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Long range correlations for stochastic lattice gases in a non-equilibrium steady state

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Abstract. We consider a system with a single locally-conserved field (≡ density) in a slab geometry with different densities maintained at the two surfaces of the slab. On the basis of fluctuating hydrodynamics we show that the static density–density correlations are long ranged and decay as $-1/|x-y|^{d-2}$ for dimension $d \geqslant 3$ over distances small compared to the size of the slab. This effect vanishes to first order in the density difference. As a particle model we investigate a stochastic lattice gas with Kawasaki dynamics. We establish the connection to fluctuating hydrodynamics. In the case of hard core interaction only we prove the validity of fluctuating hydrodynamics and obtain, presumably model dependent, corrections.

1. Introduction

As is well known, a fluid in thermal equilibrium has exponentially decaying correlations of a range comparable to the one of the intermolecular potential. Only as the phase boundary is approached the correlation length may diverge. What kind of correlations should one expect then for a fluid in a non-equilibrium steady state imposed by appropriate boundary conditions?

This problem has attracted considerable attention recently (Ronis *et al* 1979, 1980, Machta *et al* 1979, Kirkpatrick *et al* 1979, 1980, 1982, Kirkpatrick and Cohen 1980, Cohen 1980, 1981, van der Zwan and Mazur 1980, van der Zwan *et al* 1981, Tremblay *et al* 1980, 1981, Grabert 1981, Ronis and Putterman 1980, Machta and Oppenheim 1982), especially because some of the theoretically expected effects are now also accessible experimentally (Beysens *et al* 1980). When investigating this problem microscopically, i.e. on the level of an interacting particle system, a major difficulty is that the steady state is only defined as the stationary solution of a certain linear equation wih appropriate boundary conditions. From this information, properties of the steady state are not easily extracted. Therefore most theoretical treatments circumvent a microscopic theory and immediately use fluctuating hydrodynamics together with the so-called extended local equilibrium assumption. For dilute gases kinetic theory can also be used (Kirkpatrick *et al* 1982). In this particular case the link to the underlying Newtonian dynamics of particles can be made precise. It has been shown, under the restriction to short times, that the equation governing the time dependent fluctuations in the one-particle space becomes exact in the Boltzmann–Grad limit (van Beijeren *et al* 1979, Spohn 1981).

In this article I want to study the problem of nonequilibrium steady states for stochastic lattice gases. In these models one considers particles on a lattice which randomly jump to neighbouring sites at random times. Typically, one assumes a hard core exclusion of at most one particle per lattice site, and a jump rate depending on the neighbouring configuration. The number of particles is conserved in the course of time. The condition of detailed balance fixes the temperature throughout the system. Without boundary conditions the Gibbs canonical distribution is time invariant.

Compared to fluids, modelled as many classical particles, stochastic lattice gases are simpler in two essential ways. (i) The approach to equilibrium and the stochasticity is built into the model directly. (ii) Stochastic lattice gases have only one locally conserved field, namely the density. Therefore the hydrodynamic description reduces to a nonlinear diffusion equation. On the other hand, stochastic lattice gases obviously have one property in common with real fluids in that both form an interacting many particle system. As will be discussed in detail, only because of this interaction non-equilibrium steady states for stochastic lattice gases have long range correlations qualitatively of the same nature as the ones for fluids.

Since for stochastic lattice gases only the density is locally conserved, the simplest nonequilibrium steady state is maintained in a Bénard–Rayleigh type experiment. We assume a slab geometry. At the left and right boundary of the slab particles are extracted from and inserted into the system with certain rates. This fixes the boundary densities ρ_+ and ρ_-. After some transient period the system establishes a steady state. If $\rho_+ = \rho_- = \rho$, then the steady state is the grand canonical Gibbs state with fugacity $z(\rho)$ depending on the boundary density and a temperature determined through the dynamics. In this case the qualitative structure of the state is well understood. We focus our attention here on the case $\rho_+ \neq \rho_-$.

The set-up described here has been investigated numerically on a $16\times16\times16$ lattice with nearest-neighbour interaction at various densities and temperatures (Murch 1980). Only the steady state current for small density gradient was measured with the aim to determine the bulk diffusion coefficient. We are not aware of such an experiment on a real system despite the fact that a number of materials have been successfully described in terms of stochastic lattice gases, as e.g. binary mixtures, hydrogen in metals and superionic conductors.

We will first construct the purely macroscopic theory of fluctuating hydrodynamics for stochastic lattice gases, i.e. for a single locally conserved field. We find static density–density correlations which decay as $-[(\rho_+ - \rho_-)/2L]^2/|x-y|^{d-2}$ for dimension $d \geq 3$ over distances small compared to the width L of the slab. We also study the influence of boundary conditions which although essential are hardly mentioned in other papers. The effect is second order in the density gradient. For fluids one finds such a slow decay for some correlations already to first order in the, in this case, temperature gradient because of the presence of convective terms. To my knowledge fluctuating hydrodynamics with a single conserved field has been investigated in Tremblay *et al* (1981), Medina-Noyola and Keizer (1981). In Tremblay *et al* (1981) only the first-order deviations from the uniform density are considered whereas in Medina-Noyola and Keizer (1981) a very particular density dependence of the transport coefficient is assumed. In both cases the physically interesting effect does not show up.

We then indicate how the macroscopic theory can be obtained from the underlying stochastic dynamics, at least in principle. We have no idea how to carry out this programme rigorously, in general. Fortunately there is one particular but non-degenerate case for which the derivation of fluctuating hydrodynamics can be proved. This case corresponds to infinite temperature with hard core exclusion only. The equilibrium theory of this model is completely trivial. The non-equilibrium steady state shows, however, a surprisingly rich structure which has its origin *solely* in the fact that two particles are not allowed to occupy the same lattice site simultaneously.

In this simple exclusion model we will also investigate corrections to fluctuating hydrodynamics. Very likely these corrections are model dependent, but still they give us an idea of how well the macroscopic theory describes the microscopic system.

2. Stochastic lattice gases

We assume that particles jump on the d-dimensional lattice $\mathbb{Z}^d$. There is at most one particle per lattice site. (Notice that thereby the hard core exclusion is built into the model. As with other assumptions below one could be less restrictive.) The occupation variables are denoted by η_x, $x \in \mathbb{Z}^d$. $\eta_x = 1$ corresponds to site x occupied and $\eta_x = 0$ to site x empty. $\eta = \{\eta_x | x \in \mathbb{Z}^d\}$ denotes a particle configuration.

For simplicity we assume the usual nearest-neighbour interaction energy

$$H(\eta) = -\tfrac{1}{2} \sum_{|x-y|=1} \eta_x \eta_y . \tag{2.1}$$

Let

$$c(x, y, \eta) \geq 0 \tag{2.2}$$

be the rate that in the configuration η the occupations at site x and y are interchanged. Therefore $c(x, y, \eta) = c(y, x, \eta)$. If $\eta_x = 1$ and $\eta_y = 0$, then $c(x, y, \eta)$ is the rate for the particle at x to jump to y in the configuration η. If $\eta_x = \eta_y$, then we may set $c(x, y, \eta) = 0$. We make the following assumptions on the rates $c(x, y, \eta)$:

(i) $c(x, y, \eta)$ is invariant under translations, i.e. $c(x+a, y+a, \tau_a \eta) = c(x, y, \eta)$ for all $a \in \mathbb{Z}^d$, with τ_a the shift by a, and invariant under rotations.

(ii) $c(x, y, \eta) = 0$ whenever $|x-y| > 1$. This means that only nearest-neighbour jumps are allowed. To avoid degeneracies we also assume $c(x, y, \eta) > 0$ whenever $|x-y| = 1$.

(iii) $c(x, y, \eta)$ is of finite range, i.e. it depends only on a finite neighbourhood of x and y.

(iv) $c(x, y, \eta)$ satisfies the condition of detailed balance with respect to the energy (2.1), i.e.

$$c(x, y, \eta) = c(x, y, \eta^{xy}) \exp[-\beta(H(\eta^{xy}) - H(\eta))]. \tag{2.3}$$

Here η^{xy} denotes the configuration η with occupations at sites x and y interchanged,

$$(\eta^{xy})_z = \begin{cases} \eta_x & \text{for } z = y \\ \eta_y & \text{for } z = x \\ \eta_z & \text{for } z \neq x, y. \end{cases} \tag{2.4}$$

(v) We assume β to be sufficiently small such that there is only one phase at any density $0 \leq \rho \leq 1$.

If β allows the coexistence of two phases, then for $d \geq 3$ already in thermal equilibrium the system may form a stable interface. Therefore, also the steady state will have an interface provided ρ_+ and ρ_- are in the appropriate range. The average location of this interface should be determined by the balance of mass flow through the interface.

With these assumptions the generator of the dynamics is given by

$$(Lf)(\eta)=\tfrac{1}{2}\sum_{x,y} c(x,y,\eta)(f(\eta^{xy})-f(\eta)) \tag{2.5}$$

acting on functions f depending only on a finite number of occupation variables. L determines the unique Markov semigroup

$$T_t=\mathrm{e}^{Lt}, \qquad t\geq 0 \tag{2.6}$$

on the space of bounded and continuous functions on $\{0,1\}^{\mathbb{Z}^d}$ (Liggett 1977). Let χ_A be the characteristic function of a Borel set $A\subset\{0,1\}^{\mathbb{Z}^d}$. Then

$$(\mathrm{e}^{Lt}\chi_A)(\eta)=\int_A \mathrm{e}^{Lt}(\eta|\mathrm{d}\eta') \tag{2.7}$$

is the probability that, given that the system is in the configuration η at $t=0$, the system is in the set A of configurations at time t. Thus the kernel of e^{Lt} is the transition probability and, since our dynamics is Markovian, everything else is determined in terms of this transition probability.

Let $\langle\ \rangle_\rho$ denote the thermal equilibrium state at density ρ, $0\leq\rho\leq 1$, and inverse temperature β for the energy (2.1). Then because of detailed balance T_t and L are self-adjoint,

$$\begin{aligned}&\langle f(T_t g)\rangle_\rho=\langle g(T_t f)\rangle_\rho,\\ &\langle f(L_g)\rangle_\rho=\langle g(Lf)\rangle_\rho,\end{aligned} \tag{2.8}$$

in particular $\langle\ \rangle_\rho$ is time invariant, i.e.

$$\langle T_t f\rangle_\rho=\langle f\rangle_\rho. \tag{2.9}$$

The temporal evolution of the density, including its fluctuations, on a macroscopic level is determined by two microscopic quantities only.

(I) The compressibility $\chi(\rho)$ defined by

$$\chi(\rho)=\sum_x(\langle\eta_x\eta_0\rangle_\rho-\rho^2). \tag{2.10}$$

This is a purely static quantity independent of the specific jump rates.

(II) The bulk diffusion coefficient $D(\rho)$. $D(\rho)$ depends on the dynamics. In general $D(\rho)$ is a $d\times d$ matrix. Because of the assumed isotropy it is a scalar, here. $D(\rho)$ is microscopically defined by the Green–Kubo formula as the space–time integral over the current–current correlation function. The current–current correlation function has a contribution proportional to $\delta(t)$ and a regular part. Explicitly

$$D(\rho)=\frac{1}{2\chi(\rho)}\left(\langle c(0,e,\eta)(\eta_0-\eta_e)^2\rangle_\rho-\int_{-\infty}^{\infty}\mathrm{d}t\sum_{x\in\mathbb{Z}^d}\langle j(x,x+e)\,\mathrm{e}^{L|t|}j(0,e)\rangle_\rho\right). \tag{2.11}$$

Here e is a unit vector, $e\in\mathbb{Z}^d$ with $|e|=1$. The first term is the average jump rate through the bond $(0,e)$. $j(x,x+e)$ is the current function for the bond $(x,x+e)$ defined by

$$j(x,x+e)(\eta)=c(x,x+e,\eta)(\eta_x-\eta_{x+e}). \tag{2.12}$$

Since e^{Lt} is self-adjoint, $\Sigma_x\langle j(x,x+e)\,\mathrm{e}^{L|t|}j(0,e)\rangle_\rho\geq 0$. One can also show that this function is integrable in t (Spohn 1982). One has the trivial bounds

$$0\leq D(\rho)\leq(1/2\chi(\rho))\langle c(0,e)(\eta_0-\eta_e)^2\rangle_\rho. \tag{2.13}$$

At present one cannot exclude rigorously that the negative and positive contribution to $D(\rho)$ cancel each other and hence $D(\rho)=0$. Physically one certainly expects $D(\rho)>0$ away from the critical point. It is believed that as (ρ, β) tends to the critical point $D(\rho)$ tends to zero as $\chi(\rho)^{-1}$ (Hohenberg and Halperin 1977).

We are now in a position to model the physical situation described in the introduction. We consider the slab $\Lambda_N \subset \mathbb{Z}^d$. It extends from $-N$ to N in the one-direction and is infinitely extended otherwise. At the left and right boundary of Λ_N we want to allow for creation and destruction of particles. To do so we introduce the boundary rates

$$c_{+(-)}(x, \eta) \geq 0 \tag{2.14}$$

of interchanging η_x and $1-\eta_x$ when the configuration is η. Again we assume translation invariance, finite range, and detailed balance in the form

$$c_{+(-)}(x, \eta) = c_{+(-)}(x, \eta^x) \exp[-\beta(H(\eta^x) - H(\eta))] \exp[\beta\mu_{+(-)}(1-2\eta_x)]. \tag{2.15}$$

Here η^x denotes the configuration η with η_x replaced by $(1-\eta_x)$. (2.15) fixes the chemical potential $\mu_+(\mu_-)$ at the right (left) boundary which is related to the boundary density $\rho_+(\rho_-)$ in the usual way. The generator of the dynamics including boundary conditions is then given by

$$\begin{aligned}(Lf)(\eta) = \tfrac{1}{2} &\sum_{x,y\in\Lambda_N, |x-y|=1} c(x, y, \eta)(f(\eta^{xy}) - f(\eta)) \\ &+ \sum_{\substack{x_1=-N, \\ x_2,\ldots,x_d\in\mathbb{Z}^{d-1}}} c_-(x, \eta)(f(\eta^x) - f(\eta)) \\ &+ \sum_{\substack{x_1=N \\ x_2,\ldots,x_d\in\mathbb{Z}^{d-1}}} c_+(x, \eta)(f(\eta^x) - f(\eta)).\end{aligned} \tag{2.16}$$

The steady state $\langle\ \rangle_N$ is defined by

$$\langle Lf\rangle_N = 0 \tag{2.17}$$

for all strictly local functions f. The steady state depends on N and the boundary densities ρ_+ and ρ_-. If the height of the slab is finite, we have a Markov chain with finite state space and standard results guarantee uniqueness of the steady state. For the infinite slab one certainly expects uniqueness at high temperatures, but except for particular cases, we do not know of a proof.

Physically of major interest are the average density

$$\langle \eta_x \rangle_N \tag{2.18}$$

and the truncated pair-correlation function

$$\langle \eta_{x,t}\eta_{y,0}\rangle_N - \langle\eta_x\rangle_N \langle\eta_y\rangle_N. \tag{2.19}$$

(We use here the time invariance of $\langle\ \rangle_N$.) The truncated pair correlation function describes time-dependent fluctuations in the density and its space–time Fourier transform is directly measured in scattering experiments.

3. Macroscopic theory/fluctuating hydrodynamics

On a macroscopic scale the density is governed by the nonlinear diffusion equation

$$\partial\rho(q,t)/\partial t=(\partial/\partial q)D(\rho(q,t))(\partial\rho(q,t)/\partial q) \tag{3.1}$$

with $D(\rho)$ given by (2.11). There is no drift, since in equilibrium the current vanishes. We consider the slab Λ_L, $-L\leq q_1\leq L$, $-\infty<q_2,\ldots,q_d<\infty$. The steady state density ρ_s is the solution of

$$(\partial/\partial q)D(\rho_s(q))(\partial\rho_s(q)/\partial q)=0 \tag{3.2}$$

with boundary conditions

$$\rho_s(-L,q_2,\ldots,q_d)=\rho_-,\qquad \rho_s(L,q_2,\ldots,q_d)=\rho_+. \tag{3.3}$$

By symmetry the solution depends only on q_1. If $\rho_-<\rho_+$, the steady-state density increases monotonically. If $D(\rho)$ is small, the variation in $\rho_s(q)$ is large. (3.2) together with (3.3) constitutes the macroscopic approximation to (2.18).

To study the fluctuations let us briefly recall the situation for global equilibrium. We denote by $\xi(q,t)$ the deviation in the density from its uniform average value ρ at the macroscopic space–time point (q,t). (These are random variables.) $\xi(q,t)$ has mean zero and we assume that $\xi(q,t)$ is Gaussian. The exponentially correlated static fluctuations look, on a macroscopic scale, δ-correlated with weight $\chi(\rho)$. Therefore

$$\langle\xi(q,t)\xi(q',t)\rangle=\langle\xi(q,0)\xi(q',0)\rangle=\chi(\rho)\delta(q-q'), \tag{3.4}$$

where ρ is the equilibrium density. Since $\xi(q,t)$ is assumed to be small, it changes in time deterministically according to the linearised macroscopic equation. In addition $\xi(q,t)$ is driven by microscopic fluctuations, i.e. by a random force which we write as the divergence of a random current to ensure the conservation of mass. Therefore we postulate the evolution equation

$$\partial\xi(q,t)/\partial t=\frac{\partial}{\partial q}\cdot\frac{\partial}{\partial q}D(\rho)\xi(q,t)-\frac{\partial}{\partial q}\cdot j(q,t). \tag{3.5}$$

In order to have a Gaussian $\xi(q,t)$, $j(q,t)$ has to be Gaussian of mean zero. Since the stationary measure is already given through (3.4), the covariance of the random current is uniquely determined to be

$$\langle j_m(q,t)j_n(q',t')\rangle=2\delta_{mn}\delta(t-t')\delta(q-q')(D\chi)(\rho). \tag{3.6}$$

The current is white noise with strength $D\chi(\rho)$. Physically $D\chi$ just equals the electrical conductivity in linear response.

To generalise to a non-equilibrium steady state we still postulate an evolution equation of the form (3.5). The deterministic part is now the macroscopic equation linearised around the steady state. This yields

$$(\partial/\partial t)\xi(q,t)=(\partial/\partial q)\cdot(\partial/\partial q)D(\rho_s(q))\xi(q,t)-(\partial/\partial q)\cdot j(q,t). \tag{3.7}$$

The fluctuating current $j(q,t)$ still has to be Gaussian of mean zero. But we have now no additional information available to determine its covariance. To make a reasonable guess we recall that the derivation of the macroscopic equation is based on the assumption that the system is locally, in space–time, in equilibrium. Once we observe that in (3.6) the covariance of the fluctuating current is determined locally, it is natural to assume that the covariance of the fluctuating current in (3.7) is still given by

$$\langle j_m(q,t) j_n(q',t')\rangle = 2\delta_{mn}\delta(t-t')\delta(q-q')D\chi(\rho_s(q)). \tag{3.8}$$

The strength at (q, t) is determined by the local density at (q, t), i.e. by the steady state density $\rho_s(q)$, in the same way as in thermal equilibrium. Finally, we have to add to (3.7) some boundary conditions. Since at the boundary the density is fixed, the density deviations are zero and therefore

$$\xi(-L, q_2, \ldots, q_d, t) = 0 = \xi(L, q_2, \ldots, q_d, t). \tag{3.9}$$

The stationary solution of (3.7) together with (3.8) and (3.9) constitute the macroscopic approximation to (2.19).

The Gaussian process defined by (3.7), (3.8) and (3.9) has a unique stationary measure with mean zero and covariance

$$C_s(q, q') = \langle \xi(q,t)\xi(q',t)\rangle. \tag{3.10}$$

We want to divide out the local equilibrium contribution and write

$$C_s(q, q') = \delta(q-q')\chi(\rho_s(q)) + C_{\mathrm{NE}}(q, q'). \tag{3.11}$$

A straightforward computation yields then

$$C_{\mathrm{NE}}(q, q') = \int_0^\infty \mathrm{d}t \int \mathrm{d}q''\, \mathrm{e}^{At}(q, q'')[(\partial^2/\partial q_1''^2)(D\chi)(\rho_s(q''))]\, \mathrm{e}^{A^*t}(q'', q'). \tag{3.12}$$

Here

$$(A^*f)(q) = D(\rho_s(q))(\partial/\partial q)\cdot(\partial/\partial q) f(q) \tag{3.13}$$

with zero (Dirichlet) boundary conditions. $\mathrm{e}^{A^*t}(q, q')\,\mathrm{d}q'$ is the transition probability for the diffusion process with generator A^* and absorption at the boundary of the slab. Note that if we expand in the difference of the boundary densities, $\rho_+ - \rho_-$, then $C_{\mathrm{NE}} \sim (\rho_+ - \rho_-)^2$ and will pass unobserved to first order. In Medina-Noyola and Keizer (1981) $D\chi = 1$ is assumed and consequently C_{NE} vanishes.

The time-dependent fluctuations are simply obtained as

$$\langle \xi(q,t)\xi(q',0)\rangle = \int \mathrm{d}q''\, \mathrm{e}^{At}(q, q'')C_s(q'', q') \tag{3.14}$$

for $t \geqslant 0$.

To understand how C_{NE} depends on q and q' it is useful to consider the special case $D = 1$, $\chi(\rho) = \rho(1-\rho)$. This case will reappear later on when we discuss the simple exclusion model with exchange rates $c(x, y, \eta) = 1$ for $|x-y| = 1$. Since in this case D does not depend on ρ, the steady state solution is

$$\rho_s(q) = (1/2L)[(L+q_1)\rho_+ + (L-q_1)\rho_-] \tag{3.15}$$

and therefore

$$(\partial^2/\partial q_1^2)(D\chi)(\rho_s(q_1)) = -2[(\rho_+ - \rho_-)/2L]^2. \tag{3.16}$$

Using the fact that A is symmetric we obtain

$$C_{\mathrm{NE}}(q, q') = [(\rho_+ - \rho_-)/2L]^2 \Delta^{-1}(q, q') \leqslant 0, \tag{3.17}$$

where $\Delta^{-1}(q, q')$ is the kernel of the inverse of the Laplacian with zero boundary conditions (Green function). Notice that the non-equilibrium part is negatively correlated in this case. The behaviour of $\Delta^{-1}(q, q')$ is well understood: In three dimensions, if q and q' are separated by a distance small compared to L, then the influence of the boundaries is negligible and

$$\Delta^{-1}(q, q') \cong -4\pi/|q-q'|. \tag{3.18}$$

On the other hand if $|q-q'| \gg L$, then the absorption at the boundary dominates and

$$\Delta^{-1}(q, q') \cong \exp(-|q-q'|/2L). \tag{3.19}$$

The stationary density–density covariance has a δ-correlated local equilibrium contribution and a part which is negatively correlated and decays slowly as $1/|q|$. This part has the strength $[(\rho_+ - \rho_-)/2L]^2$. The long range part of the covariance is eventually cut off at distances of the order of the width of the slab.

The time-dependent fluctuations can be computed from (3.14) and are given by

$$\langle \xi(q, t)\xi(q', 0)\rangle = e^{\Delta t}(q, q')\chi(\rho_s(q')) + [(\rho_+ - \rho_-)/2L]^2 e^{\Delta t}\Delta^{-1}(q, q'). \tag{3.20}$$

Physically one typically measures the structure factor by means of a scattering experiment. For a translation invariant system this is simply the space–time Fourier transform of (3.20). For a system not invariant under translations, as the one here, one has to specify more precisely the experimental set-up. We refer to Kirkpatrick *et al* (1982) for a detailed discussion of this point. If one follows the prescription there and assumes that the scattering region is in the middle of the slab at $q_1 = 0$, then a rather good approximation to Δ with zero boundary conditions is the free Laplacian with mass $\pi^2/4L^2$. Then within that approximation

$$S(k, \omega) = \frac{k^2 + \pi^2/4L^2}{\omega^2 + (k^2 + \pi^2/4L^2)^2}\frac{1}{4}\left((\rho_+ + \rho_-)(2 - \rho_+ - \rho_-) - (\rho_+ - \rho_-)^2 \frac{1}{L^2k^2 + \pi^2/4}\right). \tag{3.21}$$

The frequency distribution is still Lorentzian, but the amplitude for small k is strongly suppressed because of the imposed density gradient.

Returning to the general case (3.12) one expects results qualitatively comparable to the special case $D(\rho) = 1$, $\chi(\rho) = \rho(1-\rho)$. This is certainly the case if $-a \leqslant (\partial^2/\partial q_1^2)(D\chi)(\rho_s(q_1)) \leqslant -b$ with strictly positive constants a, b. If $(\partial^2/\partial q_1^2)(D\chi)(\rho_s(q_1))$ takes on both signs, which does not seem to be excluded in general, then cancellations might wash out the effect found here.

4. The hydrodynamic limit/connection between microscopic and macroscopic theory

We will first consider only static, equal time functionals.

We introduce the scaling parameter ε, $\varepsilon > 0$, $\varepsilon \to 0$. It is convenient to think of ε as the lattice spacing. We approximate then the continuum slab Λ_L by a discrete slab $\varepsilon\Lambda_{N(\varepsilon)}$ with $N(\varepsilon) = [\varepsilon^{-1}L]$ and lattice spacing ε. $[a]$ denotes here the integer part of a.

One expects that for every point $q \in \Lambda_L^0$

$$\lim_{\varepsilon \to 0} \langle \eta_{[\varepsilon^{-1}q]}\rangle_{N(\varepsilon)} = \rho_s(q). \tag{4.1}$$

The average density approximates the steady state solution. We take q to be in the interior of Λ_L to avoid the boundary layer. If one spatially averages over many lattice sites, one expects to have small density fluctuations only. Let Λ_ε be a hypercube of side-length $1/\sqrt{\varepsilon}$ lattice sites. ($1/\sqrt{\varepsilon}$ is only a convention here. One wants the number $|\Lambda_\varepsilon|$ of lattice sites in Λ_ε to tend to infinity as $\varepsilon \to 0$ and $\varepsilon\Lambda_\varepsilon$, i.e. Λ_ε on the lattice with lattice spacing ε, to shrink to zero. Therefore $\varepsilon^{-\alpha}$ with $0<\alpha<1$ would do.) Then one expects that for every $q \in \Lambda_L^0$

$$\lim_{\varepsilon \to 0} \frac{1}{|\Lambda_\varepsilon|} \sum_{x \in \Lambda_\varepsilon} \eta_{[\varepsilon^{-1}q]+x} = \rho_s(q) \tag{4.2}$$

in probability with respect to the sequence of stationary measures $\langle \cdot \rangle_{N(\varepsilon)}$. Technically it is often more convenient instead of (4.2) to average spatially over a smooth test function. Let f be a test function defined on Λ_L. f is assumed to vanish rapidly at infinity and to be zero some finite distance away from the boundary. Then one expects that

$$\lim_{\varepsilon \to 0} \varepsilon^d \sum_{x \in \Lambda_{N(\varepsilon)}} f(\varepsilon x)\eta_x = \int \mathrm{d}q\, \rho_s(q) f(q) \tag{4.3}$$

in probability with respect to the stationary measure $\langle \cdot \rangle_{N(\varepsilon)}$.

The fluctuations in the density field are defined in the usual way, anticipating their normal character,

$$\xi^\varepsilon(f) = \varepsilon^{d/2} \sum_{x \in \Lambda_{N(\varepsilon)}} f(\varepsilon x)(\eta_x - \langle \eta_x \rangle_{N(\varepsilon)}) \tag{4.4}$$

in the stationary state $\langle\ \rangle_{N(\varepsilon)}$.

Conjecture 1. Let $\langle\ \rangle_{N(\varepsilon)}$ be the steady state with $N(\varepsilon) = [\varepsilon^{-1}L]$. Then

$$\lim_{\varepsilon \to 0} \xi^\varepsilon(f) = \xi(f) \tag{4.5}$$

exists. $\xi(f)$ is a Gaussian random field with mean zero and covariance

$$\langle \xi(f)\xi(g) \rangle = \int \mathrm{d}q\, \mathrm{d}q'\, f(q) g(q') C_s(q, q'), \tag{4.6}$$

where $C_s(q, q')$ is given by (3.11) and (3.12).

Since the non-equilibrium part of the steady state covariance is smooth one also expects that for $q, q' \in \Lambda_L^0$, $q \neq q'$,

$$\lim_{\varepsilon \to 0} \varepsilon^{-d}(\langle \eta_{[\varepsilon^{-1}q]} \eta_{[\varepsilon^{-1}q']} \rangle_{N(\varepsilon)} - \langle \eta_{[\varepsilon^{-1}q]} \rangle_{N(\varepsilon)} \langle \eta_{[\varepsilon^{-1}q']} \rangle_{N(\varepsilon)}) = C_{\mathrm{NE}}(q, q'). \tag{4.7}$$

Given (4.3) and (4.5) with (4.6) as a backbone the picture can be refined in several directions. One may investigate the distribution of particles in the neighbourhood of the macroscopic point $q \in \Lambda_L^0$ and should find the Gibbs measure with density $\rho_s(q)$. Instead of the density field one could consider fields of the form $\Sigma_x f(\varepsilon x)\tau_x h$ with h a local function. In the limit $\varepsilon \to 0$ their deterministic value and their fluctuations should become functionals of the density.

If one wants to include the time-dependence, then one has to speed up time as $\varepsilon^{-2}t$ and defines

$$\xi^{\varepsilon}(f,t)=\sum_{x\in\Lambda_{N(\varepsilon)}} f(\varepsilon x)(\eta_{x,\varepsilon^{-2}t}-\langle\eta_x\rangle_{N(\varepsilon)}) \tag{4.8}$$

in the stationary measure $\langle\ \rangle_{N(\varepsilon)}$. $\xi^{\varepsilon}(f,t)$ should converge as $\varepsilon\to 0$ to the stationary Gaussian process with covariance (3.14).

Unfortunately, we have no mathematical technique at present to prove even the simplest conjecture, in general. However, we will show in § 5 that there is at least one model, namely the simple exclusion model, for which the hydrodynamic limit can be established rigorously. This model is non-trivial in the sense that $C_{\mathrm{NE}}(q,q')\neq 0$. For non-interacting particle models $C_{\mathrm{NE}}(q,q')=0$ always.

5. The simple exclusion model

In this section we consider the special case $\beta=0$ and $c(x,y,\eta)=1$ for $|x-y|=1$, $c(x,y,\eta)=0$ otherwise. Then we can rewrite the generator (2.16) directly in terms of the boundary densities as

$$\begin{aligned}(Lf)(\eta)=\tfrac{1}{2}&\sum_{x,y\in\Lambda_N,|x-y|=1}(f(\eta^{xy})-f(\eta))\\&+\sum_{x\in\Lambda_N,x_1=-N}[\rho_-(1-\eta_x)+(1-\rho_-)\eta_x](f(\eta^x)-f(\eta))\\&+\sum_{x\in\Lambda_N,x_1=N}[\rho_+(1-\eta_x)+(1-\rho_+)\eta_x](f(\eta^x)-f(\eta)).\end{aligned} \tag{5.1}$$

The simplicity of this particular lattice gas at infinite temperature stems from the fact that the BBGKY-hierarchy decouples: the nth correlation function satisfies a closed equation by itself. At finite temperatures the nth correlation function is coupled to higher-order correlation functions which makes an analysis much harder. We want to exploit this simplicity here in order to investigate the steady state pair correlation function in some detail. In particular we will prove the validity of the macroscopic theory.

The argument given in Galves *et al* (1981) extends to arbitrary dimensions and proves that there is a unique stationary probability measure $\langle\ \rangle_N$, i.e. a unique state satisfying

$$\langle Lf\rangle_N=0 \tag{5.2}$$

for all local functions f. If $\rho_-=\rho=\rho_+$, then in the state $\langle\ \rangle_N$ the η_x are independent and $\eta_x=1$ with probability ρ.

We note that $\chi(\rho)$ and $D(\rho)$ as defined in (2.10) and (2.11) are given by

$$\chi(\rho)=\rho(1-\rho) \tag{5.3}$$

and

$$D(\rho)=1, \tag{5.4}$$

since $j(x,x+e)=\eta_x-\eta_{x+e}$ which implies that $\Sigma_x\langle j(x,x+e)\,\mathrm{e}^{L't}j(0,e')\rangle_\rho=0$ in global equilibrium.

5.1. *Covariance of the steady state*

To simplify notation we abbreviate $x_2, \ldots, x_d = x_\parallel$ and write $x=(x_1, x_\parallel)$. For the first correlation function one obtains

$$\Delta\langle\eta_x\rangle_N=0 \tag{5.5}$$

with the boundary conditions $\langle\eta_{(-N-1,x_\parallel)}\rangle_N=\rho_-$ and $\langle\eta_{(N+1,x_\parallel)}\rangle_N=\rho_+$. Here Δ is the lattice Laplacian,

$$(\Delta f)(x)=\sum_{e,|e|=1}(f(x+e)-f(x)). \tag{5.6}$$

The solution of (5.5) is well known and given by

$$\langle\eta_x\rangle_N=[1/(2N+2)][\rho_-(N+1-x_1)+\rho_+(N+1+x_1)]. \tag{5.7}$$

The covariance is defined by

$$c_N(x,y)=\langle\eta_x\eta_y\rangle_N-\langle\eta_x\rangle_N\langle\eta_y\rangle_N, \tag{5.8}$$

$x, y\in\Lambda_N$. At coinciding arguments

$$c_N(x,x)=\langle\eta_x\rangle_N(1-\langle\eta_x\rangle_N). \tag{5.9}$$

From now on we assume $x\neq y$.

We insert in (5.2) $f(\eta)=\eta_x\eta_y$. In the resulting equation we substitute $\langle\eta_x\eta_y\rangle_N=c_N(x,y)+\langle\eta_x\rangle_N\langle\eta_y\rangle_N$. Using the explicit average density (5.7) we obtain

$$\begin{aligned}\sum_{x'\in\Lambda_N,|x'-x|=1,x'\neq y}&(c_N(x',y)-c_N(x,y))+\sum_{y'\in\Lambda_N,|y'-y|=1,y'\neq x}(c_N(x,y')-c_N(x,y))\\&-(\delta_{x_1,-N}+\delta_{x_1,N}+\delta_{y_1,-N}+\delta_{y_1,N})c_N(x,y)\\&=[(\rho_+-\rho_-)^2/(2N+2)^2](\delta_{x_1,y_1+1}+\delta_{x_1+1,y_1})\delta_{x_\parallel,y_\parallel}.\end{aligned} \tag{5.10}$$

(5.10) has a useful probabilistic interpretation. Let $x(t)$, $y(t)$ be two random walks on $\Lambda_N\cup\{x_1=-N-1\}\cup\{x_1=N+1\}$. They jump with rate one to either one of the nearest-neighbour lattice sites provided this site is not occupied by the other random walk. $x(t)$ and $y(t)$ are absorbed whenever they hit the boundary planes $\{x_1=-N-1\}$ and $\{x_1=N+1\}$. $\mathbb{E}_{N,(x,y)}$ refers to expectation with respect to these two excluding random walks given that initially $x(0)=x$, $y(0)=y$. Let A_N be the generator of the Markov jump process $x(t)$, $y(t)$ and let $g_N(x,y)=(\delta_{x_1,y_1+1}+\delta_{x_1+1,y_1})\delta_{x_\parallel,y_\parallel}$. Then

$$(A_Nc_N)(x,y)=[(\rho_+-\rho_-)/(2N+2)]^2g_N(x,y). \tag{5.11}$$

Because of the absorbing (Dirichlet) boundary conditions A_N is invertible and

$$c_N(x,y)=[(\rho_+-\rho_-)/(2N+2)]^2(A_N^{-1}g_N)(x,y). \tag{5.12}$$

Lemma 5.1. Let $A_N^{-1}(x,y;x',y')$ be the kernel of A_N^{-1}. Then

$$-A_N^{-1}(x,y;x',y')=\mathbb{E}_{N,(x,y)}\,(\text{time which } x(t), y(t) \text{ spend at } x', y'). \tag{5.13}$$

Proof. The time spent at x', y' equals

$$\int_0^\infty \mathrm{d}t\,\delta_{x(t),x'}\delta_{y(t),y'}. \tag{5.14}$$

Taking expectations and interchanging the order of integration yields

$$\int_0^\infty \mathrm{d}t\, \mathbb{E}_{N,(x,y)}(\delta_{x(t),x'}\delta_{y(t),y'})$$

$$= \int_0^\infty \mathrm{d}t\, \mathrm{e}^{A_N t}(x, y; x', y') = -A_N^{-1}(x, y; x', y'). \tag{5.15}$$

g_N is the indicator function of the set $\Gamma_N = \{x, y \in \Lambda_N | x_1 - y_1| = 1, x_\| = y_\|\}$. Therefore lemma 5.1 together with (5.12) gives for the covariance

$$c_N(x, y) = [(\rho_+ - \rho_-)/(2N+2)]^2 \mathbb{E}_{N,(x,y)}\,(\text{time which } x(t),\ y(t) \text{ spend in } \Gamma_N). \tag{5.16}$$

In other words, up to a prefactor, $c_N(x, y)$ is the average time the two excluding random walks stay next to each other in the one-direction given that they started at x, y.

Equation (5.16) implies two simple facts.

Proposition 5.2. Particles are negatively correlated,

$$c_N(x, y) < 0. \tag{5.17}$$

Proposition 5.3. $-(2N+2)^2 c_N(x, y)$ increases monotonically as $N \to \infty$.

Proof. For $M > N, \Gamma_M \supset \Gamma_N$ and the time spent in Γ_N increases because $\Lambda_M \supset \Lambda_N$.

If we think of $x(t)$, $y(t)$ as a $2d$-dimensional random walk, then we have to know the average time it spends in a certain d-dimensional hyperplane. It follows that the average time spent in Γ_N increases as N in one dimension, increases as $\log N$ in two dimensions and stays finite for three and more dimensions as $N \to \infty$. The order of magnitude of the correlations is then

$$\begin{aligned} c_N(x, y) \approx\ & -(\rho_+ - \rho_-)^2 1/N & d = 1 \\ & -(\rho_+ - \rho_-)^2 (\log N)/N^2 & d = 2 \\ & -(\rho_+ - \rho_-)^2 1/N^2 & d \geq 3. \end{aligned} \tag{5.18}$$

We emphasise that these correlations are entirely due to the imposed boundary conditions. The trivial equilibrium correlations of the system are contained in (5.9).

In one dimension, by luck, a closed expression can be obtained. One has for $x < y$

$$c_N(x, y) = [(\rho_+ - \rho_-)/(2N+2)]^2 (\Delta_N')^{-1}(x, y-1), \tag{5.19}$$

where Δ_N' is the lattice Laplacian in the interval $[-N, N-1]$ with Dirichlet boundary conditions and $(\Delta_N')^{-1}(x, y)$ refers to the kernel of its inverse. As is well known the kernel of the inverse Laplacian increases as N in one dimension.

In higher dimensions the expression (5.16) for c_N is somewhat indirect and we could not find a simple closed form for c_N. To find out its dependence on x and y we follow three different roads. For $d \geq 3$ if $N \to \infty$, then $c_N \to 0$ as $1/N^2$. One possibility is then to take out the trivial prefactor $1/(2N+2)^2$ and to study the limit $N \to \infty$ of the remainder. This gives a reasonable approximation for $c_N(x, y)$ with $|x_1|$, $|y_1|$ and $|x - y|$ small compared to N. This approach is pursued in § 5.2. In § 5.3 we obtain upper and lower bounds on c_N in terms of non-interacting random walks, i.e. in terms of Δ_N which can be diagonalised explicitly. In § 5.5 we investigate the hydrodynamic limit.

5.2. The infinite volume limit at fixed lattice constant

We take out the trivial prefactor from c_N by defining

$$\tilde{c}_N(x, y) = [(2N+2)/(\rho_+ - \rho_-)]^2 c_N(x, y) \tag{5.20}$$

and want to investigate the limit of $\tilde{c}_N(x, y)$ as $N \to \infty$.

Let Δ be the lattice Laplacian on $\mathbb{Z}^d$, let Δ_1 be the lattice Laplacian in the direction of the 1-axis and let $\Delta_\parallel = \Delta - \Delta_1$. We Fourier transform as

$$\hat{f}(k) = \sum_{x \in \mathbb{Z}^d} f(x)\, e^{ikx}$$

with $k = (k_1, \ldots, k_d) = (k_1, k_\parallel) \in [-\pi, \pi]^d$. Then Δ transforms to multiplication by $\varepsilon(k) = \Sigma_{j=1}^d 2(\cos k_j - 1)$. To abbreviate, we set $\varepsilon(k_j) = 2(\cos k_j - 1)$ and $\varepsilon(k_\parallel) = \varepsilon(k) - \varepsilon(k_1)$.

Proposition 5.4. For $d \geq 3$ let

$$c(x, y) = \Delta^{-1}(x, y) - [(d-1)/\alpha d^2](\Delta_\parallel \Delta^{-1})(x, y) + [(d-1)^2/\alpha d^2](\Delta_1 \Delta^{-1})(x, y) \tag{5.21}$$

with

$$\alpha = -(2\pi)^{-d} \int dk\, \varepsilon(k_1)\varepsilon(k_\parallel)\varepsilon(k)^{-1}. \tag{5.22}$$

Then for $d \geq 3$ and $x \neq y$

$$\lim_{N \to \infty} \tilde{c}_N(x, y) = c(x, y). \tag{5.23}$$

Proof. We set $\mathbb{E}_{(x,y)}(\cdot) = \mathbb{E}_{N=\infty,(x,y)}(\cdot)$ and $\Gamma = \Gamma_\infty = \{x, y \in \mathbb{Z}^d \,|\, |x_1 - y_1| = 1, x_\parallel = y_\parallel\}$. By monotonicity the limit (5.23) equals

$$c(x, y) = -\mathbb{E}_{(x,y)}\,(\text{time which } x(t), y(t) \text{ spend in } \Gamma). \tag{5.24}$$

Since $(x(t), y(t))$ is a $2d$-dimensional random walk and Γ is a d-dimensional hyperplane, $d \geq 3$, the expectation is finite. Let A be the generator of the random walk $x(t)$, $y(t)$. Then

$$c(x, y) = \sum_{w \in \mathbb{Z}} [A^{-1}(x, y; w, 0, w+1, 0) + A^{-1}(x, y; w+1, 0, w, 0)], \tag{5.25}$$

where $A^{-1}(x, y; x', y')$ refers to the kernel of A^{-1}. The set of functions on $\mathbb{Z}^d \times \mathbb{Z}^d$ of the form $g(x, y) = f(x - y)$ are invariant under A. Since in (5.25) A^{-1} acts on a function of that form, we only have to know the action of A on this invariant subspace. In Fourier space, with the convention $f(0) = 0$, one obtains

$$(\hat{A}\hat{f})(k) = 2\varepsilon(k)\hat{f}(k) + \sum_{j=1}^{d} \varepsilon(k_j)(2\pi)^{-d} \int dk\, \varepsilon(k_j)\hat{f}(k), \tag{5.26}$$

$$\int dk\, \hat{f}(k) = 0.$$

Let $c(x, y) = (2\pi)^{-d} \int dk \exp[ik(x-y)]\hat{c}(k)$. Then

$$2\varepsilon(k)\hat{c}(k) + \sum_{j=1}^{d} \varepsilon(k_j)(2\pi)^{-d} \int dk\, \varepsilon(k_j)\hat{c}(k) = 2\cos k_1, \tag{5.27}$$

$$\int dk\, \hat{c}(k) = 0.$$

The solution of (5.27) is given by

$$\hat{c}(k) = (2\varepsilon(k))^{-1}(2 + a\varepsilon(k_{\|}) + b\varepsilon(k_1)) \tag{5.28}$$

with

$$2d\beta = (d-1)a + b, \qquad 2(d-1)/d\alpha = a - b, \tag{5.29}$$

where $\beta = -(2\pi)^{-d} \int dk\, \varepsilon(k)^{-1}$. Solving (5.29) for a and b, inserting in (5.28) and using the fact that $\hat{c}(k)$ and $\hat{c}(k)$ + constant give identical Fourier transforms for $x \neq y$ yields then (5.21).

5.3. Upper and lower bounds

To understand the qualitative behaviour of the correlations c_N for finite N we derive upper and lower bounds. They consist in throwing away the interaction in A_N through replacing it by $A_N^0 = \Delta_N^{(1)} + \Delta_N^{(2)}$, i.e. by replacing the two excluding random walks in (5.6) by two independent ones.

We have

$$(A_N f)(x, y) = \sum_{x' \in \Lambda_N, |x'-x|=1, x' \neq y} (f(x', y) - f(x, y)) + \sum_{y' \in \Lambda_N, |y'-y|=1, y' \neq x} (f(x, y') - f(x, y))$$
$$- (\delta_{x_1, -N} + \delta_{x_1, N} + \delta_{y_1, -N} + \delta_{y_1, N}) f(x, y). \tag{5.30}$$

This corresponds to the convention that if $x(0) = y(0)$, then with rate one each one of the two random walks jump to a neighbouring lattice site. Once $x(t) \neq y(t)$, this will persist for all times. The generator of the independent random walks is defined by

$$(A_N^0 f)(x, y) = (\Delta_N^{(1)} + \Delta_N^{(2)}) f(x, y)$$
$$= \sum_{x' \in \Lambda_N, |x'-x|=1} (f(x', y) - f(x, y)) + \sum_{y' \in \Lambda_N, |y'-y|=1} (f(x, y') - f(x, y))$$
$$- (\delta_{x_1, -N} + \delta_{x_1, N} + \delta_{y_1, -N} + \delta_{x_1, N}) f(x, y). \tag{5.31}$$

Then by standard perturbation series

$$\tilde{c}_N(x, y) = [(1/A_N) g_N](x, y)$$
$$= [(1/A_N^0) g_N](x, y) - [(1/A_N^0)(A_N - A_N^0)\tilde{c}_N](x, y). \tag{5.32}$$

By direct computation

$$[(A_N - A_N^0) f](x, y) = \delta_{|x-y|, 1}\{2f(x, y) - f(x, x) - f(y, y)\}. \tag{5.33}$$

Propositions 5.2 and 5.3 imply then the bounds

$$2\delta_{|x-y|,1}c(x,y)\leq[(A_N-A_N^0)\tilde{c}_N](x,y)\leq-\delta_{|x-y|,1}(c(x,x)+c(y,y)), \tag{5.34}$$

where $c(x,y)=\lim_{N\to\infty}\tilde{c}_N(x,y)$ with $\tilde{c}_N$ defined by (5.32). For $x\neq y$ $c(x,y)$ is given by (5.21). For coinciding arguments we use definition (5.32) to obtain

$$c(x,x)=\frac{1}{4d}\sum_{j=1}^{d}\{c(x+e_j,x)+c(x-e_j,x)+c(x,x+e_j)+c(x,x-e_j)\}. \tag{5.35}$$

In fact, there are cancellations between the positive and negative terms in (5.33) which could be used to obtain sharper bounds. Inserting (5.34) in (5.33) results in

$$[(1/A_N^0)(g_N-g_-)](x,y)\leq\tilde{c}_N(x,y)\leq[(1/A_N^0)(g_N-g_+)](x,y) \tag{5.36}$$

with $g_-(x,y)=2\delta_{|x-y|,1}c(x,y)$ and $g_+(x,y)=-2\delta_{|x-y|,1}c(x,x)$. The bounds (5.36) differ only in amplitude.

To analyse (5.36) further one can use the eigenfunction expansion of Δ_N with Dirichlet boundary conditions. We refrain from doing so, since (5.36) establishes already the desired qualitative properties. At small distances, $|x_1|$, $|y_1|$, $|x-y|<N$, $\tilde{c}_N(x,y)$ behaves as $\Delta^{-1}(x,y)$, i.e. as the Coulomb potential on the lattice, and at large distances, $|x-y|>N$, (5.36) implies the bound

$$|\tilde{c}_N(x,y)|\leq\text{constant}\exp(-|x-y|/2N). \tag{5.37}$$

5.4. *Time-dependent correlations*

To obtain the correlations in time one only has to compute

$$(\mathrm{d}/\mathrm{d}t)\langle\eta_{x,t}\eta_{y,0}\rangle_N=\langle(L\eta_x)_t\eta_y\rangle_N \tag{5.38}$$

in the steady state. Since $L\eta_x=\Delta_N\eta_x$ one finds that in the steady state

$$\langle\eta_{x,t}\eta_{y,0}\rangle_N-\langle\eta_x\rangle_N\langle\eta_y\rangle_N=(\mathrm{e}^{\Delta_N t}c_N)(x,y). \tag{5.39}$$

In particular the structure factor has the usual diffusive behaviour, up to boundary conditions. The interesting effects are contained in the static correlations $c_N(x,y)$.

5.5. *Hydrodynamic limit*

We follow the pattern of § 4. From the explicit solution

$$\lim_{\varepsilon\to0}\langle\eta_{[\varepsilon^{-1}q]}\rangle_{N(\varepsilon)}=\rho_s(q)$$

$$=(1/2L)[\rho_+(L+q_1)+\rho_-(L-q_1)] \tag{5.40}$$

for every point q inside the slab $\Lambda_L=\{q||q_1|<L\}$.

The correlations (5.9) at coinciding points yield in the limit $\varepsilon\to0$ the local equilibrium contribution $\delta(q-q')\rho_s(q)(1-\rho_s(q))$. At non-coinciding points we have:

Proposition 5.5. For $q\neq q'\in\Lambda_L^0$

$$\lim\varepsilon^{-d}c_{[\varepsilon^{-1}L]}([\varepsilon^{-1}q],[\varepsilon^{-1}q'])=[(\rho_+-\rho_-)/2L]^2\Delta^{-1}(q,q') \tag{5.41}$$

where $\Delta^{-1}(q,q')$ is the kernel of the inverse Laplacian with zero boundary conditions.

Proof. We use the perturbation expansion (5.32). Since for $q \neq q'$ $\lim_{\varepsilon \to 0} \varepsilon^{2-d} \Delta^{-1}_{[\varepsilon^{-1}L]}([\varepsilon^{-1}q], [\varepsilon^{-1}q']) = \Delta^{-1}(q, q')$ as can be seen from the eigenfunction expansion for Δ_N, we have

$$\lim_{\varepsilon \to 0} \frac{\varepsilon^{-d}}{(2[\varepsilon^{-1}L]+2)^2}\left(\frac{1}{A^0_{[\varepsilon^{-1}L]}} g_{[\varepsilon^{-1}L]}\right)([\varepsilon^{-1}q], [\varepsilon^{-1}q']) = \frac{1}{(2L)^2}\Delta^{-1}(q, q'). \tag{5.42}$$

For the second term we use Lebesgue dominated convergence to obtain

$$\lim_{\varepsilon \to 0} \frac{\varepsilon^{-d}}{(2[\varepsilon^{-1}L]+2)^2}\left(\frac{1}{A^0_{[\varepsilon^{-1}L]}} (A_{[\varepsilon^{-1}L]} - A^0_{[\varepsilon^{-1}L]})\tilde{c}_{[\varepsilon^{-1}L]}\right)([\varepsilon^{-1}q], [\varepsilon^{-1}q'])$$
$$= \frac{1}{(2L)^2}\Delta^{-1}(q, q')$$
$$\times\left\{\lim_{N \to \infty} \sum_{j=1}^{d} [\tilde{c}_N(x+e_j, x) + \tilde{c}_N(x, x+e_j) - \tilde{c}_N(x, x) - \tilde{c}_N(x+e_j, x+e_j)]\right\}. \tag{5.43}$$

According to (5.35) the term in the curly brackets vanishes as $N \to \infty$.

In the hydrodynamic limit the static correlations are then given by

$$C_s(q, q') = \delta(q-q')\rho_s(q)(1-\rho_s(q)) + [(\rho_+ - \rho_-)/2L]^2\Delta^{-1}(q, q'). \tag{5.44}$$

The time correlations are in the hydrodynamic limit

$$\lim_{\varepsilon \to 0} \varepsilon^{-d}\{\langle \eta_{[\varepsilon^{-1}q], \varepsilon^{-2}t}\eta_{[\varepsilon^{-2}q'], 0}\rangle_{[\varepsilon^{-1}L]} - \langle \eta_{[\varepsilon^{-1}q]}\rangle_{[\varepsilon^{-1}L]}\langle \eta_{[\varepsilon^{-1}q]}\rangle_{[\varepsilon^{-1}L]}\} = (e^{\Delta t}C_s)(q, q'). \tag{5.45}$$

This follows from (5.39) together with the fact that a simple random walk converges in our scaling to Brownian motion.

We conclude that in the hydrodynamic limit the covariance of the fluctuation field coincides with the one obtained from fluctuating hydrodynamics. The latter theory also asserts that the fluctuations are Gaussian. For the simple exclusion model this can also be proved in the sense that the fluctuation field (defined in (4.8)) tends to the Gaussian field with covariance (5.45) as $\varepsilon \to 0$. The mathematical techniques used in this proof are substantially more sophisticated compared to what we employed so far. Therefore we refrain from entering into details. The interested reader is referred to Galves *et al* (1983) where the Gaussian character of the time-dependent density fluctuations in a non-stationary situation is proved. The same technique can be made to work in the present case.

6. Conclusions

There is very little known about non-equilibrium steady states defined microscopically. Even if we leave the 'safe' ground of conservative (Hamiltonian) systems and, in order to simplify the problem, allow a stochastic dynamics, retaining however the original property of dealing with many interacting particles, our knowledge is very modest. The (to my knowledge) only detailed example is the steady state of the laser in a mean field type description, cf Graham (1978) for a very clear review. The aim of the present paper is to add and to investigate another non-trivial example of a non-equilibrium steady state of a stochastic many particle system. The long range static correlations found here can be predicted already on the basis of fluctuating hydrodynamics, but it is still gratifying to see them turn up in a microscopic model. These long range correlations are caused dynamically. In essence, they originate from (i) the local conservation of mass and (ii) some interaction between particles.

It seems of interest to us to investigate our problem on the level of fluctuating hydrodynamics at a temperature below the critical temperature with one boundary density in the gas phase and the other in the fluid phase. There should be a link to the hydrodynamic theory of equilibrium interface fluctuations.

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