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Hydrodynamic Limit of a Nongradient Interacting Particle Process

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A simple example of a "nongradient" stochastic interacting particle system is analyzed. In this model, symmetric simple exclusion in one dimension in a periodic environment, the dynamical term in the Green–Kubo formula contributes to the bulk diffusion constant. The law of large numbers for the density field and the central limit theorem for the density fluctuation field are proven, and the Green–Kubo expression for the diffusion constant is computed exactly. The hydrodynamic equation for the model turns out to be linear.

KEY WORDS: Nonequilibrium statistical mechanics; interacting particle systems; hydrodynamic limit; Green–Kubo formula; simple exclusion process.

INTRODUCTION

Recent results in the hydrodynamic theory of stochastic, reversible, interacting particle systems lead to the conclusion that our understanding of models enjoying the so-called "gradient" condition is in relatively good shape. For these models, with certain exceptions, one now has a scheme of general validity for proving the law of large numbers (LLN) for the density field[6,9] and the central limit theorem (CLT) for the equilibrium density fluctuation field.[1–3,14] The bulk diffusion constant is given by the first term in the Green–Kubo formula and is computable and always strictly positive.[2,13] (One exception to this picture is the interacting Brownians,[14] for which the LLN has not yet been proven, due to purely technical difficulties with unbounded densities.) Only the nonequilibrium fluctuation theory is—I refer to rigorous results—in relatively bad shape.

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What is the gradient condition? Fick's law of diffusion states that the current should be given by minus the bulk diffusion "constant" (it generally is a function of the density) times the density gradient. "Gradient" models are (stochastic) models in which the nonrandom part of the current is given by the "gradient" of a local function. The local equilibrium assumption then implies that the expected current is a "gradient" of a (generally nonlinear) function of the local density, and hence proportional to the density gradient itself. Thus, in this class of models there is a sort of exact microscopic form of Fick's law holding. In particular, there is a simple formula, involving only (derivatives of) equilibrium expectations of local functions, for the transport coefficient.

Examples of gradient models which have been considered are: symmetric simple exclusion and some one-dimensional generalizations (exclusion processes with speed change, also called "lattice gases")[2]; the zero-range process[1,16]; interacting Brownians[14]; and a model with continuous spins on the lattice called the Ginsburg–Landau model.[4,6]

Unfortunately, gradient models form only a set of low dimension (in some sense) in the space of stochastic, reversible models with local conservation laws. [This is most easily seen for the family of reversible exclusion processes with speed change, in which gradient models with nearist-neighbor jumps and interactions form a surface of codimension two in one-dimensional models and reduce to a point (symmetric simple exclusion) in higher dimensions.[13] The "generic" model is nongradient. Until recently, there were no successes (in the rigorous sense) for nongradient models. Now, however, Fritz[5] and Varadhan[17] have separately treated non-gradient generalizations of a Ginsburg–Landau type model. In this paper I treat what is probably the simplest nongradient particle model: the simple exclusion process with periodic (alternating) jump rates, in one dimension. This example was suggested several years ago to the author by H. Spohn, who also discovered that the Green–Kubo expression for the bulk diffusion constant in this model could be evaluated explicitly. Using a curious identity (which gives a useful decomposition of the current into gradient-plus-negligible term) together with the Guo–Papanicolaou–Varadhan entropy argument (ref. 6; see also ref. 16), I prove the LLN for this model, and verify that the bulk diffusion constant is indeed given by the Green–Kubo formula. I also treat the equilibrium fluctuations.

This model should not be thought of as a "generic" case. Although genuinely nongradient, there are certain simplifying features (such as the decomposition mentioned above) that one does not expect in the "generic" nongradient model. In addition, the hydrodynamic equation for the model comes out to be linear. Thus, it shares this feature with the usual simple-exclusion process (a gradient case). The bulk diffusion "constant" comes out genuinely constant, equal to the harmonic mean of the two jump rates (the author thanks H. Rost for pointing out this fact).

In the first section I introduce the model, the hydrodynamic scaling, and discuss the meaning (in mathematical terms) of the nongradient property. The hydrodynamic equation for the model is also introduced. In a second section the results are stated. A third section contains some identities used for the analysis of the model. In the fourth section the proofs of the theorems stated in Section 2 are sketched. [Since the proofs are eventually reduced to establishing for this model facts already proven in other contexts, and since these facts can be proven using the same techniques (modulo the necessary changes), only the essential points will be discussed in any detail.] A fifth section introduces the Green–Kubo formula, and evaluates it using an identity proved in Section 3. A final section contains some remarks. The reader less interested in the mathematical details of the proofs might simply skip Section 4.

1. THE MODEL

Our process will be a finite-volume, continuous-time Markov process in a space of particle configurations. The state space of our process will be

$$\mathscr{E}_{2K} = \{0, 1\}^{\{1,2,\ldots,2K\}} \tag{1.1}$$

where K is a positive integer. Thus, a configuration is a zero-or-one-valued function $\eta(x)$, where x denotes a site ($1 \leqslant x \leqslant 2K$), and $\eta(x) = 1$ (0) is interpreted as x occupied (unoccupied) by a particle. Particles jump to nearest-neighbor sites, provided they are unoccupied, with symmetrical rates which, however, depend on the site where the particle is sitting. If the particle is at an even-numbered site, the jump rate will be $\alpha > 0$; it will be $\beta > 0$ at odd-numbered sites. Thus, the infinitesimal generator of the process will be

$$\begin{aligned} Lf(\eta) = \sum_{2\mid x} & \{\alpha\eta(x)[1-\eta(x+1)] + \beta\eta(x+1)[1-\eta(x)]\} \\ & \times [f(\eta^{x,x+1}) - f(\eta)] \\ & + \sum_{2\nmid x} \{\beta\eta(x)[1-\eta(x+1)] + \alpha\eta(x+1)[1-\eta(x)]\} \\ & \times [f(\eta^{x,x+1}) - f(\eta)] \end{aligned} \tag{1.2}$$

where $\eta^{x,x+1}$ denotes η with the occupations of x and $x+1$ interchanged, and we use periodic boundary conditions so that addition is taken modulo $2K$. The transition probabilities are determined by L in the usual way:

$$p_t(\eta' \mid \eta) = e^{Lt}(\eta', \eta) \tag{1.3}$$

See, e.g., ref. 10. The corresponding continuous-time Markov process will be denoted η_t, $t \geqslant 0$. Note that particle number is conserved.

The special case $\alpha = \beta$ is the famous symmetric simple exclusion process, about which almost everything is known. (See ref. 2 and references therein.) Taking $\alpha \neq \beta$ gives our nongradient model. I will next discuss this point, and introduce hydrodynamic scaling at the same time.

Let $\varepsilon = (2K)^{-1}$, and set the lattice spacing equal to ε. Regard the configuration η as a particle configuration in the interval $[0, 1]$. We consider the limit $K \to \infty$ $(\varepsilon \to 0)$ while speeding up the time by a factor of ε^{-2}. Given a C^∞ test function ϕ with period one, define the density field by

$$X_t^\varepsilon(\phi) = \varepsilon \sum_{x=1}^{\varepsilon^{-1}} \phi(\varepsilon x)\, \eta_{\varepsilon^{-2}t}(x) \tag{1.4}$$

Now set $\alpha = \beta$ and consider the time derivative of the expected value of the density field (with arbitrary initial distribution). After an easy computation (left to the reader) one finds

$$\frac{\partial}{\partial t} EX_t^\varepsilon(\phi) = \varepsilon^{-2} ELX_t^\varepsilon(\phi) = \alpha\varepsilon \sum_x \phi''(\varepsilon x)\, E\eta_{\varepsilon^{-2}t}(x) + O(\varepsilon) \tag{1.5}$$

The "gradient condition" in its simplest form can be seen in (1.5): the factor of ε^{-2} has disappeared, absorbed into a second derivative on the test function. [In other gradient models the occupation variable $\eta(x)$ appearing on the right side of (1.5) may be replaced by a different local function, e.g., $\eta(x)\, \eta(x+1)$. The crucial point is the appearance of the second derivative].

From (1.5) one obtains easily (for suitable initial states, by a compactness argument) that the expected density satisfies the diffusion equation in the hydrodynamic limit. Much more has been proven for this case: the LLN, local equilibrium, fluctuation theory, etc. The analysis of this special case is greatly simplified by the existence of a "dual" representation for the hierarchy of correlation functions in terms of finite particle systems.[2]

Next let us consider the case $\alpha \neq \beta$. To make the calculation more transparent, I first introduce the current functions:

$$\begin{aligned} j(x, x+1) &= \alpha\eta(x)[1-\eta(x+1)] - \beta\eta(x+1)[1-\eta(x)] \qquad \text{if } x \text{ is even} \\ &= \beta\eta(x)[1-\eta(x+1)] - \alpha\eta(x+1)[1-\eta(x)] \qquad \text{if } x \text{ is odd} \end{aligned} \tag{1.6}$$

In terms of these functions one has

$$L\eta(x)=j(x-1,x)-j(x,x+1) \tag{1.7}$$

If $\alpha=\beta$, $j(\cdot,\cdot)$ is a gradient:

$$j(x,x+1)=\alpha(\eta(x)-\eta(x+1))$$

which leads to (1.5). However, if $\alpha\neq\beta$, we obtain in place of (1.5)

$$\begin{aligned}
&\varepsilon^{-2}L\left\{\varepsilon\sum_x\phi(\varepsilon x)\,\eta(x)\right\}\\
&\quad=\varepsilon^{-2}\left\{\varepsilon\sum_x\phi(\varepsilon x)[j(x-1,x)-j(x,x+1)]\right\}\\
&\quad=\varepsilon^{-2}\left\{\varepsilon\sum_{2|x}[\phi(\varepsilon x)-\phi(\varepsilon(x-1))]\,j(x-1,x)\right.\\
&\qquad\left.+\varepsilon\sum_{2|x}[\phi(\varepsilon(x+1))-\phi(\varepsilon x)]\,j(x,x+1)\right\}\\
&\quad=\varepsilon\sum_{2|x}\varepsilon^{-1}\phi'(\varepsilon x)[j(x-1,x)+j(x,x+1)]\\
&\qquad+\frac{\varepsilon}{2}\sum_{2|x}\phi''(\varepsilon x)[-j(x-1,x)+j(x,x+1)]+O(\varepsilon)
\end{aligned}\tag{1.8}$$

From (1.6) we find for x even

$$\begin{aligned}
&j(x-1,x)+j(x,x+1)\\
&\quad=\beta[\eta(x-1)-\eta(x+1)]+(\alpha-\beta)[\eta(x-1)\,\eta(x)-\eta(x)\,\eta(x+1)]
\end{aligned}\tag{1.9}$$

It is the second term on the right side of the last equality in (1.9) which causes problems. By (1.8), there is a term, if $\alpha\neq\beta$, apparently $O(\varepsilon^{-1})$ and containing only a first derivative of the test function. This is the characteristic difficulty in nongradient models. In addition, if $\alpha\neq\beta$, the duality is destroyed and one must use other methods.

I next discuss the invariant measures for our process and hydrodynamic scaling of the initial state. We will make use of "grand canonical" states, product measures with periodically varying densities. If the density of this product measure is taken to be ρ_e at even sites and ρ_o at odd sites, then this measure will be time reversible (hence time invariant) provided the detailed balance condition

$$\alpha\rho_e(1-\rho_o)=\beta(1-\rho_e)\,\rho_o \tag{1.10}$$

is satisfied. One can then define the average density by

$$\rho=\frac{1}{2}(\rho_e+\rho_o) \tag{1.11}$$

One can express ρ_e and ρ_o in terms of α, β, and ρ if one wants, but it will be more convenient for computations to parametrize these states in terms of a fugacity ζ by setting

$$\rho_e=\frac{\zeta}{\zeta+\alpha}, \qquad \rho_o=\frac{\zeta}{\zeta+\beta} \tag{1.12}$$

It is obvious that the corresponding product measure with these densities satisfies detailed balance. We denote it by μ_ζ. [The general time-invariant measure (with a fixed number of sites) is obtained by conditioning on the particle number $N\equiv\sum\eta(x)$ and taking arbitrary convex combinations.] Note that there is an invertible relation $\rho=\rho(\zeta)$ defined by

$$\rho=\frac{1}{2}\,[\mu_\zeta(\eta(0))+\mu_\zeta(\eta(1))] \tag{1.13}$$

For the first theorem we will need to make the initial density slowly varying. It is convenient to make use of the parametrization (1.12), making the fugacity slowly varying. Given a continuous function ζ: $[0, 1]\to(0, +\infty)$ with $\zeta(0)=\zeta(1)$, define

$$\mu^\varepsilon\left(\prod_{x\in A}\eta(x)\right)=\prod_{2\mid x,\, x\in A}\frac{\zeta(\varepsilon x)}{\zeta(\varepsilon x)+\alpha}\prod_{2\nmid y,\, y\in A}\frac{\zeta(\varepsilon x)}{\zeta(\varepsilon x)+\beta} \tag{1.14}$$

It is easy to see that μ^ε defines a density profile in the hydrodynamic limit in the sense that, for all $\delta>0$ and ϕ,

$$\mu^\varepsilon\left[\left|X_0^\varepsilon(\phi)-\int_0^1\phi(r)\,\rho_0(r)\,dr\right|>\delta\right]\to 0 \tag{1.15}$$

as $\varepsilon\to 0$, where $\rho_0(r)=\rho(\zeta(r))$. We write P^ε and E^ε for the path measure and expectation (respectively) with respect to the process with initial state μ^ε.

Before stating the theorems, let us recall the form of the hydrodynamic equation for a reversible model with a single conservation law. In this class of models we expect the density field to have a hydrodynamic scaling limit satisfying a (typically nonlinear) diffusion equation. Thus, we expect to find for the limiting expected density

$$\lim_{\varepsilon \to 0} E^{\varepsilon} X_t^{\varepsilon}(\phi) = \int_0^1 \phi(r)\, \rho(r, t)\, dr \tag{1.16}$$

where $\rho(\cdot, \cdot)$ satisfies

$$\begin{gathered} \frac{\partial}{\partial t} \rho = \frac{\partial}{\partial r} D(\rho) \frac{\partial \rho}{\partial r} \\ \rho(\cdot, 0) \equiv \rho_0(\cdot) \end{gathered} \tag{1.17}$$

In (1.17), $D(\rho)$, the bulk diffusion constant, should be some positive function of ρ (possibly constant). In general, $D(\rho)$ is given by the Green–Kubo formula (see Section 5), and so cannot be determined except by a detailed analysis of the model. Gradient models are the exception to this rule: the bulk diffusion constant can be determined by a time-zero computation using a local equilibrium state. I give this computation to help clarify the meaning of the gradient property.

For simplicity assume translation invariance of the rates and invariant measures (the periodic case is similar). We compute the time derivative of the expected density field at $t = 0$ in the limit $\varepsilon \to 0$. This is expressible in terms of the Dirichlet form of the process given by

$$\langle f(-L) f \rangle = \frac{1}{2} \sum_x \langle c_{x,x+1} (f^{x,x+1} - f)^2 \rangle \tag{1.18}$$

In (1.18), $\langle \cdot \rangle$ denotes equilibrium expectation and $c_{x,x+1}$ is the rate function for interchanging the occupations at x and $x+1$. For convenience, introduce a chemical potential λ, i.e., write $\zeta = \exp(\lambda)$. Making the chemical potential slowly varying in the initial state and using the bilinear form of (1.18), we obtain

$$\begin{aligned} -\frac{d}{dt}\bigg|_0 E^{\varepsilon} X_t^{\varepsilon}(\phi) &= \left\langle \frac{\exp[\sum \lambda(\varepsilon x)\, \eta(x)]}{Z^{\varepsilon}}\, \varepsilon^{-2} (-L)\, X^{\varepsilon}(\phi) \right\rangle \\ &= \frac{1}{2} \varepsilon \sum_x \lambda'(\varepsilon x)\, \phi'(\varepsilon x)\, \mu^{\varepsilon} \{ c_{x,x+1} [\eta(x) - \eta(x+1)]^2 \} + O(\varepsilon) \\ &\xrightarrow[\varepsilon \to 0]{} \int_0^1 \lambda'(r)\, \phi'(r) \langle c_{0,1} [\eta(0) - \eta(1)]^2 \rangle\, dr \\ &= \int_0^1 \rho'(r)\, \phi'(r)\, \hat{D}(\rho)\, dr \end{aligned} \tag{1.19}$$

In (1.19), $\hat{D}(\rho)$ is given by

$$\hat{D}(\rho) = [\chi(\rho)]^{-1} \langle c_{0,1}[\eta(0) - \eta(1)]^2 \rangle(\rho) \tag{1.20}$$

and $\chi(\rho)$, the equilibrium compressibility, is defined to be $d\rho/d\lambda$.

Comparing (1.17) with (1.19) and ignoring (at our peril) the problem of interchanging the time derivative with the hydrodynamic limit, we conclude that $D(\rho) = \hat{D}(\rho)$. However, we shall see in Section 5 that $\hat{D}(\rho)$ contains only the first term in the Green–Kubo formula for D. In the gradient case this is correct, as the second term vanishes. In the nongradient case the second term makes a nonvanishing contribution to D, so the interchange of derivative with limit above is faulty. In particular, the calculation above gives the wrong answer for our model. (It predicts that the hydrodynamic equation is nonlinear, while in fact it turns out to be linear.) Clearly, in the nongradient case the diffusion constant cannot be correctly computed from a local-equilibrium hypothesis alone. [One can also see the problem by computing the time derivative on the left side of (1.19) in terms of the current functions. To compute the limit, one needs to know the ε correction to the local equilibrium state. But this is of dynamical origin.]

2. RESULTS

Theorem 1 (LLN for the density field). For all $\delta > 0$ and $t \geqslant 0$

$$P_\varepsilon\left[\left|X_t^\varepsilon(\phi) - \int_0^1 \phi(r)\,\rho(r,t)\,dr\right| > \delta\right] \to 0 \tag{2.1}$$

as $\varepsilon \to 0$. Here $\rho(\cdot, \cdot)$ is the solution of the diffusion equation

$$\frac{\partial}{\partial t}\rho(r,t) = \frac{2\alpha\beta}{\alpha+\beta}\frac{\partial^2}{\partial r^2}\rho(r,t) \tag{2.2}$$

with initial condition

$$\rho(\cdot, 0) = \rho_0(\cdot) \tag{2.3}$$

Remarks. (i) Actually we will obtain the following stronger result: let Q_ε be the path measure of the process $X^\varepsilon(\cdot)$, regarded as a process in the space of positive measures on [0, 1], and let Q be the measure of the deterministic process supported on the single path $t \to \rho(\cdot, t)\,dr$. Then $Q_\varepsilon \to Q$ weakly as $\varepsilon \to 0$. (ii) We do not need to insist on the particular form of the initial state specified in (1.14). All that is necessary is that the initial state define an initial density profile and satisfy an entropy bound; see Section 4.

For the next theorem we need to define the density fluctuation field for the equilibrium process. Given a test function ϕ and $t \geqslant 0$, let

$$
\begin{aligned}
Y_t^\varepsilon(\phi) &= \varepsilon^{-1/2}\{X_t^\varepsilon(\phi) - EX_t^\varepsilon(\phi)\} \\
&= \varepsilon^{1/2}\left\{\sum_{2\mid x} \phi(\varepsilon x)[\eta_{\varepsilon^{-2}t}(x) - \rho_e] + \sum_{2\nmid x} \phi(\varepsilon x)[\eta_{\varepsilon^{-2}t}(x) - \rho_o]\right\} \qquad (2.4)
\end{aligned}
$$

Theorem 2 (CLT for the density fluctuation field). For the equilibrium process and every ϕ and $t \geqslant 0$

$$
Y_t^\varepsilon(\phi) \xrightarrow{d} Y_t(\phi) \qquad (2.5)
$$

(convergence in distribution), where $Y_\cdot(\cdot)$ is the Gaussian generalized Ornstein–Uhlenbeck process[7] with covariance

$$
EY_t^\varepsilon(\phi)\, Y_s^\varepsilon(\psi) = \chi(\rho)(\phi, e^{[2\alpha\beta/(\alpha+\beta)]\Delta t}\psi)_2 \qquad (2.6)
$$

where Δ denotes $\partial^2/\partial r^2$, $(\cdot, \cdot)_2$ is the inner product in $L_2([0, 1])$, and $\chi(\rho)$ is given by

$$
\chi(\rho) \equiv \frac{d\rho}{d\lambda} = \frac{1}{2}[\rho_e(1-\rho_e) + \rho_o(1-\rho_o)] \qquad (2.7)
$$

Remark. Again, the result actually proven is considerably stronger (weak convergence of path measures).

3. A KEY IDENTITY

In Section 2 we found a term in the time derivative of the density field apparently of order $O(\varepsilon^{-1})$. Here is a trick which allows one to overcome this apparent difficulty. By an explicit computation one discovers that

$$
\begin{aligned}
L\{\eta(-1)\eta(0) - \eta(0)\eta(1)\} &= \alpha[\eta(-2)\,\eta(0) - \eta(0)\,\eta(2)] \\
&\quad + (\beta-\alpha)[\eta(-2)\,\eta(-1)\,\eta(0) - \eta(0)\,\eta(1)\,\eta(2)] \\
&\quad - (\alpha+\beta)[\eta(-1)\,\eta(0) - \eta(0)\,\eta(1)] \qquad (3.1)
\end{aligned}
$$

This curious equation solve our main problem, for it allows us to express the troublesome term in (1.8) as the sum of "gradients" (over two lattice sites) of local functions and a time derivative. In fact, from the computations above we have

$$EX_t^\varepsilon(\phi) = EX_0^\varepsilon(\phi) + \int_0^t \left\{ \varepsilon \sum_{2|x} \phi''(\varepsilon x)\, Eh_x(\eta_{\varepsilon^{-2}\tau}) \right\} d\tau$$
$$+ \int_0^t \left\{ \varepsilon \sum_{2|x} \varepsilon^{-1} \phi'(\varepsilon x)\, ELg_x(\eta_{\varepsilon^{-2}\tau}) \right\} d\tau + O(\varepsilon) \qquad (3.2)$$

In (3.2) a subscript x on a function denotes that function shifted in space by x, and g and h are local functions given by

$$g = \frac{\beta - \alpha}{\alpha + \beta} [\eta(-1)\, \eta(0) - \eta(0)\, \eta(1)] \qquad (3.3)$$

and

$$h = 2 \left\{ \beta\eta(-1) + \frac{\alpha - \beta}{\alpha + \beta} [\alpha\eta(-2)\, \eta(0) - (\alpha - \beta)\, \eta(-2)\, \eta(-1)\ \ \eta(0)] \right\}$$
$$+ \frac{1}{2} \{ -j(-1, 0) + j(0, 1) \} \qquad (3.4)$$

The third term on the right side of (3.2) is negligible since it equals

$$\varepsilon^2 \sum_{2|x} \phi'(\varepsilon x)\, Eg_x(\eta_{\varepsilon^{-2}t}) - \varepsilon^2 \sum_{2|x} \phi'(\varepsilon x)\, Eg_x(\eta_0) \qquad (3.5)$$

which is of order ε.

Since only the first two terms in (3.2) will contribute in the limit, one can determine the bulk diffusion constant from (3.2), (3.4), and a local equilibrium ansatz. Assuming that the state at macroscopic time t (microscopic time $\varepsilon^{-2}t$) and macroscopic location r (microscopic location $[\varepsilon^{-1}r]$) is an invariant measure with parameter adjusted so that the local density is $\rho(r, t)$, $\rho(\cdot, \cdot)$, the solution of (2.2), we find that in the hydrodynamic limit (3.2) should yield

$$\int_0^1 \phi(r)\, \rho(r, t)\, dr = \int_0^1 \phi(r)\, \rho(r, 0)\, dr + \frac{1}{2} \int_0^t \int_0^1 \phi''(r)\, a(\rho(r, s))\, ds \qquad (3.6)$$

where $a(\rho)$ is given by

$$a(\rho) = \mu_{\zeta(\rho)}(h) \qquad (3.7)$$

Equation (3.6) is a weak version of the equation

$$\frac{\partial}{\partial t} \rho(r, t) = \frac{1}{2} \frac{\partial^2}{\partial r^2} a(\rho(r, t)) \qquad (3.8)$$

We conclude that the diffusion constant should be given by

$$D(\rho)=\frac{1}{2}\frac{\partial}{\partial\rho}a(\rho) \tag{3.9}$$

The latter can be computed with the help of the parametrization given in (2.3).

We first compute the right side of (3.7) as a function of ζ. Noting that the current functions in (3.4) do not contribute (they have mean zero by the detailed balance condition), we obtain, after some algebra,

$$\begin{aligned}\mu_\zeta(h)&=2\frac{\alpha\beta}{\alpha+\beta}\frac{\zeta(2\zeta+\alpha+\beta)}{(\zeta+\beta)(\zeta+\alpha)}\\&=2\frac{\alpha\beta}{\alpha+\beta}(\rho_e+\rho_o)\end{aligned} \tag{3.10}$$

This gives

$$D(\rho)=\frac{2\alpha\beta}{\alpha+\beta} \tag{3.11}$$

Thus we expect to get a linear diffusion equation in the hydrodynamic limit, as stated in theorem one.

4. PROOFS OF THE THEOREMS

Proof of Theorem 1. We have from standard Markov process theory[2,10]

$$X_t^\varepsilon(\phi)-X_0^\varepsilon(\phi)=\int_0^t\varepsilon^{-2}LX_\tau^\varepsilon(\phi)\,d\tau+M_t^\varepsilon(\phi) \tag{4.1}$$

where $M_t^\varepsilon(\phi)$ is a martingale satisfying

$$E(M_t^\varepsilon(\phi))^2=\int_0^t\varepsilon^{-2}E[L(X^\varepsilon(\phi))^2-2X^\varepsilon LX^\varepsilon]_{\varepsilon^{-2}\tau}\,d\tau \tag{4.2}$$

By direct calculation, the right side of (4.2) equals

$$\int_0^t E\left\{\varepsilon^2\sum_x c_{x,x+1}[\phi'(\varepsilon x)]^2\,[\eta_{\varepsilon^{-2}\tau}(x+1)-\eta_{\varepsilon^{-2}\tau}(x)]^2\right\}d\tau+O(\varepsilon)$$

($c_{x,x+1}$ are the rate functions), which is $O(\varepsilon)$.

To treat the drift term in (4.1), we use the trick introduced in Section 3. Let

$$G^{\varepsilon}(\eta)=\varepsilon^2 \sum_{2\mid x} \phi'(\varepsilon x)\, g_x(\eta) \tag{4.3}$$

Adding and subtracting $G_0^{\varepsilon}-G_{\varepsilon^{-2}t}^{\varepsilon}$ (which is of order ε) in (4.1), we have

$$X_t^{\varepsilon}(\phi)-X_0^{\varepsilon}(\phi)=\int_0^t \left\{\varepsilon \sum_{2\mid x} \phi''(\varepsilon x)\, h_x(\eta_{\varepsilon^{-2}\tau})\right\} d\tau$$
$$+M_t^{\varepsilon}(\phi)-N_t^{\varepsilon}(\phi)+O(\varepsilon) \tag{4.4}$$

In (4.3), $N_t^{\varepsilon}(\phi)$ is another martingale (the one associated with the function G^{ε}), with quadratic variation

$$E(N_t^{\varepsilon})^2=\int_0^t \varepsilon^{-2} E[L(G^{\varepsilon})^2-2G^{\varepsilon}LG^{\varepsilon}]_{\varepsilon^{-2}\tau}\, d\tau \tag{4.5}$$

The first term in square brackets in (4.5) integrates to a difference which is $O(\varepsilon)$. For the second term apply (3.1) again, which states that

$$Lg=-(\alpha+\beta)\, g+(\text{gradients over two lattice sites})$$

Since G^{ε} is $O(\varepsilon)$, the gradients contribute $O(\varepsilon)$, while the term in g contributes

$$2(\alpha+\beta)\int_0^t E\left\{\varepsilon \sum_{2\mid x} \phi'(\varepsilon x)\, g_x\right\}^2_{\varepsilon^{-2}\tau} d\tau \tag{4.6}$$

which will be shown later to vanish as $\varepsilon \to 0$.

Given these facts, Kolmogorov's inequality for martingales tells us that, for all $\delta>0$ and T,

$$P\left[\sup_{0\leqslant t\leqslant T}\left|X_t^{\varepsilon}(\phi)-X_0^{\varepsilon}(\phi)-\int_0^t \left\{\varepsilon \sum_{2\mid x} \phi''(\varepsilon x)\, h_x\right\}_{\varepsilon^{-2}\tau} d\tau\right|>\delta\right]\to 0 \tag{4.7}$$

We have reduced the problem—the reader may balk at this expression—to treating properly normalized integrated drift terms of the type present in (4.4) and (4.6). This is now standard, using either large-deviation methods[9] or entropy arguments.[6] These arguments yield

$$\lim_{l\to 0}\lim_{\varepsilon\to 0}\int_0^t E\left|\varepsilon \sum_{2\mid x} \phi(\varepsilon x)\left[f_x(\eta_{\varepsilon^{-2}\tau})\right.\right.$$
$$\left.\left.-\hat{f}\left(\frac{\varepsilon}{2l}\sum_{x\leqslant y\leqslant x+\varepsilon^{-1}2l} \eta_{\varepsilon^{-2}\tau}(y)\right)\right]\right| d\tau \to 0 \tag{4.8}$$

In (4.8), f is a local function and $\hat{f}$ is a function of one variable given by

$$\hat{f}(\rho) = \mu_\rho(f) \tag{4.9}$$

[I remark in passing that the only assumption on the initial state needed for (4.8) in our context is a bound on the relative entropy with respect to an invariant measure; see refs. 6 and 16.] Equation (4.8) allows us to replace a properly normalized space-and-time average of a local function by a similar average of a function of the local density. It is this result which allows one to close the equation for the density field.

We can now complete the proof of the theorem. The expression in (4.6) vanishes by (4.8)–(4.9) and the fact that

$$\mu_\rho(g) = 0 \qquad \text{for all } \rho$$

The LLN follows from a compactness argument (note that due to the exclusion, a bound on the density field is trivial), (4.1)–(4.9), and uniqueness of the solution of (a weak version of) the PDE (2.8), which is standard, since the equation is linear.[6,16] This completes the (sketch of) the proof of Theorem 1.

Proof of Theorem 2. The proof of Theorem 2 uses the Holley–Stroock martingale characterization of generalized Ornstein–Uhlenbeck processes[7] and the "Boltzmann–Gibbs" principle introduced in ref. 1. I follow the line of argument developed in refs. 3 and 14. Let us begin by decomposing the fluctuation field into drift-plus-martingale in the usual way. We find

$$Y_t^\varepsilon(\phi) = Y_0^\varepsilon(\phi) + \int_0^t \varepsilon^{-2} [L Y^\varepsilon(\phi)]_{\varepsilon^{-2}\tau} \, d\tau + \hat{M}_t^\varepsilon(\phi) \tag{4.10}$$

$\hat{M}_t^\varepsilon(\phi)$ in (4.10) is a martingale.

In gradient cases one proves that the two terms in (4.10) seperately have a limit which moreover give the corresponding objects in the decomposition of the Ornstein–Uhlenbeck process. This process is characterized precisely in ref. 7, but informally it has a decomposition

$$Y_t(\phi) = Y_0(\phi) + \int_0^t Y_\tau(A\phi) \, d\tau + W_t(B\phi) \tag{4.11}$$

where $W_\cdot(\cdot)$ is a Gaussian generalized process (the time integral of white noise in spacetime) with covariance

$$E W_t(\phi) \, W_s(\psi) = s \wedge t \int_0^1 \phi(r) \, \psi(r) \, dr \tag{4.12}$$

and the operators A and B are given by

$$A = \frac{2\alpha\beta}{\alpha+\beta} \frac{\partial^2}{\partial r^2}$$
$$B = \left\{\chi(\rho) \frac{2\alpha\beta}{\alpha+\beta}\right\}^{1/2} \frac{\partial}{\partial r} \tag{4.13}$$

The choice of A here reflects the accepted wisdom that fluctuations propagate by the linearized hydrodynamic evolution and the choice of B follows from the fluctuation-dissipation theorem (a consequence of stationarity):

$$A\chi(\rho) + \chi(\rho) A^* = -B^*B$$

In the nongradient case neither term in (4.10) has the proper form to have the expected limit. Computing as in (1.8), the drift in the original process equals

$$\int_0^t \varepsilon^{1/2} \left\{ \sum_{2|x} \varepsilon^{-1} \phi'(\varepsilon x)[j(x-1, x) + j(x, x+1)] + \frac{1}{2} \sum_{2|x} \phi''(\varepsilon x)[-j(x-1, x) + j(x, x+1)] \right\}_{\varepsilon^{-2}\tau} d\tau + O(\varepsilon) \tag{4.14}$$

The first term in (4.14) is not a properly normalized fluctuation field. (The second is, but will not contribute in the limit; see below.) Additionally, the quadratic variation of the martingale in (4.10) equals [computing as in (4.2)]

$$E(\hat{M}_t^\varepsilon)^2 = t\varepsilon \sum_x \langle c_{x,x+1}[\eta(x+1) - \eta(x)]^2 \rangle (\phi'(\varepsilon x))^2 + O(\varepsilon)$$

($\langle \cdot \rangle$ denotes equilibrium expectation), which tends to

$$\frac{1}{2} \langle c_{-1,0}[\eta(-1) - \eta(0)]^2 + c_{0,1}[\eta(0) - \eta(1)]^2 \rangle \int_0^1 [\phi'(r)]^2 \, dr \tag{4.15}$$

The prefactor of the integral in (4.15), which should be $\chi(\rho) D(\rho)$, is not correct. (We shall see that it contains only the first term in the Green–Kubo expression for the diffusion constant; see the next section.)

We conclude from this analysis that we must somehow split the integrated drift term in (4.10) into a properly normalized fluctuation field and a martingale. Again the identity (3.1) comes to our rescue. The drift term splits as

$$\int_0^t \varepsilon^{1/2} \sum_{2|x} \phi''(\varepsilon x)(h_x - \langle h \rangle)_{\varepsilon^{-2}\tau}\, d\tau$$
$$+\int_0^t \varepsilon^{-1/2} \sum_{2|x} \phi'(\varepsilon x)(Lg_x)_{\varepsilon^{-2}\tau}\, d\tau + O(\varepsilon) \tag{4.16}$$

For convenience, let us use the notation, given a local function f,

$$\hat{Y}_t^\varepsilon(f;\phi) \equiv \varepsilon^{1/2} \sum_{2|x} \phi(\varepsilon x)(f_x - \langle f \rangle)_{\varepsilon^{-2}t}$$

With this notation and adding and subtracting

$$\varepsilon \hat{Y}_t^\varepsilon(g;\phi') - \varepsilon \hat{Y}_0^\varepsilon(g;\phi')$$

in (4.16), we obtain the decomposition of the fluctuation field

$$Y_t^\varepsilon(\phi) = \int_0^t \hat{Y}_\tau^\varepsilon(h;\phi'')\, d\tau + \varepsilon \hat{Y}_0^\varepsilon(g;\phi') - \varepsilon \hat{Y}_t^\varepsilon(g;\phi')$$
$$+ \hat{M}_t^\varepsilon(\phi) - \hat{N}_t^\varepsilon(g;\phi') + O(\varepsilon) \tag{4.17}$$

In (4.17), $\hat{N}_\cdot^\varepsilon(\cdot)$ is another martingale, and the second and third terms on the right side are $O(\varepsilon)$.

Given a decomposition of the type given in (4.17), the proof of Theorem 2 is (almost) standard. I shall confine myself to a discussion of how the drift term in (4.17) can be replaced by a multiple of the density fluctuation field when passing to the hydrodynamic limit (the so-called "Boltzmann–Gibbs" principle), and to a computation of the total quadratic variation of the two martingales. Given these results, the proof of Theorem 2 then follows essentially the identical route as for gradient models treated previously.[1–3,14]

Just as for the density field, to close the equation we must replace the integrated drift term by a (in this case linear) function of the original field. The following result does the job: For every local function h and test function ϕ

$$\lim_{\varepsilon\to 0}\left(E\left\{\int_0^t [\hat{Y}_\tau^\varepsilon(h;\phi) - a'(h;\rho)\, \hat{Y}_\tau^\varepsilon(\eta(0)+\eta(1);\phi)]\, d\tau\right\}^2\right) = 0 \tag{4.18}$$

where

$$a'(h;\rho)\equiv\frac{d}{d\rho}\,\mu_{\zeta(\rho)}(h) \tag{4.19}$$

Note that the second field in square brackets in (4.18) is essentially the original fluctuation field. (4.18) says that the only component of $\hat{Y}_t^\varepsilon(h;\phi)$ which matters in the limit is the component along the density fluctuation field. The proof of (4.18) is the same as that in ref. 3, with the minor difference that translation invariance is replaced by invariance under translations by two lattice sites, and the considerable simplification that the Gibbs state in our case is a product measure. Equations (4.18)–(4.19) also yield that the second term in (4.14) vanishes in the limit.

Finally, let us compute the limiting quadratic variation (mean square) of the difference of the two martingales in (4.17). We have already computed the quadratic variation for $\hat{M}_\cdot$. Since $\hat{N}_\cdot$ is the martingale associated with the function $\varepsilon\hat{Y}_t^\varepsilon(g;\phi)$, we have

$$\begin{aligned}
E(\hat{N}_t^\varepsilon)^2 &= 2t\langle\hat{Y}^\varepsilon(g;\phi'),\,(-L)\,\hat{Y}^\varepsilon(g;\phi')\rangle\\
&= 2(\alpha+\beta)\left\langle\left(\varepsilon^{1/2}\sum_{2\mid x}\phi'(\varepsilon x)\,g_x\right)^2\right\rangle\\
&\xrightarrow[\varepsilon\to 0]{} 2(\alpha+\beta)\int_0^1[\phi'(r)]^2\,dr\sum_x\langle gg_x\rangle
\end{aligned}\tag{4.20}$$

In the third line we have used that g is an eigenfunction of L (except for a gradient). In a similar fashion we obtain for the cross term

$$\begin{aligned}
(-2)\,E\hat{M}_t^\varepsilon\hat{N}_t^\varepsilon &= 4t\left\langle\left[\sum_{2\mid x}\phi'(\varepsilon x)\,g_x\right]\left[\sum_x\phi(\varepsilon x)\,L\eta(x)\right]\right\rangle\\
&= 4t\varepsilon\left\langle\left[\sum_{2\mid x}\phi'(\varepsilon x)\,g_x\right]\left[\sum_{2\mid x}\phi'(\varepsilon x)\,Lg_x\right]\right\rangle+O(\varepsilon)\\
&= (-4t)(\alpha+\beta)\varepsilon\left\langle\left[\sum_{2\mid x}\phi'(\varepsilon x)\,g_x\right]^2\right\rangle+O(\varepsilon)\\
&\xrightarrow[\varepsilon\to 0]{} (-4t)(\alpha+\beta)\int_0^1[\phi'(r)]^2\,dr\sum_x\langle gg_x\rangle
\end{aligned}\tag{4.21}$$

Combining, we have

$$\lim_{\varepsilon \to 0} E(\hat{M}_t^\varepsilon - \hat{N}_t^\varepsilon)^2$$
$$= \int_0^1 [\phi'(r)]^2 \, dr \left\{ \frac{1}{2} \langle c_{-1,0}[\eta(-1) - \eta(0)]^2 + c_{0,1}[\eta(0) - \eta(1)]^2 \rangle \right.$$
$$\left. - 2(\alpha + \beta) \sum_{2|x} \langle g g_x \rangle \right\} \tag{4.22}$$

In the next section I show that the expression in curly brackets in (4.22) equals $\chi(\rho)\, D(\rho)$, as one expects. This completes the partial sketch of the proof of Theorem 2; see the indicated references for the full treatment.

5. THE GREEN–KUBO FORMULA

The Green–Kubo formula gives the bulk diffusion constant in terms of current–current correlations.(2,13) For reversible stochastic models it has two terms with opposite sign. For our model it reads

$$2\chi(\rho)\, D_{\mathrm{GK}}(\rho) = \frac{1}{2} \langle j(-1, 0)[\eta(-1) - \eta(0)] + j(0, 1)[\eta(0) - \eta(1)] \rangle_\rho$$
$$- \lim_{T \to \infty} \lim_{\varepsilon \to 0} E\left(\frac{1}{(\varepsilon^{-1} T)^{1/2}} \sum_{x=1}^{\varepsilon^{-1}} \int_0^T j_t(x, x+1)\, dt \right)^2 \tag{5.1}$$

In (5.1), $\langle \cdot \rangle_\rho$ denotes an equilibrium average and the expectation in the second term is with respect to the equilibrium process with density ρ.

Curiously, in our model the second term can be explicitly calculated. This is because the total current is an eigenfunction of the generator. From (1.9) we find, defining

$$\sum j = \sum_x j(x, x+1) \tag{5.2}$$

that

$$L\left(\sum j\right) = -(\alpha + \beta)\left(\sum j\right) \tag{5.3}$$

This gives for the second term in (5.1)

$$\lim_{T \to \infty} \lim_{\varepsilon \to 0} \frac{2}{T} \int_0^T d\tau \int_0^\tau d\tau' \, \varepsilon \left\langle \sum j, T_{\tau'} \sum j \right\rangle$$
$$= \lim_{T \to \infty} \lim_{\varepsilon \to 0} \left\{ \frac{2}{T} \int_0^T d\tau \int_0^\tau d\tau' \, \varepsilon^{-(\alpha+\beta)\tau'} \right\} \varepsilon \left\langle \sum j, \sum j \right\rangle$$

$$= 2(\alpha+\beta)^{-1} \left\langle \frac{1}{2} j(-1, 0)^2 + \frac{1}{2} j(0, 1)^2 + j(-1, 0)\, j(0, 1) + j(0, 1)\, j(1, 2) \right\rangle \tag{5.4}$$

One finds, by explicit computation using (1.6), that the terms involving $j(\cdot, \cdot)^2$ in (5.4) exactly cancel the first term in the Green–Kubo formula (5.1). Computing the remaining terms using (1.6) and (1.12), one finds after a little algebra

$$D_{\mathrm{GK}} = 2\alpha\beta/(\alpha+\beta) \tag{5.5}$$

in agreement with the bulk diffusion constant, as physical reasoning predicts.

We must also check that D_{GK} agrees with the diffusion constant we found in fluctuation theory. This is easily done; starting again with (5.1) and using (1.8), (1.9), and (3.1), we have

$$\sum_{x} j(x, x+1) = \sum_{2 \mid x} Lg_x \tag{5.6}$$

and remembering that

$$Lg = -(\alpha+\beta) + (\text{gradients over two lattice sites})$$

we see that the second term in Green–Kubo comes out to be

$$-2(\alpha+\beta) \sum_{2 \mid x} \langle g g_x \rangle$$

in agreement with (4.22).

6. REMARKS

1. The attentive reader may have noticed that I used the basic decomposition given in (3.1) in two different ways. In proving Theorem 1, I kept the contribution from the gradient but the contribution from the term containing the generator proved to be negligible. But in computing D_{GK} just the reverse held: the gradient made no contribution, but the term in Lg contributed the second term in the Green–Kubo formula.

2. One might ask whether or not the situation changes if the period

is chosen to be three or higher. One might conjecture that the diffusion constant is given in general by

$$n\left(\sum_{i=1}^{n} \frac{1}{1/\alpha_{i-1} + 1/\alpha_i}\right) \tag{6.1}$$

where n is the period. This amounts to the belief that the only effect of putting a model in a periodic (or perhaps random) inhomogeneous environment is to modify the diffusion constant by a (constant) factor. (A result supporting this conjecture has been announced by Fritz,[5] who discussed a Ginsburg–Landau type model in a random environment.)

Unfortunately, I have not been able to find an analogue of the identity (3.1) for higher periodicity and it is possible that no decomposition of the sum of the n current functions in terms of local functions exists for $n \geqslant 3$. That such a decomposition in terms of possibly nonlocal functions always exists can be seen by using the Hilbert space introduced in ref. 1. Defining an inner product by

$$\langle\langle f, g \rangle\rangle \equiv \sum_{n|x} \langle f g_x \rangle \tag{6.2}$$

one finds that L is still a self-adjoint nonpositive operator in the Hilbert space with this inner product and that $\sum_1^n j(x, x+1)$ is orthogonal to the eigenspace of eigenvalue zero. Therefore, one can always solve the equation

$$\sum_{i=1}^{n} j(x, x+1) = Lg \tag{6.3}$$

up to a zero element in this norm, which is a "gradient" over n lattice sites. However, there is no guarantee that the functions so defined are local (i.e., they may vary with ε). In this case the argument would become much more delicate than in this paper.

Lacking a generalization of (3.1), I have no convincing argument for the conjecture that D is given by (6.1) and the hydrodynamic equation remains linear for $n \geqslant 3$.

NOTE ADDED

I thank a referee for pointing out previous work on the same model.[18–20]

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