# Navier-Stokes equations for stochastic lattice gases


R. Esposito

*Dipartimento di Matematica Pura ed Applicata, Università di L'Aquila*

R. Marra

*Dipartimento di Fisica, Università di Roma Tor Vergata*

H.T. Yau

*Courant Institute, New York University*



(May 22, 1996)



We discuss the diffusive limit of a class of stochastic lattice gases on the cubic lattice $Z^d$. If the initial conditions correspond to a local equilibrium with small deviations from a spatially constant profile, we prove the law of large numbers for the rescaled empirical velocity field. The limiting field satisfies the Navier-Stokes equation and the viscosity is characterized by variational formulas, formally equivalent to the Green-Kubo formula.



05.20.-y 05.70.Ln 02.50.-R 47.10.+g


A major open problem in non-equilibrium statistical physics is a derivation of hydrodynamical equations, such as the Euler or the Navier-Stokes equations, from the microscopic Hamiltonian dynamics. Formally the Euler equations can be understood with the simple local equilibrium assumption [1]. A proof can indeed be achieved by adding some noise to the Newtonian dynamics [2], helping to establish the local equilibrium. For longer time scale, such as the diffusive scale, it is necessary to compute the transport coefficients which depend on the first order corrections to the local equilibrium. The corrections can be determined by formal expansions, as in [3], [4]. Unlike the Euler equations, even with the addition of noise to the Newtonian dynamics, a rigorous treatment of this formal expansions for general Hamiltonian systems is beyond the present mathematical technique. A major difficulty is the lack of control on the relaxation rate to equilibrium for general Hamiltonian systems, a problem much harder than proving local equilibrium assumption. Estimates of this kind are essential for a derivation of the Navier-Stokes equations.

The only systems that we have sufficient estimates for are the lattice gas models. In this Letter we present a rigorous derivation of the incompressible Navier-Stokes equation for stochastic particle systems on the lattice. The transport coefficients, as a byproduct, are characterized via variational formulas, following the approach pioneered by [5] and developed by, among others, [6], [7], [8], [9]. These variational formulas are formally equivalent to the Green-Kubo formula. But unlike the Green-Kubo formula, the variational formulas are analytically more tractable and they can be used for numerical approximations of the transport coefficients. We remark that the convergence of the Green-Kubo integrals is always very difficult to obtain while the transport coefficients are automatically finite by the variational formulation.

We now introduce the models. Let $\Lambda_L \in Z^d$ be the cubic sublattice $\{-L, \dots, L\}^d$ with periodic boundary conditions. We set $L = \varepsilon^{-1}$. Let $e_i$, $i = 1, \dots, d$ be the unit vectors in the positive coordinate directions and $\mathcal{E} = \{e = \pm e_i \text{ for some } i = 1, \dots, d\}$. Let $\mathcal{V}$ be a finite subset of $R^d$ representing the possible velocities and $N$ the numbers of elements in $\mathcal{V}$. Assume that $\mathcal{V}$ is invariant under reflections and permutations of the coordinate axes. Assume for simplicity that all velocities have a fixed modulus, say, $\kappa$. The simplest choice is to take the velocities along the coordinate directions, namely $\mathcal{V} = \mathcal{E}$. We will refer to that case as Model I. Since this model does not provide the correct isotropy property for the non linear term in the Navier-Stokes equation, we introduce also a more complex model (Model II) by choosing as $\mathcal{V}$ the set of the vectors with two components $\pm 1$ and a component $\pm\varpi$, to be fixed later to get the right hydrodynamical equations. In Model II we have $N = 24$.

On each site of the lattice at most one particle for each velocity is allowed, so that there are at most $N$ particles per site (exclusion rule only between particles with the same velocity). A configuration of particles on the lattice is denoted by $\eta = \{\eta_x, x \in \Lambda_L\}$ where $\eta_x = \{\eta(x, v), v \in \mathcal{V}\}$ and $\eta(x, v) = 0, 1$, $x \in Z^d$, $v \in \mathcal{V}$ is the occupation number of particles at $x$ with velocity $v$. The dynamics consists of the following two parts:

1- The *free motion* of the particles with velocity $v$ is modeled by a simple exclusion process (SEP) with drift $v$. In other words, particles with velocity $v$ jump at (independent) exponential times from a site $x$ to a neighboring site $x + e$, $e \in \mathcal{E}$, with intensity $p(x, x + e, v)$ provided that there is no particle with velocity $v$ at $x + e$. The intensity is chosen so that the drift $\sum_{e \in \mathcal{E}} e p(0, e, v) = v$. This is the way we associate a notion of velocity to particles on the lattice and one can obtain any velocity $v$ by choosing the jump rate correctly even if the underlying lattice is the standard square lattice. We choose $p(x, y, v) = [\gamma + (y - x) \cdot v/2]$, where $\gamma$ is a constant large enough so that the jump rates are nonnegative. One can characterize this dynamics formally by the generator

$$\mathcal{L}^{free} f(\eta) = \sum_{v\in\mathcal{V}} \sum_{x\in Z^d, e\in\mathcal{E}} \eta(x,v)(1-\eta(x+e,v)) \times p(x,x+e,v)\left[f(\eta^{x,x+e,v}) - f(\eta)\right] \quad (1)$$

where $\eta^{x,y,v}$ is the configuration obtained from $\eta$ by exchanging the occupation numbers of particles with velocity $v$ at $x$ and $y$.

2- The velocity of the particles change by means of binary collisions. By *collisions* we mean all the quadruples $\mathcal{Q} = \{q = (v,w,v',w') \in \mathcal{V}^4 : v+w = v'+w'\}$ conserving the total momentum; here $v, w$ are the incoming velocities and $v', w'$ the outgoing velocities. These binary collisions occur at a site $y$ at independent exponential times, provided the exclusion rule is not violated. Since the moduli of velocities are fixed, the energy coincides with the mass in our setup and collisions conserve energy as well. The generator is given by

$$\mathcal{L}^c f(\eta) = \sum_{y\in Z^d} \sum_{q\in\mathcal{Q}} C(y,q.\eta)\left[f(\eta^{y,q}) - f(\eta)\right], \quad (2)$$

where $C(y,q.\eta) = 1$ if $\eta(y,v) = \eta(y,w) = 1$ and $\eta(y,v') = \eta(y,w') = 0$ and $C(y,q.\eta) = 0$ otherwise. Note that $C(y,q.\eta) = 0$ when in the configuration $\eta$ there is no particle with velocity $v$ or $w$ at $y$ or there is already a particle with velocity $v'$ or $w'$ at $y$. The configuration $\eta^{y,q}$ is constructed by setting $\eta^{y,q}(y,v) = \eta^{y,q}(y,w) = 0$, $\eta^{y,q}(y,v') = \eta^{y,q}(y,w') = 1$ and $\eta^{y,q}(z,u) = \eta(z,u)$ if $z \neq y$ or $u \notin q$. Note that the only possible collisions in Model I are those $q = (v,w,v',w')$ such that $v + w = 0$ and $v' + w' = 0$ (head-on collisions).

The generator of the full dynamics is defined by

$$\mathcal{L}f = \mathcal{L}^{free} f + \mathcal{L}^c f \quad (3)$$

There are $d+1$ conserved quantities for this dynamics, namely, the total mass and the total momentum. Define the local mass and momentum by

$$I_0(\eta_x) = \sum_{v\in\mathcal{V}} \eta(x,v), \quad I_i(\eta_x) = \sum_{v\in\mathcal{V}} (v\cdot e_i)\eta(x,v), \quad (4)$$

for $i = 1, \ldots, d$. The product Gibbs measure

$$\mu_{L,r,n} = \frac{1}{Z_{L,r,n}} \prod_{x\in\Lambda_L} \exp\left\{ rI_0(\eta_x) + \sum_{i=1}^d n_i I_i(\eta_x)\right\}, \quad (5)$$

is invariant for $\mathcal{L}$. It is parametrized by the "chemical potentials" $r, n$, $r \in R$ and $n$ a $d$-dimensional vector $(n_1, \ldots, n_d)$, namely the conjugate variables to the mass and momentum. In (6) the *partition function* $Z_{L,r,n}$ is the normalization factor. When $n = 0$, we denote the measure by $\mu_r$ and the corresponding average by $\langle\cdot\rangle$. We shall say that a model has the local ergodic property if and only if all the invariant measures in a finite cube are of the form (5). The specific form of $\mathcal{V}$ is needed only in the proof of the local ergodic property. The rest of our method is valid under quite general conditions. Like general Hamiltonian systems, our dynamics is not reversible with respect to the measure (5), i.e., the detailed balance condition is not satisfied.

Let $f_t$ be the density w.r.t. $\mu_r$ of the process on the diffusive time scale. Then $f_t$ satisfies the forward (Fokker-Plank) equation

$$\frac{\partial}{\partial t} f_t = \varepsilon^{-2} \mathcal{L}^* f_t. \quad (6)$$

The factor $\varepsilon^{-2}$ is due to the diffusive time scaling and $\mathcal{L}^*$ is the formal adjoint of $\mathcal{L}$ in $L^2(\mu_r)$. We consider the initial data, $f_{t=0}$, given by the *local equilibrium state* $\psi_0$

$$\psi_0 = Z_\varepsilon^{-1} \exp\left[\varepsilon \sum_{x\in\Lambda_L} \sum_{i=1}^d \lambda_i(\varepsilon x) I_i(x)\right] \quad (7)$$

with $\lambda_i$ smooth periodic functions. The corresponding density is $\langle I_0(\eta_x)\rangle_{\psi_0} = N\theta + O(\varepsilon^2)$ where $\theta = e^r/(1+e^r) = \langle \eta_x \rangle_{\mu_r}$ is a constant. The mean velocity field is $u_0^i = \langle I_i(\eta_x)\rangle_{\psi_0} \propto \varepsilon\lambda_i$. This special choice corresponds to assume a Mach number of order $\varepsilon$, namely we are considering the incompressible regime (see [10], [3] for more discussions on this point).

It is possible to obtain the Navier-Stokes equations by a formal calculation assuming suitable approximations for $f_t$. Introduce the *empirical velocity fields*

$$\nu_i^\varepsilon(z,t) = \varepsilon^{d-1} \sum_{x\in\Lambda_L} \delta(z - \varepsilon x) I_i(\eta_x(t)), \quad (8)$$

for $i = 1, \ldots, d$ and $z$ the macroscopic coordinates, which are expected to approximate the velocity profile for $\varepsilon$ small, namely $\nu_i^\varepsilon(z,t) \approx u_i(z,t)$, as $\varepsilon \to 0$. They satisfy the following local conservation laws

$$\frac{\partial}{\partial t} \nu_i^\varepsilon(z,t) = -\sum_{j=1}^d \partial_{z_j} w_j^i(z,t). \quad (9)$$

Here $w_j^i(z,t) = \varepsilon^{d-1} \sum_{x\in\Lambda_L} \delta(z-\varepsilon x) w_{x,j}^i$. The currents $w_{x,j}^i$, $i,j = 1, \ldots, d$ are given explicitly by (with $\nabla_j g(x) \equiv g(x+e_j) - g(x)$)

$$w_{x,j}^i = \sum_{v\in\mathcal{V}} (e_i\cdot v) w_{x,j}(v) = \gamma \nabla_j I_i + \sum_{v\in\mathcal{V}} (e_i\cdot v)(e_j\cdot v) b_{x,j}(v)$$

$$b_{x,j}(v) = \eta(x+e_j,v)\eta(x,v) - \frac{1}{2}\Big[\eta(x+e_j,v) + \eta(x,v)\Big]$$

Strictly speaking, there is a martingale term on the r.h.s. of (9), vanishing in the limit discussed here.

To the first approximation, one can assume that the non-equilibrium density $f_t$ is a local equilibrium state similar to (7). This is *not* sufficient to obtain the Navier-Stokes equation. The correct assumption is that the density $f_t$ can be approximated (up to order $\varepsilon^2$) by the density

$$\Psi_t = Z_t^{-1} \exp\Big[\varepsilon \sum_{x\in\Lambda_L} \sum_{i=1}^{d} \lambda_i(\varepsilon x,t) I_i(x) + \varepsilon^2 \{ \sum_{x\in\Lambda_L} \lambda_0(\varepsilon x,t) I_0(x) + \Phi(\eta) \} \Big], \tag{10}$$

where $\Phi(\eta) = \sum_{x\in\Lambda_L}\sum_{i,j}\partial_j\lambda_i F^i_j$, for some local function $F^i_j$. The correct choice of $F^i_j$ will be discussed later on and is the key step of the rigorous derivation. Suffice to say that $F^i_j$ determine the fluctuations and they appear only in the transport coefficient. Note that because of the $\Phi$ term $\Psi_t$ is not a product measure.

If we average eq. (9) versus $\Psi_t$ we have the Navier-Stokes equations below in the limit $\varepsilon \to 0$:

$$\text{div } u = 0, \tag{11}$$

$$\frac{\partial}{\partial t}u_i + \frac{h(\theta)}{At(\theta)}[B\partial_{z_i}u_i^2 + C\sum_{j=1}^{d} u_j \partial_{z_j} u_i] = -\partial_{z_i}p + \sum_{j,\ell,k=1}^{d} D^{i,\ell}_{j,k}\partial_{z_j}\partial_{z_k}u_\ell, \tag{12}$$

where $u_i = At(\theta)$ and the constants are defined as:

$$t(\theta) = \theta(1-\theta),\ h(\theta) = \frac{t(\theta)}{2}(1-6t(\theta)),$$

$$A = \sum_{v\in\mathcal{V}} v_1^2,\ B = \sum_{v\in\mathcal{V}}[v_1^4 - 3v_1^2v_2^2],\ C = 2\sum_{v\in\mathcal{V}} v_1^2 v_2^2.$$

We have, for Model I, $A = 2$, $B = 2$, $C = 0$, and for Model II, $A = 8(2+\varpi^2)$, $B = \varpi^4 - 6\varpi^2 - 1$, $C = 16(1+2\varpi^2)$. The anisotropic term, $\partial_{z_i}u_i^2$, disappears by choosing $\varpi$ as the positive root of the equation $B = \varpi^4 - 6\varpi^2 - 1 = 0$ so that eq. (12) becomes the usual incompressible Navier-Stokes equation. This fixes the constant $\varpi$. The corrections $\Phi$ to the local equilibrium determine the viscosity matrix $D^{i,\ell}_{j,k}$. We summarize the main result proved in [9]:

**Theorem**. *Let $d \geq 3$ and $\mathcal{V}$ as in Model I or Model II. Then there is a bounded positive matrix $D$ such that the following holds: Suppose the incompressible Navier-Stokes equations (11), (12) have a smooth solution $p(x,t), u(x,t)$ for $t \in [0,T]$ with initial value $u_0$. Then the empirical field $\nu^\varepsilon$ converges weakly in probability to $u$ as $\varepsilon \to 0$. Furthermore, the ansatz (10) holds in the sense that the specific relative entropy $s(f_t \mid \Psi_t)$ satisfies*

$$s(f_t \mid \Psi_t) \equiv \varepsilon^d \int f_t \log(f_t/\Psi_t) d\mu_r = o(\varepsilon^2), \tag{13}$$

*provided that the chemical potential is chosen to give the correct velocity and $F^i_j$ approximate solutions of (14)* below.

This is, to our knowledge, the only example of rigorous derivation of the Navier-Stokes equations from a many body system. Our result actually holds in dimensions strictly bigger than 2. In fact, note that the rescaled velocity field $\nu^\varepsilon$ is the local average of velocity blown up by a factor $\varepsilon^{-1}$. Since the typical fluctuations of the sum in (8) are of order $\varepsilon^{-d/2}$, it is reasonable to expect a law of large numbers for $\nu^\varepsilon$ only for $d > 2$ . In dimension 2, one expects logarithmic corrections to the simple diffusive scaling due to the long time tails [1], [11].

The main point in the proof is to find the functions $F^i_j$. We use the approach of [5], [6], [7]. The strategy is to decompose the currents $w^i_j$ into the sum of a gradient term and a term of the form $\mathcal{L}g$, i.e.,

$$w^i_j - \sum_{k,\ell} D^{i,\ell}_{j,k}\nabla_k I_\ell - \mathcal{L}F^i_j = 0 \tag{14}$$

The coefficients $D^{i,\ell}_{j,k}$ will be identified as the viscosity. The last term represents the contribution of the fast modes and will not appear in the macroscopic equations; the function $F^i_j$ appears in the ansatz (10) for the nonequilibrium density $f_t$. Equation (14) will be understood as an equation in a suitable Hilbert space and $D^{i,\ell}_{j,k}$ has a geometric interpretation as "the component of the currents in the gradient directions". Hence the calculation of the transport coefficients $D^{i,\ell}_{j,k}$ involves solving the many-body equation (14) and is no simpler than the Green-Kubo formula. We shall give variational formulas bypassing this difficulty. We first describe the Hilbert space.

Define the space $\mathcal{G}$ as the space of the local functions satisfying $E^{\mu_r}[g] = 0$, $\partial E^{\mu_m}[g]/\partial m_\alpha|_{m=(r,0)} = 0$, for $\alpha = 0,\ldots,d$, where $\mu_m$ denotes the product measure (5) with chemical potentials chosen so that $E^{\mu_m}[I_\alpha(\eta_x)] = m_\alpha$. This means that functions in $\mathcal{G}$ have null projection on the invariant space of the generator $\mathcal{L}$. The currents $w^i_{x,j}$ are *not* in $\mathcal{G}$, so that we need to subtract the components of the currents on the space of the hydrodynamic variables. We denote by $\sigma^i_{x,j}$ the part of the current $w^i_{x,j}$ in $\mathcal{G}$: $\sigma^i_j = w^i_j - \sum_{\alpha\geq 0} a^i_{j,\alpha} I_\alpha$. In the case of Hamiltonian particle systems this subtraction procedure has been proposed to avoid infinite contributions to the Green-Kubo integrals and the coefficients $a^i_{j,\alpha}$ are given by the Zwanzig-Mori projectors ( see for example [4]).

We introduce a scalar product on $\mathcal{G}$, formally given by the expression

$$\ll f, g \gg_{-1} = \langle \sum_x \tau_x f,\ (\mathcal{L}_s)^{-1} g \rangle,$$

where $\mathcal{L}_s = (1/2)(\mathcal{L} + \mathcal{L}^*)$ is the symmetric part of the generator, the average is taken w.r.t. $\mu_r$ in the infinite volume and $\tau_x$ denotes spatial translation by $x$ on the lattice. This expression is formal because the r.h.s. may not even be finite due to the tail of the Green function $(\mathcal{L}_s)^{-1}$. We are able to control this tail for dimension $d \geq 3$ and it indeed defines a scalar product [7]. We obtain the Hilbert space $\bar{\mathcal{G}}$ by completing $\mathcal{G}$ with the associated norm.

Let $\chi = \langle [I_\alpha - < I_\alpha >]^2 \rangle$ denote the "susceptibility". For $a = (a^i_j), i, j = 1, \ldots, 3$, let $(Da)^i_j = \sum_{k,\ell} D^{i,k}_{j,\ell} a^k_\ell$ and let $a \cdot b = \sum_{i,j} a^i_j b^i_j$. $D$ can be characterized by

$$a \cdot Da = \frac{1}{\chi} \inf_{h \in \mathcal{G}} \ll \sigma \cdot a + \mathcal{L}h, \sigma \cdot a + \mathcal{L}h \gg_{-1}, \qquad (15)$$

$$a \cdot D^{-1} a = \frac{1}{\chi} \inf_{h \in \mathcal{G}} \ll \nabla I \cdot a + \mathcal{L}h, \nabla I \cdot a + \mathcal{L}h \gg_{-1} \qquad (16)$$

These formulas provide upper and lower bounds for the diffusion coefficients. Variational formulation for the diffusivity is common in homogenization theory. In particle systems context, it was first introduced by [5] for reversible systems. Expressions similar to (15,16) were previously derived in [8] for the asymmetric simple exclusion process.

We can show (following the arguments in [7], [8]) that (15, 16) are formally equivalent to the Green-Kubo formula

$$D^{i,\ell}_{j,k} = \gamma \delta_{i,\ell} \delta_{j,k} + \chi^{-1} \gamma \int_0^\infty dt \sum_x \left\langle \sigma^i_j e^{\mathcal{L}t} \tau_x \sigma^\ell_k \right\rangle, \qquad (17)$$

in the sense that, if the time integral in (17) is finite, then the expression (17) of the diffusion coefficient coincides with (15) and (16). The first term in (17) is the viscosity due to the symmetric simple exclusion ($\gamma$ is the jump rate of the symmetric part); the second one is the so-called dynamical part of the viscosity. Similar Green-Kubo formulas for "deterministic" cellular automata have been heuristically obtained using the fluctuation-dissipation approach [11].

The formulas (15) and (16) give finite transport coefficients and provide an efficient way to approximate them from above and below. The Green function $(\mathcal{L}_s)^{-1}$ appearing in the definition of $\ll \cdot, \cdot \gg_{-1}$ can be eliminated using $\langle u, S^{-1} u \rangle = \sup_v 2\langle u, v \rangle - \langle v, Sv \rangle$, true for any positive symmetric operator $S$. The symmetry properties of the model and previous representation formulas show that $D$ has the form

$$D^{i,\ell}_{j,k} = \delta_{j,k} \delta_{i,\ell} [D_1 + D_2 \delta_{i,j})] + D_3 \delta_{i,j} \delta_{\ell,k} + D_4 \delta_{j,\ell} \delta_{i,k}$$

and that $D > \gamma\, \mathbb{I}$ in matrix sense; in other words, the "dynamical part" of the viscosity is strictly positive. The bulk viscosity $\zeta = D_3 + D_4$ does not appear in the limiting equation because $\mathrm{div} u = 0$. The effective diffusivity is the shear viscosity due to $D_1$ and an anisotropic term $D_2$. We do not know if the anisotropic term $D_2$ is zero. Similar anisotropy appeared in the deterministic cellular automaton FCHC [11], introduced to obtain an isotropic nonlinear transport term.

Our method is general enough to work also for different models, e.g., different lattice geometry or thermal stochastic cellular automata, provided the local ergodic property holds. It also provide a rigorous derivation for the law of fluctuations in equilibrium and hence proves a fluctuation-dissipation relation. We will report on this in a future paper.

Work partially supported by GNFM-CNR, MURST, U. S. National Science Foundation grant 9403462 and David and Lucile Packard Foundation Fellowship


[1] H. Spohn, *Large Scale Dynamics of Interacting Particles*, Springer-Verlag New York (1991).

[2] S. Olla, R. Varadhan, H. T. Yau, Commun. Math. Phys., **155**, 523–560, (1993).

[3] R. Esposito, R. Marra, Jour. Stat. Phys., **74**, 981, (1993).

[4] G. L. Eyink, J. L. Lebowitz and H. Spohn, *Hydrodynamics and fluctuations outside local equilibrium*, Electr. Texas archive n. 95-168, and references therein.

[5] S. R. S. Varadhan, *Nonlinear diffusion limit for a system with nearest neighbor interactions II*, p 75-130, Taniguchi Symp., ed. K. D. Elworthy and N. Ikeda, Longman Scientific & Technical, (1990).

[6] L. Xu, *Diffusion limit for the lattice gas with short range interactions*, Thesis, N. Y. Univ. (1993).

[7] R. Esposito, R. Marra and H. T. Yau, Rev.Math.Phys., **6**, 1233-1267, (1994); Nato ASI Series B: Physics **324**, 43–53, M. Fannes edt. (1994).

[8] C. Landim, S. Olla and H. T. Yau, *First order correction for the hydrodynamic limit of asymmetric simple exclusion processes* CMAP preprint, **307**,(1994); *Some properties of the diffusion coefficient for asymmetric simple exclusion processes*; Ecole Polytechnique CMAP preprint, **327**, (1995).

[9] R. Esposito, R. Marra and H. T. Yau, *Navier-Stokes equations for stochastic particle systems on the lattice*, Electr. Texas archive n.95-290.

[10] A. De Masi, R. Esposito, J. L. Lebowitz, Commun. Pure and Appl. Math., **42**,1189–1214, (1989).

[11] U. Frisch, D. d'Humieres, B. Hasslacher, P. Lallemand, Y. Pomeau and J. P. Rivet Complex Systems **1**, 649–707, (1987) and references therein.