\nu_\theta[F(\rho, \eta)]$ vanishes at $\theta = \rho$:

$$\nu_\rho[F(\rho, \eta)] = 0$$

and

$$\frac{d}{d\theta}\nu_\theta[F(\rho, \eta)]\bigg|_{\theta=\rho} = 0.$$

The next result concerns the regularity in m of the function $\mathbb{V}_m(F(m, \cdot))$.

LEMMA 4.3. *For each function $F(m, \eta)$ in $\mathfrak{F}$, $\mathbb{V}_m(F(m, \cdot))$ is continuous in m in* $(0,1)$.

PROOF. From Proposition 3.3 we have that $\mathbb{V}_m(F_{(L)})$ converges to $\mathbb{V}_m(F)$ uniformly. Hence it suffices to prove that $\mathbb{V}_m(F_{(L)})$ is continuous. However, this is a corollary of Lemma 4.2. □

In fact, a little more work shows that $\mathbb{V}_m(F(m, \cdot))$ is continuous in $[0,1]$.

5. The diffusion coefficient. Recall from Section 3 the definitions of the space $\mathscr{G}_m$ and the variance $\mathbb{V}_m$ for $0 \le m \le 1$. From the definition of $\mathbb{V}_m$ we may introduce the bilinear form $\mathbb{V}_m(\cdot, \cdot)$ on $\mathscr{G}_m$ by polarization

$$\mathbb{V}_m(g, h) = \tfrac{1}{4}\{\mathbb{V}_m(g+h) - \mathbb{V}_m(g-h)\}.$$

Denote by $\overline{\mathscr{G}_m}$ the closure of $\mathscr{G}_m$ with respect to $\mathbb{V}_m$ and by $\mathscr{N}_m$ the kernel of $\mathbb{V}_m$. Hence $(\overline{\mathscr{G}_m}|_{\mathscr{N}_m}, \mathbb{V}_m)$ is a Hilbert space. The following relations, valid for every $1 \le i \le d$ and all cylinder functions g and h in $\mathcal{G}_m$, are easily obtained from the definition of $\mathbb{V}_m$:

$$
\begin{aligned}
\mathbb{V}_m\big(L^* g, \nabla_{e_i}\eta(0)\big) &= -2\langle w_i, g\rangle_{m,0},\\
\mathbb{V}_m\big(Lg, \nabla_{e_i}\eta(0)\big) &= -2\langle w_i^*, g\rangle_{m,0},\\
\mathbb{V}_m\big(\nabla_{e_i}\eta(0), L_s g\big) &= 0,\\
\mathbb{V}_m(L_s g, h) &= -\langle g, h\rangle_{m,0},\\
\mathbb{V}_m\big(\nabla_{e_i}\eta(0), \nabla_{e_j}\eta(0)\big) &= 2\chi\delta_{i,j}.
\end{aligned}
\tag{5.1}
$$

Recall that $\chi = m(1-m)$ stands for the static compressibility and that w_i^*, w_i represent the normalized currents defined by

$$
\begin{aligned}
w_i &= \tfrac{1}{2}\nabla_{e_i}\eta(0) - \gamma_i[\eta(e_i) - m][\eta(0) - m],\\
w_i^* &= \tfrac{1}{2}\nabla_{e_i}\eta(0) + \gamma_i[\eta(e_i) - m][\eta(0) - m]
\end{aligned}
\tag{5.2}
$$

for $1 \le i \le d$. Here γ is the mean drift of each particle, defined in (1.2). Notice that we changed the coefficient in front of the gradient to keep the notation simple.

We start this section by investigating the structure of the Hilbert space $\overline{\mathcal{G}_m}$. The next result follows straightforwardly from the definition of the inner product $\mathbb{V}_m(\cdot,\cdot)$. The proof can be found in [2] [cf. Theorem 5.9(i)].

LEMMA 5.1. *Denote by* $\mathcal{G}_g$ *the space generated by the gradients*: $\mathcal{G}_g = \{\sum_i \alpha_i \nabla_{e_i}\eta(0);\ \alpha \in \mathbb{R}^d\}$. *Furthermore, denote by* $\mathcal{G}_c, \mathcal{G}_{c,*}$ *the space generated by the normalized currents*: $\mathcal{G}_c = \{\sum_i \alpha_i w_i;\ \alpha \in \mathbb{R}^d\}$, $\mathcal{G}_{c,*} = \{\sum_i \alpha_i w_i^*;\ \alpha \in \mathbb{R}^d\}$. *Then*

$$
\begin{aligned}
\overline{\mathcal{G}_m} &= \overline{L\mathcal{G}_m + \mathcal{G}_g} = \overline{L^*\mathcal{G}_m + \mathcal{G}_g} = \overline{L_s\mathcal{G}_m + \mathcal{G}_g},\\
\overline{\mathcal{G}_m} &= \overline{L\mathcal{G}_m + \mathcal{G}_c} = \overline{L_s\mathcal{G}_m + \mathcal{G}_c},\\
\overline{\mathcal{G}_m} &= \overline{L^*\mathcal{G}_m + \mathcal{G}_{c,*}} = \overline{L_s\mathcal{G}_m + \mathcal{G}_{c,*}}.
\end{aligned}
$$

From this lemma we obtain that there exists a unique matrix $a(m)$ such that

$$
w_i^* - \sum_{k=1}^{d} a^{i,k}(m)\nabla_{e_k}\eta(0) \in \overline{L^*\mathcal{G}_m}. \tag{5.3}
$$

Here $a(m)$ is the diffusion coefficient of the Navier–Stokes equation (1.3). Alternatively, the diffusion coefficient can be characterized by the following lemma.

LEMMA 5.2. *The diffusion coefficient* $a(m)$ *is such that*

$$
w_i - \sum_{j=1}^{d} a^{i,j}(m)\nabla_{e_j}\eta(0) \in \overline{L\mathcal{G}_m}. \tag{5.4}
$$

PROOF. Denote by θ: $\mathbb{Z} \to \mathbb{Z}$ the reflection with respect to the origin: $\theta(x) = -x$. We may extend θ to the space of configurations in the natural way: $(\theta\eta)(x) = \eta(\theta(x))$. Similarly, we may extend θ to the space of continuous functions on $\{0,1\}^{\mathbb{Z}^d}$: $(\theta f)(\eta) = f(\theta\eta)$. Notice that $\theta(\mathscr{G}_m) = \mathscr{G}_m$ and that

$$\theta(w_j^*) = -\tau_{-e_j} w_j,$$
$$\theta\big(\nabla_{e_j}\eta(0)\big) = -\tau_{-e_j}\nabla_{e_j}\eta(0),$$
$$\theta(L^* f) = L(\theta f)$$

for $1 \le j \le d$ and $f \in \mathscr{G}_m$. In particular, (5.4) follows from (5.3). □

In Lemma 5.3 below we prove that in the *isotropic* case the diffusion coefficient is symmetric: $a^{i,j}(m) = a^{j,i}(m)$. An example is the totally asymmetric case where $p(e_i) = 1$ for $1 \le i \le d$.

LEMMA 5.3. *The diffusion coefficient, $a^{i,j}(m)$, is symmetric in the isotropic case.*

PROOF. Fix $1 \le i, j \le d$ and define $\theta_{i,j}$: $\mathbb{Z}^d \to \mathbb{Z}^d$ as the transformation that interchanges coordinates i and j: $(\theta_{i,j}x)_k = x_k$ for $k \ne i, j$, $(\theta_{i,j}x)_i = x_j$ and $(\theta_{i,j}x)_j = x_i$. We may extend $\theta_{i,j}$ to the space of configurations and to the space of continuous functions on $\{0,1\}^{\mathbb{Z}^d}$ in a natural way setting $(\theta_{i,j}\eta)(x) = \eta(\theta_{i,j}x)$, $(\theta_{i,j}f)(\eta) = f(\theta_{i,j}\eta)$. Since the process is rotationally invariant,

$$\theta_{i,j} w_i^* = w_j^*, \qquad \theta_{i,j}(L^* f)(\eta) = L^*\big(\theta_{i,j} f\big)$$

and

$$\theta_{i,j}\nabla_{e_k}\eta(0) = \nabla_{\theta_{i,j}e_k}\eta(0) = \begin{cases} \nabla_{e_k}\eta(0), & \text{if } k \ne i, j, \\ \nabla_{e_i}\eta(0), & \text{if } k = j, \\ \nabla_{e_j}\eta(0), & \text{if } k = i. \end{cases}$$

Since $\theta_{i,j}(\mathscr{G}_m) = \mathscr{G}_m$, applying the transformation $\theta_{i,j}$ to (5.3), we obtain

$$w_j^* - \sum_{k=1}^{d} a^{i,k}(m)\nabla_{\theta_{i,j}e_k}\eta(0) \in \overline{L^*\mathscr{G}_m}.$$

From the uniqueness we then get that $a^{i,k}(m) = a^{j,k}(m)$ for $k \ne i, j$; $a^{i,j}(m) = a^{j,i}(m)$ and $a^{i,i}(m) = a^{j,j}(m)$. Therefore, there exist $a^d(m)$ and $a^{nd}(m)$ such that $a^{i,i}(m) = a^d(m)$ for every $1 \le i \le d$ and $a^{i,j}(m) = a^{nd}(m)$ for $i \ne j$. □

To keep the notation simple, for $1 \le i \le d$, define the cylinder functions $\sigma_i(\eta)$ and $\sigma_i^*(\eta)$ by

$$\sigma_i(\eta) = 2w_i(\eta), \qquad \sigma_i^*(\eta) = 2w_i^*(\eta).$$

Let T be the linear transformation from $\mathscr{G}_m$ to $\mathscr{G}_m$ such that

$$T\left(\sum_{i=1}^{d}\alpha_i\sigma_i + Lh\right) = \sum_{i=1}^{d}\alpha_i \nabla_{e_i}\eta(0) + L^s h.$$

In the next lemma we recall a few properties of T. The inverse of T, denoted by R, was introduced in [2]. It was claimed there that R is bounded. The proof is in fact incorrect. We shall not use R in this article. The next lemma and its proof are taken from [2].

LEMMA 5.4. *The linear transformation T has norm bounded above by* 1. *The linear transformation T^*: $\mathscr{G}_m \to \mathscr{G}_m$, defined by*

$$T^*\left(\sum_{i=1}^{d}\alpha_i\sigma_i^* + L^* h\right) = \sum_{i=1}^{d}\alpha_i \nabla_{e_i}\eta(0) + L^s h,$$

is the adjoint of T with respect to the inner product $\mathbb{V}_m(\cdot,\cdot)$. Moreover, $T\nabla_{e_i}\eta(0)$ is orthogonal to the space $\overline{L^*\mathscr{G}_m}$:

$$T\nabla_{e_i}\eta(0) \perp \overline{L^*\mathscr{G}_m}$$

and

$$\mathbb{V}_m\big(\sigma_i^*(\eta), T\nabla_{e_j}\eta(0)\big) = 2\chi\delta_{i,j}.$$

PROOF. We start by proving that T has norm bounded above by 1. By Lemma 5.1, it is enough to show that

$$\mathbb{V}_m\left(\sum_{i=1}^{d}\alpha_i\sigma_i + Lh\right) \ge \mathbb{V}_m\left(\sum_{i=1}^{d}\alpha_i \nabla_{e_i}\eta(0) + L_s h\right) \tag{5.5}$$

for all α in $\mathbb{R}^d$ and h and $\mathscr{G}_m$. The right-hand side is easy to compute because $\nabla_{e_i}\eta(0)$ is orthogonal to $L_s\mathscr{G}_m$. It is enough to $2\chi\sum_i\alpha_i^2 - \langle h, L^s h\rangle_{m,0}$. To estimate the left-hand side, notice that

$$\sup_{\alpha\in\mathbb{R}}\left\{2\alpha t_i\left(\sum_{j=1}^{d}\alpha_j\sigma_j + Lh\right) - \frac{\alpha^2\chi}{2}\right\} = \frac{2}{\chi}\big(\alpha_i\chi - \langle h, w_i^*\rangle_{m,0}\big)^2.$$

On the other hand, choosing $g = -h$, we get that

$$\sup_{g\in\mathscr{C}}\left\{2\left\langle\sum_{i=1}^{d}\alpha_i\sigma_i + Lh, g\right\rangle_{m,0} + \langle g, L^s g\rangle_{m,0}\right\}$$
$$\ge -2\sum_{i=1}^{d}\alpha_i\langle\sigma_i, h\rangle_{m,0} - \langle h, L_s h\rangle_{m,0}.$$

It is now easy to conclude the proof of inequality (5.5) if we recall that $\sigma_i = 2w_i$ and that $\langle w_i, h\rangle_{m,0} = -\langle w_i^*, h\rangle_{m,0}$.

To very that T^* is the adjoint of T, by Lemma 5.1 we just need to check that

$$\mathbb{V}_m\left(T\left(\sum_{i=1}^{d} \alpha_i \sigma_i + Lh\right), \sum_{i=1}^{d} \beta_i \sigma_i^* + L^* g\right)$$
$$= \mathbb{V}_m\left(\sum_{i=1}^{d} \alpha_i \sigma_i + Lh, T^*\left(\sum_{i=1}^{d} \beta_i \sigma_i^* + L^* g\right)\right).$$

This is a simple computation if one recalls that $\sigma_j^* = 2w_j^*$.

In particular,

$$\mathbb{V}_m\big(T\,\nabla_{e_i}\eta(0), L^* h\big) = \mathbb{V}_m\big(\nabla_{e_i}\eta(0), T^* L^* h\big) = \mathbb{V}_m\big(\nabla_{e_i}\eta(0), L_s h\big) = 0.$$

Analogously,

$$\mathbb{V}_m\big(T\,\nabla_{e_i}\eta(0), \sigma_j^*\big) = \mathbb{V}_m\big(\nabla_{e_i}\eta(0), T^*\sigma_j^*\big) = \mathbb{V}_m\big(\nabla_{e_i}\eta(0), \nabla_{e_j}\eta(0)\big) = 2\chi\delta_{i,j}. \quad \square$$

Denote by T^s the symmetrization of T with respect to the inner product $\mathbb{V}_m$:

$$T^s = \tfrac{1}{2}(T + T^*).$$

In the next lemma we show that $T^s = T^* T$.

LEMMA 5.5. *For every g in $\mathscr{G}_m$,*

$$\mathbb{V}_m(g, Tg) = \mathbb{V}_m(T_g, Tg). \tag{5.6}$$

In particular, by polarization, $\mathbb{V}_m(T^s g, h) = \mathbb{V}_m(TT^* g, h)$ for every g and h in $\mathscr{G}_m$ because T^s and TT^* are symmetric.

PROOF. By Lemma 5.1, we just need to check identity (5.6) for $g = \sum_i \alpha_i \sigma_i + Lh$ for α in $\mathbb{R}^d$ and h in $\mathscr{G}_m$. This is elementary if one recalls that $\sigma_i = 2w_i$. $\square$

We are now ready to obtain an explicit formula (cf. [2]) for the inverse of the diffusion coefficient a. Let Q denote the matrix with entries $(Q_{i,j})_{1\le i,j\le d}$ defined by

$$Q_{i,j} = \mathbb{V}_m\big(\nabla_{e_i}\eta(0), T\,\nabla_{e_j}\eta(0)\big).$$

We claim that Q is invertible. Indeed, assume $\alpha^* Q\alpha = 0$ for some α in $\mathbb{R}^d$. By the definition of Q and Lemma 5.5,

$$\alpha^* Q\alpha = \mathbb{V}_m\left(T\sum_i \alpha_i\,\nabla_{e_i}\eta(0), T\sum_i \alpha_i\,\nabla_{e_i}\eta(0)\right).$$

Thus $T\sum_i \alpha_i\,\nabla_{e_i}\eta(0) = 0$ for the inner product $\mathbb{V}_m$. In particular, $0 = \mathbb{V}_m(T\sum_i \alpha_i\,\nabla_{e_i}\eta(0), \sigma_j^*) = 2\chi\alpha_j$. This implies that $\alpha = 0$. In fact, Q is related to the inverse of the diffusion matrix a by the following formula:

$$a = \chi Q^{-1}. \tag{5.7}$$

Indeed, since $w_j^* = (1/2)\sigma_j^*$, by the definition of a, $(1/2)\sigma_j^* - \sum_k a^{j,k}(m)\nabla_{e_k}\eta(0)$ belongs to $\overline{L^*\mathscr{G}_m}$. Taking the inner product with respect to $T\nabla_{e_i}\eta(0)$, we obtain, by Lemma 5.4,

$$\chi\delta_{i,j} - \sum_k a^{j,k}(m)Q_{k,i} = 0.$$

This proves identity (5.7).

Again there is a factor of 2 difference between (5.7) and the formula obtained by Esposito, Marra and Yau [2] due to their generator being accelerated by a factor of 2.

Denote by Q^* the adjoint of Q and by Q^s the symmetric part. Notice that the matrix $B = (B_{i,j})_{1\le i,j\le d}$, defined by $B_{i,j} = \mathbb{V}_m(T\nabla_{e_i}\eta(0), T\nabla_{e_j}\eta(0))$, is symmetric so that $\alpha^* B\alpha = \alpha^* Q\alpha$ by virtue of Lemma 5.5. Therefore,

$$\big((a^{-1})^s\big)_{i,j} = \chi^{-1}(Q^s)_{i,j} = \chi^{-1}\mathbb{V}_m\big(T\nabla_{e_i}\eta(0), T\nabla_{e_j}\eta(0)\big). \tag{5.8}$$

Because, by Lemma 5.4, T is bounded above by 1 and $\mathbb{V}_m(\nabla_{e_i}\eta(0), \nabla_{e_i}\eta(0)) = 2\chi\delta_{i,j}$, $(a^{-1})^s$ is bounded above by 2. Therefore,

$$\big((a^{-1})^s\big)^{-1} \ge \tfrac{1}{2}I$$

in the matrix sense. In the next section we shall prove in fact that $a^s \ge (1/2)I$.

Note that the proof of $a^s(1/2)I$ presented in [2] is correct only in the case where a is symmetric.

6. Variational formulas for the diffusion coefficient. In this section, from Lemma 5.5 and the definition of Q, we obtain two variational formulas for the symmetric part of the diffusion coefficient a and its inverse a^{-1}. A variational formula for the symmetric part of (a^{-1}) is also given in [2].

THEOREM 6.1. *For every α in $\mathbb{R}^d$,*

$$\begin{aligned} \alpha^*\big((a^{-1})^s\big)^{-1}\alpha &= \frac{1}{\chi}\inf_{g\in\mathscr{G}_m}\mathbb{V}_m\Big(\sum_i \alpha_i w_i^* - L^*g\Big),\\ \alpha^*(a^s)^{-1}\alpha &= \frac{1}{\chi}\inf_{g\in\mathscr{G}_m}\mathbb{V}_m\Big(\sum_i \alpha_i\nabla_{e_i}\eta(0) - L^*g\Big). \end{aligned} \tag{6.1}$$

PROOF. Since the codimension of $L^*\mathscr{G}_m$ is d and $T\nabla_{e_j}\eta(0)$ are linearly independent and orthogonal to $L^*\mathscr{G}_m$, $T\nabla_{e_j}\eta(0)$ and $L^*\mathscr{G}_m$ generate $\overline{\mathscr{G}_m}$. There exists therefore a matrix $b = (b_{i,j})_{1\le i,j\le d}$ such that

$$w_i^* - \sum_{j=1}^d b_{i,j}T\nabla_{e_j}\eta(0) \text{ belongs to } \overline{L^*\mathscr{G}_m}.$$

Taking the inner product with $T\nabla_{e_k}\eta(0)$, we obtain that $b = \chi(Q^s)^{-1} = \chi((a^{-1})^s)^{-1}$ because $\mathbb{V}_m(w_i^*, T\nabla_{e_k}\eta(0)) = \chi\delta_{i,k}$, $(Q^s)_{i,j} = \mathbb{V}_m(T\nabla_{e_i}\eta(0), T\nabla_{e_j}\eta(0))$ and $T\nabla_{e_k}\eta(0)$ is orthogonal to $L^*\mathscr{G}_m$.

Therefore,

$$0 = \inf_{g \in \mathcal{G}_m} \mathbb{V}_m\left(\sum_{i=1}^{d} \alpha_i w_i^* - \sum_{1 \le i, j \le d} \alpha_i b^{i,j} T \, \nabla_{e_j} \eta(0) - L^* g \right).$$

Computing the inner product with the help of the identities proved in Lemma 5.4, we obtain

$$\alpha^* b \alpha = \frac{1}{\chi} \inf_{g \in \mathcal{G}_m} \mathbb{V}_m\left(\sum_i \alpha_i w_i^* - L^* g \right).$$

To prove the second formula, since, by (5.3), $w_i^* - \sum_j a^{i,j} \nabla_{e_j} \eta(0)$ belongs to $L^* \mathcal{G}_m$, from the previous formula, we have

$$\alpha^* \left((a^{-1})^s \right)^{-1} \alpha = \frac{1}{\chi} \inf_{g \in \mathcal{G}_m} \mathbb{V}_m\left(\sum_{i,j} \alpha_i a^{i,j} \, \nabla_{e_j} \eta(0) - L^* g \right).$$

Define β in $\mathbb{R}^d$ as $a^* \alpha$: $\beta_i = \sum_j a^{j,i} \alpha_i$. Since $((a^{-1})^s)^{-1} = a(a^s)^{-1} a^*$, the left-hand side of the last formula can be written as $(a^* \alpha)^* (a^s)^{-1} a^* \alpha = \beta^* (a^s)^{-1} \beta$. Therefore,

$$\beta^* (a^s)^{-1} \beta = \frac{1}{\chi} \inf_{g \in \mathcal{G}_m} \mathbb{V}_m\left(\sum_j \beta \, \nabla_{e_j} \eta(0) - L^* g \right).$$

This concludes the proof of the lemma. □

These two variational formulas provide a numerical method to check if the diffusion coefficient is symmetric, which we shall explain later. Moreover, they provide an upper bound and a lower bound for the diffusion coefficient and a simple proof of the continuity of the diffusion coefficient in the case where it is symmetric. More precisely, we have the following three corollaries.

COROLLARY 6.2. *For each β in $\mathbb{R}^d$*,

$$\begin{aligned} \beta^* a^s \beta - \frac{1}{2} \beta^* \beta &= \frac{1}{\chi} \sup_{g \in \mathcal{G}_m} \Bigg\{ \sum_{i=1}^{d} \beta_i \mathbb{V}_m\left(\nabla_{e_i} \eta(0), L^* g \right) \\ &\qquad + \frac{1}{2\chi} \sum_i \left(\mathbb{V}_m\left(\nabla_{e_i} \eta(0), L^* g \right) \right)^2 - \mathbb{V}_m(L^* g, L^* g) \Bigg\}. \end{aligned}$$

PROOF. From the variational principle, we have

$$\beta^* a^s \beta = \sup_{\alpha} \left\{ 2 \alpha^* \beta - \alpha^* (a^s)^{-1} \alpha \right\}$$

for every β in $\mathbb{R}^d$. From the previous theorem this last expression is equal to

$$\frac{1}{\chi} \sup_{\alpha \in \mathbb{R}^d,\, g \in \mathscr{G}_m} \Big\{ 2\chi\alpha^*\beta - 2\chi\alpha^*\alpha + 2\sum_i \alpha_i \mathbb{V}_m\big(\nabla_{e_i}\eta(0), L^*g\big) - \mathbb{V}_m(L^*g, L^*g) \Big\}.$$

To conclude the proof of the lemma, we need just to maximize over α. □

Since the supremum is positive, a^s is bounded below below by $(1/2)I$ in the matrix sense:

$$\alpha^* a \alpha \geq \tfrac{1}{2}|\alpha|^2$$

for every α in $\mathbb{R}^d$.

Since $((a^{-1})^s)^{-1} \geq a^s$ and the equality holds if and only if a is symmetric, from (6.1) and Corollary 6.2 we have that a is not symmetric if and only if, for some α and $g, h \in \mathscr{G}_m$,

$$\begin{aligned} &\frac{1}{\chi}\mathbb{V}_m\Big(\sum_i \alpha_i w_i^* - L^*g\Big) - \frac{1}{2}\alpha^*\alpha \\ &\quad \geq \frac{1}{\chi}\Big\{ \sum_{i=1}^d \alpha_i \mathbb{V}_m\big(\nabla_{e_i}\eta(0), L^*h\big) \\ &\qquad + \frac{1}{2\chi}\sum_i \Big(\mathbb{V}_m\big(\nabla_{e_i}\eta(0), L^*h\big)\Big)^2 - \mathbb{V}_m(L^*h, L^*h)\Big\}. \end{aligned} \tag{6.2}$$

Since in the first formula of (6.1) the diffusion coefficient is expressed as an infimum, an upper bound is very easy to prove.

COROLLARY 6.3. *There exists a universal constant C_1 such that*

$$\alpha^* a \alpha \leq C_1 (2\chi)^{-1} |\alpha|^2$$

for every $\alpha \in \mathbb{R}^d$.

PROOF. Take $g = 0$ in the variational formula for $b = ((a^{-1})^s)^{-1}$. We get that

$$\alpha^* b \alpha \leq \frac{1}{\chi}\mathbb{V}_m\Big(\sum_i \alpha_i w_i^*\Big) \leq \frac{d}{\chi}\sum_i \alpha_i^2 \mathbb{V}_m(w_1^*).$$

A bound on $\mathbb{V}_m(w_1^*)$, uniform on m, is easy to obtain from the integration-by-parts formula and the characterization of $\mathbb{V}_m$ as a limit of finite-volume variances (cf. Lemma 7.4 and Theorem 3.2). In fact,

$$\mathbb{V}_m(w_1^*) \leq \sum_{b \in \mathbb{Z}^d} |b|^{d+(1/2)} \Big\langle \big(\Phi_b(w_1^*)\big)^2 \Big\rangle_m,$$

where $\Phi_b(\sigma_1)$ is the function given by the integration-by-parts formula.

Up to this point we proved that there exists a finite constant C_1 such that

$$\alpha^*\big((a^{-1})^s\big)^{-1}\alpha \leq C_1(2\chi)^{-1}|\alpha|^2$$

for every $\alpha \in \mathbb{R}^d$. To conclude the proof, we just have to recall that $((a^{-1})^s)^{-1} \geq a^s$. □

Finally, in the case where the diffusion coefficient is symmetric, the first variational formula obtained in Theorem 6.1 and the one obtained in Corollary 6.2 reduce to two variational formulas for a. This will permit us to prove that the diffusion coefficient is continuous provided it is symmetric.

COROLLARY 6.4. *Assume that the diffusion coefficient* a *is symmetric. Then it is continuous in* $(0, 1)$.

PROOF. In the case where the matrix a is symmetric, the first relation in (6.1) provides a variational formula for a. Since, by Lemma 4.2, $\mathbb{V}_m(\cdot)$ is continuous, this proves that $a^{i,i}(\cdot)$ and $a^{i,i}(\cdot) + 2a^{i,j}(\cdot) + a^{j,j}(\cdot)$ are upper semicontinuous functions in $(0, 1)$ for $1 \leq i, j \leq d$. On the other hand, by the same reasoning, Corollary 6.2 shows that $a^{i,i}(\cdot)$ and $a^{i,i}(\cdot) + 2a^{i,j}(\cdot) + a^{j,j}(\cdot)$ are lower semicontinuous functions in $(0, 1)$ for $1 \leq i, j \leq d$. This proves that $a^{i,j}(\cdot)$ is continuous in $(0, 1)$ for $1 \leq i, j \leq d$. □

7. Regularity properties of the diffusion coefficient. In this section we prove that the diffusion coefficient is continuous in the general case and give some technical results needed to fill in the gaps left in [7].

Recall the definition of $\mathfrak{F}$ defined in Section 4. The proof of the continuity of the diffusion coefficient a follows essentially from the continuity in m of $\mathbb{V}_m(F(m, \cdot))$ for every function F in $\mathfrak{F}$ proved in Section 4.

THEOREM 7.1. *The diffusion coefficient* a *is continuous in* $(0, 1)$.

PROOF. Fix $\varepsilon > 0$ and m in $[0, 1]$. Since $w_i^* - \sum_j a^{i,j}(m) \nabla_{e_j} \eta(0)$ belongs to $\overline{L^* \mathscr{G}_m}$, there exists a cylinder function $H_i(m, \eta)$ in $\mathscr{G}_m$ such that

$$\mathbb{V}_m\left(w_i^* - \sum_j a^{i,j}(m) \nabla_{e_j} \eta(0) - L^* H_i(m, \eta)\right) \leq \varepsilon.$$

Up to the end of this proof, we will denote w_i^* by $w_i^*(m)$ to stress the dependence of w_i^* on m.

Fix $0 \leq m_0 \leq 1$. For $0 \leq m \leq 1$, define $F_{i, m_0}(m, \eta)$ by

$$F_{i, m_0}(m, \eta) = H_i(m_0, \eta) - \langle H_i(m_0, \eta) \rangle_m - \partial_\rho \langle H_i(m_0, \eta) \rangle_\rho |_{\rho = m} [\eta(0) - m].$$

Notice that $F_{i, m_0}(m, \eta)$ belongs to $\mathscr{G}_m$. Moreover, $F_{i, m_0}(m, \cdot)$ is a cylinder function with uniform support and $F_{i, m_0}(\cdot, \eta)$ is smooth. Therefore, $F_{i, m_0}(m, \eta)$ belongs to $\mathfrak{F}$.

To keep the notation simple, we introduce the following notation:

$$\tilde{H}_{i, m_0}(m) = \partial_\rho \langle H_i(m_0, \eta) \rangle_\rho |_{\rho = m}.$$

Recall that $\tilde{H}_{i, m_0}(m_0) = 0$ since $H_i(m_0, \eta)$ belongs to $\mathscr{G}_{m_0}$.

From Lemma 4.3, for each fixed m_0,

$$\mathbb{V}_m\Big(w_i^*(m) - \sum_j a^{i,j}(m_0)\,\nabla_{e_j}\eta(0) - L^* F_{i,m_0}(m,\eta)\Big)$$
$$= \mathbb{V}_m\Big(w_i^*(m) - \sum_j a^{i,j}(m_0)\,\nabla_{e_j}\eta(0) - L^* H_i(m_0,\eta) - \tilde{H}_{i,m_0}(m) L^*\eta(0)\Big)$$

is continuous in m. At m_0 this function is bounded by ε. In particular, there exists a neighborhood N_{m_0} of m_0 such that the above continuous function is bounded by 2ε. In this way, for each m_0 in $[0,1]$, we obtain a function $F_{i,m_0}(m,\eta)$ in $\mathfrak{F}$ such that

$$\mathbb{V}_m\Big(w_i^*(m) - \sum_j a^{i,j}(m_0)\,\nabla_{e_j}\eta(0) - L^* F_{i,m_0}(m,\eta)\Big) \le 2\varepsilon$$

for m in N_{m_0}. The family $\{N_{m_0}, m_0 \in [0,1]\}$ constitutes an open covering of $[0,1]$ and we may therefore find a finite open subcovering. Since $\mathfrak{F}$ is closed under addition, by interpolation we may construct smooth functions $a_\varepsilon^{i,j}(m)$ and $H_i^\varepsilon(m,\eta)$ in $\mathfrak{F}$ such that

$$\mathbb{V}_m\Big(w_i^*(m) - \sum_j a_\varepsilon^{i,j}(m)\,\nabla_{e_j}\eta(0) - L^* H_i^\varepsilon(m,\eta)\Big) \le 2\varepsilon.$$

From the triangle inequality it follows that

$$\mathbb{V}_m\Big(\sum_j \big[a_\varepsilon^{i,j}(m) - a^{i,j}(m)\big]\,\nabla_{e_j}\eta(0) + L^* H_i^\varepsilon(m,\eta) - L^* H_i(m,\eta)\Big)$$
$$\le 2\mathbb{V}_m\Big(w_i^*(m) - \sum_j a_\varepsilon^{i,j}(m)\,\nabla_{e_j}\eta(0) - L^* H_i^\varepsilon(m,\eta)\Big)$$
$$+ 2\mathbb{V}_m\Big(w_i^*(m) - \sum_j a^{i,j}(m)\,\nabla_{e_j}\eta(0) - L^* H_i(m,\eta)\Big) \le 6\varepsilon.$$

From this inequality we want to conclude that on each compact subset of $(0,1)$ the difference $a_\varepsilon^{i,j}(m) - a^{i,j}(m)$ is uniformly bounded by $C\sqrt{\varepsilon}$. This will prove that the diffusion coefficient $a^{i,j}(m)$ can be uniformly approximated by smooth functions on each compact subset of $(0,1)$ and is therefore continuous in $(0,1)$.

To keep the notation simple, denote the difference $a_\varepsilon^{i,j}(m) - a^{i,j}(m)$ by $b_\varepsilon^{i,j}(m)$ and the cylinder function $H_i^\varepsilon(m,\eta) - H_i(m,\eta)$ by $G_i^\varepsilon(m,\eta)$. Recall the definition of the matrix Q defined just before (5.7). We will now evaluate the inner product

$$\mathbb{V}_m\Big(\sum_j b_\varepsilon^{i,j}(m)\,\nabla_{e_j}\eta(0) + L^* G_i^\varepsilon(m,\eta),\ \sum_k a^{k,l}(m) T\,\nabla_{e_k}\eta(0)\Big)$$

for fixed i and l. From the definition of Q and the fact that $T\nabla_{e_k}\eta(0)$ is orthogonal to $L^*\mathcal{G}_m$, this expression is equal to

$$\sum_{j,k} b_\varepsilon^{i,j}(m) Q_{j,k} a^{k,l}(m) = 2\chi \sum_j b_\varepsilon^{i,j}(m)\,\delta_{j,l} = 2\chi b_\varepsilon^{i,l}(m).$$

On the other hand, by the Schwarz inequality and the previous bounds, the inner product is bounded above by

$$(6\varepsilon)^{1/2}\left\{\mathbb{V}_m\left(T\sum_k a^{k,l}(m)\,\nabla_{e_k}\eta(0)\right)\right\}^{1/2}.$$

From the definition of the matrix Q and the proof of Theorem 6.1, this last inner product is equal to

$$\sum_{j,k} a^{j,l}(m) Q_{j,k} a^{k,l}(m) = 2\chi \sum_j a^{j,l}(m)\,\delta_{j,l} = 2\chi a^{l,l}(m).$$

In conclusion, we showed that $|a_\varepsilon^{i,l}(m) - a^{i,l}(m)|$ is bounded above by

$$\sqrt{12\chi^{-1}a^{l,l}(m)}\,\sqrt{\varepsilon}.$$

In Corollary 6.3 above we proved that $a^{l,l}(m)$ is uniformly bounded on each compact subset of $(0,1)$. This concludes the proof of the theorem. □

With the same ideas we prove a useful result.

COROLLARY 7.2. *For each* $1 \le i \le d$ *and* $\delta > 0$,

$$\inf_{F\in\mathfrak{F}} \sup_{\delta\le m\le 1-\delta} \mathbb{V}_m\left(w_i^* - \sum_{j=1}^d a^{i,j}(m)\,\nabla_{e_i}\eta(0) - L^*F\right) = 0.$$

PROOF. We have to avoid both ends of the interval $[0,1]$ because we proved the continuity of the diffusion coefficient a only on $(0,1)$.

Fix $1 \le i \le d$. From Lemma 5.1 we know that, for each m in $[0,1]$,

$$\inf_{F\in\mathcal{G}_m} \mathbb{V}_m\left(w_i^* - \sum_{j=1}^d a^{i,j}(m)\,\nabla_{e_i}\eta(0) - L^*F\right) = 0.$$

The corollary thus states that we may interchange the order of supremum and infimum. Fix $\varepsilon > 0$. For m_0 in $[\delta, 1-\delta]$, there exists a function G_{m_0} in $\mathcal{G}_{m_0}$ such that

$$\mathbb{V}_{m_0}\left(w_i^*(m_0) - \sum_{j=1}^d a^{i,j}(m_0)\,\nabla_{e_i}\eta(0) - L^*G_{m_0}\right) \le \varepsilon.$$

To keep the notation as simple as possible, until the end of the proof we denote the function $w_i^*(m) - \sum_{j=1}^d a^{i,j}(m)\nabla_{e_i}\eta(0)$ by $Z_m(\eta)$. Recall the notation introduced in the beginning of this section. For m in $[0,1]$, define the cylinder function F_m as

$$F_m(\eta) = G_{m_0}(\eta) - \tilde{G}_{m_0}(m) - \tilde{G}'_{m_0}(m)[\eta(0) - m].$$

We defined F_m in such a way that F_m belongs to $\mathcal{G}_m$ for every m in $[0,1]$. More than that, $F(m,\eta)$ belongs in fact to $\mathfrak{F}$ since it is smooth in the first variable and has a uniform support.

We claim that, near m_0,

$$\mathbb{V}_m(Z_m - L^* F_m)$$

is small. Indeed, this expression, which is equal to

$$\mathbb{V}_m\Big(Z_m - L^* G_{m_0} - \tilde{G}'_{m_0}(m) L^*[\eta(0) - m]\Big),$$

is bounded above by

$$\Big|\mathbb{V}_m\Big(Z_m - L^* G_{m_0} - \tilde{G}'_{m_0}(m) L^*\eta(0)\Big) - \mathbb{V}_{m_0}\Big(Z_{m_0} - L^* G_{m_0} - \tilde{G}'_{m_0}(m_0) L^*\eta(0)\Big)\Big|$$
$$+ \mathbb{V}_{m_0}\big(Z_{m_0} - L^* G_{m_0}\big).$$

From Lemma 4.3 and Theorem 7.1, the first line vanishes in the limit as m converges to m_0. On the other hand, the second line is bounded by ε by construction.

Therefore, there exists a neighborhood N_{m_0} of m_0 such that

$$\mathbb{V}_m(Z_m - L^* F_m) \le 2\varepsilon$$

for m in N_{m_0}. The family $\{N_{m_0},\ m_0 \in [\delta, 1-\delta]\}$ constitutes an open covering of $[\delta, 1-\delta]$ and we may therefore extract a finite subcovering. In this way we obtain a finite family of open intervals $(N_i)_{1\le i\le n_0}$ whose union is equal to $[\delta, 1-\delta]$ and an associated family of functions $(F_i)_{1\le i\le n_0}$ in $\mathfrak{F}$ such that

$$\mathbb{V}_m(Z_m - L^* F_i(m,\eta)) \le 2\varepsilon$$

if $m \in N_i$. By interpolation, we obtain from this family a function F in $\mathfrak{F}$ such that

$$\sup_{m\in[\delta,1-\delta]} \mathbb{V}_m(Z_m - L^* F(m,\eta)) \le 2\varepsilon.$$

This concludes the proof of the lemma. □

The following lemma is used in Section 7 of [7].

LEMMA 7.3. *For $\delta > 0$ and $1 \le i \le d$, let $\{H_k^i(m,\eta);\ k > 1\}$ be a sequence of functions in $\mathfrak{F}$ such that*

$$\lim_{k\to\infty} \sup_{\delta\le m\le 1-\delta} \mathbb{V}_m\left(w_i^* - \sum_{j=1}^{d} a^{i,j}(m)\,\nabla_{e_i}\eta(0) - L^* H_k^i(m)\right) = 0.$$

Such a sequence exists by virtue of Corollary 7.2.

For every $v \in \mathbb{R}^d$ and $\delta \le m \le 1-\delta$,

$$\lim_{k\to\infty} \frac{1}{4\chi} \sum_i \left\langle \left\{\nabla_{e_i} \sum_j v_j \sum_x \tau_x H_k^j\right\}^2 \right\rangle_m = \sum_{i,j} v_i a^{i,j}(m) v_j - \frac{1}{2}|v|^2.$$

PROOF. We compute the inner product of $w_i^* - \sum_{j=1}^{d} a^{i,j}(m)\nabla_{e_i}\eta(0) - L^* H_k^i(m)$ with respect to $\nabla_{e_l}\eta(0)$, using identity (5.2) and relation (5.1). In this way, we obtain, applying the Schwarz inequality,

$$\left| \chi\delta_{i,l} - 2a^{i,l}(m)\chi + 2\langle w_l, H_k^i\rangle_{m,0}\right| \le o_k(1)(2\chi)^{1/2}.$$

Repeating the same procedure with $L_s H_k^l$ instead of $\nabla_{e_l}\eta(0)$, we obtain

$$\left| -\langle w_i^*, H_k^l\rangle_{m,0} + \langle L^* H_k^i, H_k^l\rangle_{m,0}\right| \le o_k(1)\left\{\mathbb{V}_m\left(L_s H_k^l\right)\right\}^{1/2} \tag{7.1}$$

because $L_s\mathscr{G}_m$ is orthogonal to the space generated by $\nabla_{e_i}\eta(0)$ for $1 \le i \le d$. A simple computation shows that $\mathbb{V}_m(L_s H_k^l) \le \mathbb{V}_m(L^* H_k^l)$. By the Schwarz inequality we have

$$\mathbb{V}_m\left(L^* H_k^l\right) \le o_k(1) + 2\mathbb{V}_m\left(w_i^* - \sum_{j=1}^{d} a^{i,j}(m)\nabla_{e_i}\eta(0)\right).$$

Since a is continuous, the right-hand side of this expression is bounded. This shows that the right-hand side of (7.1) is of order $o_k(1)$.

Since $\langle w_i + w_i^*, H_k^l\rangle_{m,0} = 0$, from the two previous equalities we get

$$\tfrac{1}{2}\delta_{i,j} - a^{i,j}(m) - \chi^{-1}\langle L^* H_k^i, H_k^j\rangle_{m,0} = o_k(1).$$

Thus, for every $v \in \mathbb{R}^d$,

$$\tfrac{1}{2}|v|^2 - \sum_{i,j} v_i a^{i,j} v_j = \chi^{-1}\left\langle L^* \sum_i v_i H_k^i, \sum_j v_j H_k^j\right\rangle_{m,0} + o_k(1). \tag{7.2}$$

Since the first term on the right-hand side is equal to

$$\chi^{-1}\left\langle L^s \sum_i v_i H_k^i, \sum_j v_j H_k^j\right\rangle_{m,0} = -\frac{1}{4\chi}\sum_i\left\langle\left\{\nabla_{e_i}\sum_j v_j \sum_x \tau_x H_k^j\right\}^2\right\rangle_m,$$

the lemma is proved. □

We conclude this section with the statement of the integration-by-parts formula. The proof is omitted since it is similar to the proof of Lemma 6.1 in [2].

LEMMA 7.4 (Integration-by-parts formula). *Let g be a cylinder function. Denote by ℓ the smallest integer such that Λ_ℓ contains the support of g. Fix $K \ge \ell$ and x such that $\tau_x g$ is measurable with respect to $\{\eta(z),\ z \in \Lambda_K\}$. Recall the definition of $\tilde{g}_K$ given in Definition* 3.1. *Assume that*:

(i) $\tilde{g}(j/\overline{K}^d) = 0$;
(ii) $\tilde{g}'(j/\overline{K}^d) = 0$ *for some* $0 \le j \le \overline{K}^d$.

Then there exists a family of functions $\{\Phi_b(x, g);\ b \in \Lambda_K\}$ *such that*

$$\left\langle \tau_x g - \tilde{g}_K\left(j/\overline{K}^d\right), h\right\rangle_{K,\,j/\overline{K}^d} = \sum_{b \in \Lambda_K} \left\langle \Phi_b(x, g), \nabla_b h\right\rangle_{K,\,j/\overline{K}^d} \tag{7.3}$$

and

$$\sum_{b \in \Lambda_K} |b - x|^{d+(1/2)} \left\langle \left(\Phi_b(x, g)\right)^2\right\rangle_{K,\,j/\overline{K}^d} \le C(g)$$

for some constant $C(g)$ *that does not depend on* K *or* x. *In fact*, $C(g)$ *depends only on* g *through the length of the support of* g, *denoted by* ℓ, *and through* $\|g\|_\infty$.

Instead, *assume that* g *satisfies*:

(i) $\tilde{g}(m) = 0$;
(ii) $\tilde{g}'(m) = 0$ *for some* m *in* $[0, 1]$.

Then there exists a family of functions $\{\Phi_b(x, g);\ b \in \Lambda_K\}$ *satisfying* (7.3) *and such that*

$$\sum_{b \in \Lambda_K} |b - x|^{d+(1/2)} \left\langle \left(\Phi_b(x, g)\right)^2\right\rangle_m \le C(g)$$

for some constant $C(g)$ *satisfying the same properties mentioned above*.

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REFERENCES

[1] ESPOSITO, R., MARRA, R. and YAU, H. T. (1994). Diffusive limit of asymmetric simple exclusion. *NATO Adv. Sci. Inst. Ser. B: Phys.* **324** 43–53.

[2] ESPOSITO, R., MARRA, R. and YAU, H. T. (1994). Diffusive limit of asymmetric simple exclusion. *Rev. Math. Phys.* **6** (Special Issue) 1233–1267.

[3] EYINK, G. L., LEBOWITZ, J. L. and SPOHN, H. (1995). Hydrodynamics and fluctuations outside local equilibrium: driven diffusive systems. Preprint.

[4] FUNAKI, T., UCHIYAMA, K. and YAU, H. T. (1995). Hydrodynamic limit for lattice gas under Bernoulli measures. In *Nonlinear Stochastic PDE's* (T. Funaki and W. Woyczinky, eds.) 1–40. Springer, New York.

[5] KATZ, S., LEBOWITZ, J. L. and SPOHN, H. (1984). Non equilibrium steady state of stochastic lattice gas models of fast ionic conductors. *J. Statist. Phys.* **34** 497–537.

[6] KIPNIS, C. and LANDIM, C. (1995). Hydrodynamic limit of interacting particle systems. Preprint.

[7] LANDIM, C., OLLA, S. and YAU, H. T. (1996). First order correction for the hydrodynamic limit of asymmetric simple exclusion processes in dimension $d \ge 3$. *Comm. Pure Appl. Math.* To appear.

[8] QUASTEL, J. (1992). Diffusion of colors in the simple exclusion process. *Comm. Pure Appl. Math.* **45** 321–379.

[9] REZAKHANLOU, F. (1990). Hydrodynamic limit for attractive particle systems on Z^d. *Comm. Math. Phys.* **140** 417–448.

[10] SPOHN, H. (1991). *Large Scale Dynamics of Interacting Particles*. Springer, New York.

[11] VARADHAN, S. R. S. (1993). Nonlinear diffusion limit for a system with nearest neighbor interactions. II. In *Asymptotic Problems in Probability Theory: Stochastic Models and Diffusion on Fractals* (K. Elworthy and N. Ikeda, eds.) 75–128. Longman, Harlow, UK.

[12] VARADHAN, S. R. S. (1994). Regularity of self diffusion coefficient. In *The Dynkin Festschrift* (M. Freidlin, ed.) 387–397. Birkhäuser, Boston.

[13] XU, L. (1993). Diffusion limit for the lattice gas with short range interactions. Ph.D. dissertation, Courant Institute, New York Univ.

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