

EQUILIBRIUM FLUCTUATIONS OF STOCHASTIC PARTICLE SYSTEMS: THE ROLE OF CONSERVED QUANTITIES¹

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In the particular model of a zero range jump process in equilibrium, the asymptotic covariances of the—spatially and temporally rescaled—particle number field are computed. The main tool in that computation is a general theorem, whose validity is established for the given class of processes, which states that the asymptotic behaviour of the covariances of any field corresponding to a local function is determined by a suitable projection of that field on the linear (here one-dimensional) space spanned by the fields of conserved quantities (here: the particle number).

1. Introduction. One of the goals in studying stochastic particle systems is to derive rigorously typical features of hydrodynamic behaviour, in particular to establish macroscopic laws for those systems. Before, however, entering into the difficulties of nonequilibrium theory, one may first try to understand how small deviations from equilibrium, which occur at random (“fluctuations”), spread out in space and time. It has been believed by physicists for a long time (see e.g. [1]), that nonequilibrium transport properties can be recognized already from the characteristics of the fluctuation process at different equilibria.

In this paper we will analyze a special particle jump process on \mathbb{Z}^d i.e. a process without creation or annihilation of particles. We consider it in equilibrium at a given density ρ ; it will be stationary in time, even reversible, and invariant under spatial shifts. One expects that an additional mass (particles) added at the origin at time 0 spreads out on a large scale like Brownian motion; the problem is to prove this fact and to identify the diffusion constant, usually called bulk diffusion coefficient ([2]). In more precise terms: if we denote by $X(j, t)$ the number of particles present at site j at time t , we want to study the behaviour of the time delayed covariances

$$(1.1) \quad A(j, t) = \mathcal{L}(X(j, t) - \rho)(X(0, 0) - \rho),$$

as t tends to infinity, $j \cdot t^{-1/2}$ to a fixed limit. The correct formulation in Fourier analytic terms is the following: we prove that

$$(1.2) \quad \lim_{t \rightarrow \infty} \sum_j A(j, t) \exp(ij \cdot \vartheta \cdot t^{-(1/2)}) = \chi \cdot \exp(-(\frac{1}{2})\kappa\vartheta^2)$$

for all $\vartheta \in R^d$, with some constants χ and κ . We will say that (1.2) expresses diffusive behaviour of additional mass and will call κ the corresponding bulk

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diffusion coefficient, which, of course, depends on ρ , the chosen equilibrium state. (The symmetry inherent to our specific model gives an isotropic diffusive behaviour; otherwise one could also imagine an arbitrary positive quadratic form in ϑ at the r.h.s. of (1.2).)

In the special case of the so-called symmetric simple exclusion process ([3]), due to the algebraic structure of the system and the method of duality one knows the covariances explicitly:

$$(1.3) \quad A(j, t) = \rho(1 - \rho)p(t; j),$$

with $p(t; \cdot)$ being the transition probability of a symmetric random walk on \mathbb{Z}^d . So, there, diffusive behaviour follows from the classical central limit theorem. In the present paper, we will instead consider a different type of evolution, which might be qualified as the simplest interacting particle model which is not explicitly solvable: the zero range symmetric jump process ([4]; for precise definitions see Section 2 below).

To arrive at (1.2) a certain calculus of what we call local functions and formal Hamiltonians has been proven useful. We present it in detail in Section 3 and the Appendix. The main result there is Theorem 1 which underlines the role of the conserved quantity (here particle number) in equilibrium processes. Its content may be stated as follows: consider a local function f , i.e. a cylindrical function on the state space, of expectation zero; denote by $S_k f$ the function f shifted by a vector $k \in \mathbb{Z}^d$. Then there exists an $\alpha \in \mathbb{R}$ such that for each local g one has

$$(1.4) \quad \lim_{t \rightarrow \infty} \sum_k \mathcal{E} g(X(0)) \cdot S_k f(X(t)) = \alpha \sum_k \mathcal{E} g(X(0)) \cdot (X(k, 0) - \rho).$$

In that sense the time evolution semigroup acts on f asymptotically like a projection onto the one-dimensional space spanned by $f_0(x) = x_0 - \rho$, the “conserved quantity”. We remark that scalar products of the form (1.4) occur also in the renormalization of certain spin-flip processes ([11]).

In Section 4 one applies Theorem 1 to compute the asymptotics of $A(j, t)$ and to establish (1.2). The method is Fourier analytical: scalar products

$$(1.5) \quad \sum_j \mathcal{E} g(X(0)) \cdot S_k f(X(t)) \cdot \exp(i\vartheta \cdot k)$$

and analyzed for t large and ϑ small.

In Section 5 one translates the Fourier analytic statements into the language of fluctuation fields: these are \mathcal{S}' -valued processes $N^\epsilon(f)$, associated to a centered local function f and a scale parameter $\epsilon > 0$,

$$(1.6) \quad N^\epsilon(f; \varphi, s) := \epsilon^{d/2} \sum_j s_j f(X(s\epsilon^{-2})) \cdot \varphi(\epsilon j), \quad \varphi \in \mathcal{S}, \quad s \geq 0.$$

The theory developed in Section 3 not only allows then to compute time delayed covariances of $N^\epsilon(f_0)$, for $f_0(x) = x_0 - \rho$, in the limit $\epsilon \rightarrow 0$, but also to show that the time averages

$$(1.7) \quad S^{-1} \cdot \int_0^S N^\epsilon(f - \alpha f_0; \varphi, s) ds$$

converge in L^2 -norm to zero for α chosen as in (1.4), as soon as the observation time length S is large compared to the “microscopic time unit” ϵ^2 (Theorem 3).

This last result is in close analogy to a classical principle in hydrodynamics: if f is local, not necessarily centered, one believes that even in a nonequilibrium process, at any fixed time t the r.v.

$$(1.8) \quad \varepsilon^d \cdot \sum_j S_j f(X(t)) \cdot \varphi(\varepsilon j)$$

is close to the deterministic quantity

$$(1.9) \quad \int \langle f \rangle_{\rho(r,t)} \cdot \varphi(r) \cdot dr,$$

where $\rho(r, t)$ is the particle density at the macroscopic position r and $\langle f \rangle_{\rho}$ the mean of f under the equilibrium state with density ρ . That means that (1.8) is in principle known, if one knows the function $\rho(\cdot, t)$. In our approximation we use a finer scale to measure the deviation from (1.8) to (1.9), at least in the equilibrium situation of constant ρ . Theorem 3 then says that the fluctuations corresponding to f can be expressed in a linear way by the fluctuations corresponding to the conserved quantity f_0 . It is easily verified, in our class of models, that the coefficient α in (1.4) and (1.7), which relates $N^\varepsilon(f)$ to $N^\varepsilon(f_0)$ for ε small, satisfies the identity

$$(1.10) \quad \alpha = (d/d\rho)\langle f \rangle_{\rho}.$$

It should be noted, however, that the linear approximation of $N^\varepsilon(f)$ by $N^\varepsilon(f_0)$ is not valid at a fixed instant t , but only in the sense of (1.7). (For more details see [5].)

2. Preliminaries and notations. The example to be analyzed in this paper is the so-called zero range symmetric jump process. We mention some facts about it which will be needed later (see [4], [6]).

The process $X = X(t), t \geq 0$, has as its state space a suitable subset \mathfrak{X} of $N^{\mathbb{Z}^d}$; we denote an element of \mathfrak{X} by x , its coordinates by $x_j, j \in \mathbb{Z}^d$, and the coordinates of the process at time t by $X(j, t)$. On \mathfrak{X} we have the group of shifts, which in a natural way also acts on functions f defined on \mathfrak{X} ; if e.g. $f = F(x_{j_1}, \dots, x_{j_n})$ the function f shifted by k is $S_k f$:

$$(2.1) \quad S_k f(x) = F(x_{j_1+k}, \dots, x_{j_n+k}).$$

The following mappings of \mathfrak{X} into itself will be considered

$$(2.2) \quad x \rightarrow x^j \quad \text{where} \quad (x^j)_k = x_k + \delta_{jk},$$

$$(2.3) \quad x \rightarrow x^{jk} \quad \text{where} \quad (x^{jk})_{\ell} = x_{\ell} + \delta_{k\ell} - \delta_{j\ell}.$$

(The latter is only defined on $\{x_j > 0\}$.)

The process X is determined by its generator L :

$$(2.4) \quad Lf(x) = \sum_{j \in \mathbb{Z}^d} c(x_j) \sum_{|k-j|=1} (f(x^{jk}) - f(x));$$

here $c(\cdot)$ is a function on N which satisfies the following conditions:

- (i) $c(0) = 0 < c(1)$,
- (2.5) (ii) $c(k + 1) - c(k) \geq 0$ for all k ,
- (iii) $\sup_k [c(k + 1) - c(k)] =: c^* < \infty$.

Intuitively, (2.4) means that a particle jumps from j to a neighbouring site k with an intensity depending on how many other particles are on site j at that time. The semigroup of transition operators is denoted by (T_t) , $t \geq 0$; it has the Feller property. The order structure on \mathfrak{X} (coordinatewise) and the corresponding notion of monotonicity of functions and stochastic order of measures play an important role: as a consequence of (2.5 (ii)) we have preservation of stochastic order by T_t . To fix ideas we will prove something only in the special case below, which allows us to present the method of coupling in a simple way.

PROPOSITION 2.1. *Let f monotonic be given; then*

$$(2.6) \quad T_t f(x) \leq T_t f(x') \quad \text{for } x \in \mathfrak{X}, \ell \in \mathbb{Z}^d.$$

PROOF. Let X be the process with initial state x ; define a process W , which conditioned on X is in a random walk on \mathbb{Z}^d with the following generator \tilde{L}

$$(2.7) \quad \tilde{L}h(j) = (c(X(j, t) + 1) - c(X(j, t))) \cdot \sum_{|k-j|=1} (h(k) - h(j)),$$

and which starts at ℓ . Define the process Y by

$$(2.8) \quad Y(j, t) = X(j, t) + \delta(j, W(t));$$

then it is easy to see that Y is Markovian with semigroup (T_t) , too. Since $Y \geq X$ by construction, the assertion follows. \square

It is known ([6]) that the measures μ_u , $u < u^*$, described below, are extremal invariant under (T_t) : μ_u is a product measure and

$$(2.9) \quad \mu_u(x_j = n) = Z(u)^{-1} \cdot u^n \cdot \prod_{1 \leq m \leq n} c(m)^{-1}.$$

Here $Z(u)$ is a normalizing constant and u^* the radius of convergence of the power series at the r.h.s. of (2.9).

We fix a value of u ; unless stated otherwise the process X will in the sequel always be stationary with initial measure $\mu = \mu_u$. We denote its density by ρ :

$$(2.10) \quad \rho = \mathcal{L} X(i, t).$$

We remark that X is also invariant in law under the shifts S_j and that X is reversible, i.e.

$$(2.11) \quad \int f T_t g \, d\mu = \int g T_t f \, d\mu \quad \text{for all } f, g \in L^2(\mu).$$

Reversibility is an important structure, since it allows us to use spectral argu-

ments. So, for example, one gets immediately that the process X is also mixing: the spectral theorem applied to the generator L of (T_t) in $L^2(\mu)$ gives the representation

$$(2.12) \quad \int f \cdot T_t f \, d\mu = \int_0^\infty e^{-\lambda t} \sigma_f(d\lambda), \quad t \geq 0,$$

with

$$\sigma_f(d\lambda) = \langle f, \Pi(d\lambda)f \rangle,$$

where $\Pi(d\lambda)$ is the spectral measure of $-L$ and $\langle \cdot, \cdot \rangle$ denotes the scalar product in $L^2(\mu)$. From (2.12) it follows that Cesàro convergence of the l.h.s. to zero, as $t \rightarrow \infty$, is equivalent to ordinary convergence; but the former holds, since X is ergodic, for every f with $\int f \, d\mu = 0$. So we arrive at

$$(2.13) \quad \lim_{t \rightarrow \infty} \int f \cdot T_t g \, d\mu = 0, \quad \text{whenever} \quad \int f \, d\mu = \int g \, d\mu = 0,$$

which means that X is mixing.

3. The Euclidean structure of local quantities and its time evolution.

General ideas. Consider functions f , centered, depending only on finitely many coordinates and—for the moment—square integrable. To each such f we associate the stationary (in space) process

$$(3.1) \quad S_j f, \quad j \in \mathbb{Z}^d,$$

and the “formal Hamiltonian”

$$(3.2) \quad \sum_j S_j f.$$

What we intend to develop is kind of a calculus of those Hamiltonians, better: of their linear structure; in particular we want to investigate how the semigroup (T_t) acts on the process (3.1), resp. its Hamiltonian (3.2).

The space of functions f of the above type is given a Euclidean structure by means of the (degenerate) scalar product

$$(3.3) \quad E_0(f, g) = \sum_j \int f \cdot S_j g \, d\mu$$

which is well defined, since the sum converges absolutely. The first step is to construct a domain for E_0 as well as for E_t , which is formally defined by

$$(3.4) \quad E_t(f, g) = \sum_j \int f \cdot S_j T_t g \, d\mu.$$

At the same time, one tries to make visible the formal Hamiltonian itself; at least something like its conditional expectations on local σ -fields are shown to be meaningful (Proposition 3.2). (In the Appendix, when we prove Theorem 1,

this aspect will become more important.) The rest of this paragraph deals with the “conserved quantity” $f_0 = x_0 - \rho$, whose Hamiltonian is

$$(3.5) \quad \sum_j S_j f_0 = \sum_j (x_j - \rho),$$

the total number of particles, and its invariance under T_t . Finally we state the main theorem, which says that in the metric of E_0 the time evolution T_t acts like a projection onto the space spanned by f_0 .

Notations.

\mathcal{F}_Γ : the σ -field generated by $x_j, j \in \Gamma$;

$L^2(\Gamma)$: the set of μ -square integrable and \mathcal{F}_Γ -measurable functions;

$\mathcal{D}^+(\Gamma)$: the set of centered \mathcal{F}_Γ -measurable functions, which are increasing and for which

$$(3.6) \quad \sum_j \sup_x (f(x^j) - f(x)) < \infty;$$

$$\mathcal{D}^+ := \bigcup_{\Gamma \text{ finite}} \mathcal{D}^+(\Gamma),$$

$$\mathcal{D} := \mathcal{D}^+ - \mathcal{D}^+, \text{ similarly } \mathcal{D}(\Gamma).$$

DEFINITION 3.1. The elements of \mathcal{D} will be called *local quantities* (functions).

PROPOSITION 3.1. Let $f \in \mathcal{D}^+$ be given; put $a(j) = \sup_x (f(x^j) - f(x))$, $a = \sum a(j)$. Then

$$(3.7) \quad \sum_j \int f S_j f \, d\mu \leq \chi \cdot a^2$$

where $\chi = \int (x_0 - \rho)^2 \, d\mu$.

PROOF. The increasing functions are positively correlated since μ is a product measure (elementary; special case of FKG-inequality [12]). So all terms in the sum (3.7) are positive.

But also $g(x) := \sum_k a(k)(x_k - \rho)$, as well as $g - f$ and $S_j(g - f)$ are increasing functions. Applying twice FKG we obtain

$$\int f S_j f \, d\mu \leq \int g S_j g \, d\mu = \chi \cdot \sum_k a(k)a(j - k).$$

Summation over j yields (3.7). \square

COROLLARY. For $f, g \in \mathcal{D}$ the symmetric bilinear form

$$(3.8) \quad E_0(f, g) = \sum_j \int f \cdot S_j g \, d\mu$$

is well defined; the r.h.s. converges absolutely.

PROPOSITION 3.2. Same assumptions as Proposition 3.1. Fix $t \geq 0$ and a finite

Γ . Then there exists a function F with the properties

- (i) F is \mathcal{F}_Γ -measurable;
- (ii) $0 \leq F(x^k) - F(x) \leq a$;
- (3.9) (iii) for each increasing $g \in L^2(\Gamma)$; $\int gF \, d\mu = \sum_j \int gS_jT_if \, d\mu$;
- (iv) $\int F \, d\mu = 0$.

PROOF. We choose $|\Lambda| < \infty$ and set $h_\Lambda := \sum_{j \in \Lambda} S_j f$. For each x and k one gets

$$(3.10) \quad 0 \leq h_\Lambda(x^k) - h_\Lambda(x) \leq \sum_{j \in \Lambda} a(k - j) \leq a.$$

As in Proposition 2.1, we conclude that (3.10) remains valid with $T_t h_\Lambda$ instead of h_Λ . Further, also

$$\tilde{h}_\Lambda := \mathcal{L}(T_t h_\Lambda | \mathcal{F}_\Gamma)$$

satisfies the same estimates. The FKG-argument then yields

$$(3.11) \quad \int \tilde{h}_\Lambda^2 \cdot d\mu \leq a^2 \int (\sum_{k \in \Gamma} (x_k - \rho))^2 d\mu = a^2 \cdot \chi | \Gamma |.$$

By Schwarz' inequality for each $g \in L^2(\Gamma)$ we get thus

$$(3.12) \quad \sum_{j \in \Lambda} \int g \cdot S_j T_i f \, d\mu = \int g \tilde{h}_\Lambda \, d\mu \leq \|g\| \cdot \text{const.}$$

The sum on the l.h.s. consists of positive terms if we require in addition g to be increasing; for all such g we have thus

$$(3.13) \quad \sum_j \int g S_j T_i f \, d\mu < \infty.$$

On the other hand, the value (3.13) can be written as

$$\int g \cdot F \cdot d\mu,$$

where F is the weak limit in $L^2(\Gamma)$ of \tilde{h}_Λ , as $\Lambda \rightarrow \mathbb{Z}^d$. This proves (i), (iii); the statement (ii) follows from (3.10) by integrating

$$0 \leq \tilde{h}_\Lambda(x^k) - \tilde{h}_\Lambda(x) \leq a$$

over the cylinder sets $\{y: y_j = x_j, j \in \Gamma\}$ and taking the limit in Λ ; (iv) is an immediate consequence of (iii). \square

COROLLARY. *The symmetric bilinear form*

$$(3.14) \quad E_t(g, f) := \sum_j \int g \cdot S_j T_t f \, d\mu$$

is well defined for $f, g \in \mathcal{D}$, since the r.h.s. is absolutely convergent.

PROPOSITION 3.3. *The function $t \rightarrow E_t(f, f)$ is for each $f \in \mathcal{D}$ positive and decreasing. The limit*

$$(3.15) \quad E(g, f) := \lim_{t \rightarrow \infty} E_t(g, f)$$

exists for each $f, g \in \mathcal{D}$.

PROOF. Because of the absolute convergence of the series (3.14) its value can also be identified as

$$(3.16) \quad \lim_{\Lambda} E_t^\Lambda(g, f),$$

where $E_t^\Lambda(g, f) = |\Lambda|^{-1} \cdot \int (\sum_{\Lambda} S_j g) T_t (\sum_{\Lambda} S_j f) \, d\mu$ and Λ runs through an increasing sequence of cubes. Using spectral arguments, since X is reversible, we write

$$(3.17) \quad E_t^\Lambda(f, f) = \int_0^\infty e^{-\lambda t} \sigma_\Lambda(d\lambda)$$

with σ_Λ a positive measure. Hence $E_t^\Lambda(f, f)$ is positive and decreasing, even alternating of any order, which properties are preserved in the limit $\Lambda \rightarrow \mathbb{Z}^d$. The rest is obvious. \square

REMARK. The bilinear form E on \mathcal{D} , which is well defined by Proposition 3.3, can for each finite Γ be extended to $L^2(\Gamma)$, since for each $f \in \mathcal{D}(\Gamma)$

$$(3.18) \quad E(f, f) \leq E_0(f, f) \leq c(\Gamma) \cdot \|f\|^2.$$

PROPOSITION 3.4. *Define $f_0(x) = x_0 - \rho$. Then*

$$(3.19) \quad E_t(g, f_0) = E_0(g, f_0) \quad \text{for all } t \geq 0, \quad g \in \mathcal{D}.$$

PROOF. By means of the interpretation (3.16) we get

$$(3.20) \quad (E_t - E_0)(g, f_0) = \lim_{\Lambda} |\Lambda|^{-1} \cdot \int_0^t \left[\int G^\Lambda \cdot T_s L F_0^\Lambda \, d\mu \right] ds$$

with $F_0^\Lambda = \sum_{j \in \Lambda} S_j f_0$, G^Λ similarly. Since

$$(3.21) \quad L F_0^\Lambda = \sum_{|j-k|=1} 1_{\{j \in \Lambda, k \notin \Lambda\}} (c(x_k) - c(x_j))$$

we have $\|L F_0^\Lambda\| = O(n^{(d-1)/2})$ for the L^2 -norm of $L F_0^\Lambda$, if Λ is a cube of length $2n$. Since $\|G^\Lambda\| = O(n^{d/2})$ and T_s is a contraction, the expression under the limit is of order $O(n^{-1/2})$ for each fixed t , by Schwarz' inequality. Hence the l.h.s. in (3.20) is zero.

DEFINITION 3.2. The multiples of f_0 are called *conserved quantities*.

The reason for this name is that, in the sense of the E_0 -metric, $T_t f_0$ is equal to f_0 , by Proposition 3.4; if one likes, one might define also scalar products $E_0(T_t f, T_t g)$, since the series in (3.14) converges absolutely and, by reversibility,

$$\int T_t g \cdot T_t h \, d\mu = \int g \cdot T_{2t} h \, d\mu.$$

THEOREM 1. If $f \in \mathcal{D}$ and if one sets

$$(3.22) \quad \alpha = E_0(f, f_0) \cdot \chi^{-1},$$

then

$$(3.23) \quad E(g, f) = \alpha \cdot E_0(g, f_0) \quad \text{for all } g \in \mathcal{D}.$$

(Equivalent formulations are:

$$\lim_t E_t(f - \alpha f_0, f - \alpha f_0) = 0, \quad \text{or}$$

$$\lim_t E_t(g, f - \alpha f_0) = 0 \quad \text{for all } g \in \mathcal{D}.)$$

The statement made in this theorem, that T_t acts like a projection onto the multiples of f_0 as $t \rightarrow \infty$, implies in particular that there are no nontrivial other conserved quantities, i.e. functions f_1 satisfying

$$(3.24) \quad E_t(g, f_1) = E_0(g, f_1) \quad \text{for all } g \in \mathcal{D}, \quad t \geq 0,$$

besides f_0 . Proposition 3.4 and Theorem 1 can also be viewed as “linearizations” for small β of the fact that the measure ρ_β , formally written as

$$(3.25) \quad c \cdot \mu_u \cdot \exp(\beta \sum_j (x_j - \rho)),$$

(which is of the form μ_v for some v) is invariant under T_t , and of the conjecture—not yet proven to our knowledge—that for reasonable f the measures $c \cdot \mu_u \cdot \exp(\beta \sum_j S_j f) T_t$ converge weakly as $t \rightarrow \infty$ to some ρ_β . The proof of Theorem 1 is postponed to the Appendix.

4. The Fourier picture. This paragraph is devoted to an asymptotic calculation of the family of time delayed covariances

$$(4.1) \quad A(j, t) = \mathcal{L}(X(0, 0) - \rho)(X(j, t) - \rho).$$

The method of Fourier transformation allows us to formulate the result precisely and provides a very useful technique to prove it. First, we have to extend the scalar products E_t by adding an additional argument.

DEFINITION 4.1. For $f, g \in \mathcal{L}$, $t \geq 0$ and $\vartheta \in R^d$, we put

$$(4.2) \quad E(t, \vartheta; f, g) = \sum_j \int f \cdot e^{i\vartheta j} T_t S_j g \, d\mu.$$

($j\vartheta$ is understood as scalar product in R^d .)

PROPOSITION 4.1. *The expression $E(t, \vartheta; f, f)$ is continuous in ϑ for fixed t and decreasing in t for fixed ϑ . It is positive and bounded uniformly in t and ϑ .*

PROOF. We represent once more $E(t, \vartheta; f, f)$ as $\lim_{\Lambda} \int HT_t \bar{H} d\mu$ with $H = |\Lambda|^{-1/2} \cdot \sum_{j \in \Lambda} e^{ij\vartheta} S_j f$. Everything follows from there; the boundedness is a consequence of the absolute convergence of the series in (4.2), resp. (3.14). \square

The representation used in the proof shows that $E(t, \cdot; f, f)$, if understood as function on the d -dimensional torus, is nothing but the spectral density of the stationary (in space) process $S_j(T_{t/2} f), j \in \mathbb{Z}^d$.

PROPOSITION 4.2. *Let $f \in \mathcal{D}$ be given, suppose $E_0(f, f_0) = 0$. Then we have*

$$(4.3) \quad \lim_{t \rightarrow \infty, \vartheta \rightarrow 0} E(t, \vartheta; f, f) = 0 \quad \text{and}$$

$$(4.4) \quad \lim_{t \rightarrow \infty, \vartheta \rightarrow 0} E(t, \vartheta; f, g) = 0 \quad \text{for all } g \in \mathcal{D},$$

where the limit may be taken in any order.

PROOF. By Theorem 1, we know that $\lim_t E(t, 0; f, f) = 0$. Given $\varepsilon > 0$, by Proposition 4.1 we can find a t_0 and $\eta > 0$ such that for all $t \geq t_0$ and $|\vartheta| \leq \eta$ we have

$$(4.5) \quad 0 \leq E(t, \vartheta; f, f) \leq E(t_0, \vartheta; f, f) \leq E(t_0, 0; f, f) + \varepsilon \leq 2\varepsilon.$$

This proves (4.3); assertion (4.4) follows from Schwarz' inequality, since $E(t, \vartheta; \cdot, \cdot)$ is a nonnegative bilinear form. \square

We proceed now to the computation of the covariance

$$(4.6) \quad A(j, t) := \mathcal{L}(X(0, 0) - \rho)(X(j, t) - \rho).$$

For that purpose we introduce another covariance:

$$(4.7) \quad B(j, t) := \mathcal{L}(X(0, 0) - \rho)c(X(j, t)) = \mathcal{L}(X(0, 0) - \rho)(c(X(j, t)) - u).$$

(Take into account that $\int c(x_0) d\mu = Z(u)^{-1} \cdot \sum_n u^n \cdot \prod_{1 \leq m \leq n} c(m)^{-1} \cdot c(n) = u$.)

$$\text{PROPOSITION 4.3.} \quad (d/dt)A(j, t) = \sum_{|k-j|=1} (B(k, t) - B(j, t)).$$

PROOF. Obvious. One just counts the expected net flow between j and its neighbours in the time interval $(t, t + dt)$, given some condition on $X(0, 0)$. \square

If we take the Fourier transforms of A and B ,

$$(4.8) \quad \hat{A}(\vartheta, t) := \sum_j A(j, t)e^{ij\vartheta},$$

\hat{B} analogously, Proposition 4.3 reads as

$$(4.9) \quad (d/dt)\hat{A}(\vartheta, t) = \hat{B}(\vartheta, t) \cdot 2 \cdot \sum_{m=1}^d (\cos \vartheta_m - 1).$$

If in addition we rescale space and time, defining

$$(4.10) \quad \hat{a}_\varepsilon(\vartheta, s) := \hat{A}(\varepsilon\vartheta, s\varepsilon^{-2}),$$

similarly \hat{b}_ε , the evolution equation is

$$(4.11) \quad (d/dt)\hat{a}_\varepsilon(\vartheta, s) = \hat{b}_\varepsilon(\vartheta, s) \cdot 2\varepsilon^{-2} \cdot \sum_m (\cos(\varepsilon\vartheta_m) - 1).$$

THEOREM 2. *For fixed ϑ and s one has*

$$(4.12) \quad \lim_{\varepsilon \rightarrow 0} \hat{a}_\varepsilon(\vartheta, s) = \chi \cdot \exp(-1/2 \cdot \kappa \cdot s \cdot \vartheta^2)$$

where $\kappa = 2u \cdot \chi^{-1}$.

An equivalent formulation is the one given in the introduction:

$$(4.13) \quad \lim_{t \rightarrow \infty} \sum_j A(j, t) \exp(ij \cdot \vartheta t^{-1/2}) = \chi \cdot \exp(-u\chi^{-1} \cdot \vartheta^2).$$

(ϑ^2 stands for $\sum_1^d \vartheta_m^2$.)

PROOF. The idea of proving (4.12) is to apply Theorem 1 and to replace in the limit $\varepsilon \rightarrow 0$ the right hand side of (4.11) by

$$\alpha \cdot \hat{a}_\varepsilon(\vartheta, s) \cdot \vartheta^2;$$

the thus modified equation (4.11) is easily solved and has the right type of solution.

a) The coefficient α suggested by Theorem 1 is

$$\left(\int c(x_0)(x_0 - \rho) d\mu \right) \cdot \left(\int (x_0 - \rho)^2 d\mu \right)^{-1}.$$

The denominator has been called χ , the numerator is computed as

$$\begin{aligned} Z^{-1} \cdot \sum_{n \geq 0} u^n \cdot \prod_{m \leq n} c(m)^{-1} \cdot c(n)(n - \rho) \\ = Z^{-1} \cdot \sum_{n \geq 0} u^n \cdot \prod_{m \leq n} c(m)^{-1} \cdot u \cdot (n + 1 - \rho) = u. \end{aligned}$$

We set therefore

$$(4.14) \quad \alpha := u \cdot \chi^{-1}.$$

We can thus write

$$(4.15) \quad \hat{b}_\varepsilon(\vartheta, s) = \alpha \hat{a}_\varepsilon(\vartheta, s) + r(\varepsilon, \vartheta, s)$$

where r is of the form

$$E(s\varepsilon^{-2}, \varepsilon\vartheta; f_0, g) \quad \text{with } g \text{ satisfying } \lim_t E(t, 0; f_0, g) = 0.$$

From Proposition 4.2 we conclude that

$$(4.16) \quad \lim_\varepsilon r(\varepsilon, \vartheta, s) = 0 \quad \text{for } \vartheta \text{ fixed,}$$

even uniformly in $s \geq s_0 > 0$.

b) We fix $\vartheta \in R^d$ and write (4.11) in integral form

$$(4.17) \quad \hat{a}_\epsilon(\vartheta, s) = \hat{a}_\epsilon(\vartheta, 0) + \int_0^s \hat{b}_\epsilon(\vartheta, s') \cdot \sum_m 2\epsilon^{-2}(\cos(\epsilon\vartheta_m) - 1) ds'.$$

The integrand on the right is bounded (Proposition 4.1), $\hat{a}_\epsilon(\vartheta, 0) = \chi$ for all ϵ . Hence the family $\hat{a}_\epsilon(\vartheta, \cdot)$, $\epsilon > 0$, is precompact in the supremum-metric in the space of continuous functions on $[0, S]$, for any fixed S . Due to a), the boundedness of \hat{b} and the fact that

$$\lim_\epsilon \sum_m 2\epsilon^{-2}(\cos(\epsilon\vartheta_m) - 1) = -\vartheta^2,$$

any limit function \hat{a} must satisfy

$$(4.18) \quad \hat{a}(s) = \chi - \int_0^s \alpha \cdot \hat{a}(s')\vartheta^2 ds'.$$

But (4.18) has a unique solution, namely $\hat{a}(s) = \chi \cdot \exp(-\alpha\vartheta^2s)$, which thus turns out to be the limit of $\hat{a}_\epsilon(\vartheta, s)$. \square

REMARK. The diffusion constant $\kappa = 2u\chi^{-1}$ can be understood also by another, heuristic argument. One easily verifies the identity

$$u \cdot \chi^{-1} = \left(\frac{d\rho}{du}\right)^{-1}.$$

Further, we have seen that

$$u = \int c(x_0) d\mu.$$

So, the statement of Theorem 2

$$(4.19) \quad \kappa = 2 \cdot \frac{du}{d\rho}$$

equates $\kappa/2$ to the rate at which the intensity of jumps over a given bond in one direction changes if the density is increased. It is very natural to believe that this quantity tells us at which average speed *additional particles* will diffuse. That is, in our opinion, the most appealing interpretation of the *bulk diffusion* coefficient. If we ask instead for the *self diffusion* coefficient, the speed at which a *tagged* particle diffuses, which from a pile of height n jumps over a given bond with rate $c(n)/n$, the theorem of Spitzer and Harris ([7], [8]) tells us what the average jump rate of this particle in one direction is: the expectation of $c(x_0)/x_0$ under the Palm measure, which equals

$$\rho^{-1} \cdot \int c(x_0) \cdot x_0^{-1}x_0 d\mu = u \cdot \rho^{-1}.$$

That means that the self diffusion coefficient is $2u\rho^{-1}$ compared to $2 \cdot (du/d\rho)$, the bulk diffusion coefficient.

5. The fluctuation field. We are going to restate Theorem 2 in this paragraph, using a somehow different language without any Fourier terminology. In the new context, however, we are able to state also a new fact (indeed an easy consequence of Theorem 1), the “Boltzmann-Gibbs principle” ([5], [9]) about the behaviour of time averages of fluctuating variables.

DEFINITION 5.1. Let f be a local function; we associate to f and $\varepsilon > 0$ the following \mathcal{S}' -valued process $N^\varepsilon(f)$, whose evaluation at time s and $\varphi \in \mathcal{S}$ is the random variable

$$(5.1) \quad N^\varepsilon(f; s, \varphi) := \varepsilon^{d/2} \sum_j \varphi(\varepsilon j) S_j f(X(s\varepsilon^{-2})).$$

If $f = f_0$ we will write simply $N^\varepsilon(s, \varphi)$. The process $N^\varepsilon(f)$ can be interpreted as the properly rescaled deviation of an extensive quantity from its mean value. Together with X , $N^\varepsilon(f)$ is stationary also.

THEOREM 2a. For $\varphi, \psi \in \mathcal{S}$ and $s \geq 0$ we have

$$(5.2) \quad \lim_{\varepsilon \rightarrow 0} \mathcal{L} N^\varepsilon(0, \varphi) N^\varepsilon(s, \psi) = \chi \cdot \int \int \varphi(v) \psi(w) g_{\kappa s}(w - v) \, dv \, dw,$$

where $g_{\sigma^2}(\cdot)$ is d -dimensional Gaussian density with mean 0 and covariance $\sigma^2 \cdot \mathbb{1}$.

PROOF. The quantity under the limit sign is equal to

$$(5.3) \quad \sum_{j,k} \varepsilon^d \cdot \varphi(\varepsilon j) \psi(\varepsilon(j + k)) \cdot A(k, s\varepsilon^{-2}).$$

Theorem 2 is a weak convergence statement for the discrete measure with weight $A(k, s\varepsilon^{-2})$ at $\varepsilon \cdot k$: it converges to $\chi g_{\kappa \cdot s}(dw)$. The rest is obvious. \square

THEOREM 3. (“Boltzmann-Gibbs principle” for fluctuation processes). Let f be a local function; assume that $E_0(f, f_0) = 0$. Let $S(\varepsilon)$, $\varepsilon > 0$, be a family of positive numbers with

$$(5.4) \quad \lim_{\varepsilon \rightarrow 0} S \cdot \varepsilon^{-2} = \infty.$$

Then for each $\varphi \in \mathcal{S}$ the time average

$$(5.5) \quad S^{-1} \cdot \int_0^S N^\varepsilon(f; s', \varphi) \, ds'$$

converges to zero in quadratic mean.

PROOF. Using “microscopic” time $T = S\varepsilon^{-2}$ we express (5.5) as

$$(5.6) \quad T^{-1} \cdot \int_0^T \varepsilon^{d/2} \cdot \sum_j \varphi(\varepsilon j) S_j f(X(t)) \, dt,$$

whose square integral, by Fubini, is equal to

$$(5.7) \quad T^{-2} \cdot \int \int K_\epsilon(|t_1 - t_2|) dt_1 dt_2,$$

where

$$K_\epsilon(t) = \int H_\epsilon T_t H_\epsilon d\mu \quad \text{and} \quad H_\epsilon = \epsilon^{d/2} \cdot \sum_j \varphi(\epsilon j) S_j f.$$

Sufficient for the theorem to hold is that

$$(5.8) \quad \lim_\epsilon K_\epsilon(t) = 0, \quad \text{whenever} \quad t = t(\epsilon) \rightarrow \infty.$$

Now we argue as in Proposition 4.2 to establish (5.8):

- a) $K_\epsilon(\cdot)$ is positive and decreasing
- b) $\lim_\epsilon K_\epsilon(t) = (\int \varphi^2 dw) \cdot E_t(f, f)$;

the r.h.s. in (b) goes to zero by assumption on f . Therefore

$$(5.9) \quad \lim_{\epsilon \rightarrow 0, t \rightarrow \infty} K_\epsilon(t) = 0$$

as desired, which proves Theorem 3. \square

REMARK. We have made no statement about the Gaussian character of the field N^ϵ in the limit $\epsilon \rightarrow 0$. It is easy, since μ is a product measure, to see that for fixed t the r.v.'s $N^\epsilon(t, \varphi)$, $\varphi \in \mathcal{L}$, get jointly Gaussian in the limit; the limiting field is Gaussian white noise with covariance kernel

$$(5.10) \quad \mathcal{L}N(t, \varphi)^2 = \chi \cdot \int \varphi^2(w) dw, \quad \varphi \in \mathcal{L}.$$

What has not been shown is the *joint* Gaussian character of $N^\epsilon(t_1, \varphi_1) \dots N^\epsilon(t_n, \varphi_n)$ for $t_1, \dots, t_n \in R$, $\varphi_1, \dots, \varphi_n \in \mathcal{L}$ in the limit $\epsilon \rightarrow 0$. But since we know its covariance structure (Theorem 2a), the limiting field, if it is Gaussian, can be identified. It is easy to see that the covariance structure is that of a stationary Ornstein-Uhlenbeck process $N(t, \varphi)$, $\varphi \in \mathcal{L}$, $t \geq 0$, which is characterized by (5.10) together with

for each $\varphi \in \mathcal{L}$, the process

$$(5.11) \quad t \rightarrow N(t, \varphi) - N(0, \varphi) - \int_0^t N\left(s, \frac{\kappa}{2} \cdot \Delta\varphi\right) ds$$

is a Brownian motion with diffusion constant $2u \cdot \int |\nabla\varphi|^2 dw$.

(See [10] for the case of independently moving particles.)

APPENDIX

PROOF OF THEOREM 1. We assume that $f \in \mathcal{D}^+$ and set $a := \sum_j \sup_x (f(x^j) - f(x))$. Major steps in the proof are

- a) the identification of $(d/dt)E_t(g, f)$ (Proposition A.1);

- b) the construction of functions F_Γ , $|\Gamma| < \infty$, which may be thought of as conditional expectations of the limit Hamiltonian given \mathcal{F}_Γ (Proposition A.2);
- c) a Liapounov argument in terms of F_Γ : its increments $F_\Gamma(x^k) - F_\Gamma(x)$ do not depend on k , for $k \in \Gamma$ (Proposition A.3/4);
- d) the identification of F_Γ by a martingale argument.

PROPOSITION A.1 For $g \in \mathcal{D}$ and $t > 0$ one has

$$(A.1) \quad (d/dt)E_t(g, f) = E_t(Lg, f),$$

where the r.h.s. is defined as the absolutely convergent series

$$(A.2) \quad \sum_j \int Lg \cdot S_j T_t f \, d\mu.$$

PROOF. Assume $g \in \mathcal{D}^+$ and take Γ so that g and Lg are \mathcal{F}_Γ measurable. By Proposition 3.2 the series in (A.2) converges absolutely, because Lg is the difference of increasing functions belonging to $L^2(\Gamma)$. Consequently, the value of the sum can be identified as

$$(A.3) \quad \lim_\Lambda E_t^\wedge(Lg, f)$$

in the notation of (3.16). Since for finite Λ , obviously,

$$(A.4) \quad (d/dt)E_t^\wedge(g, f) = E_t^\wedge(Lg, f),$$

everything is reduced to show that for the functions $E_t^\wedge(g, f)$, differentiation and Λ -limit can be interchanged. But that is indeed true: these functions are, together with its limit, alternating of any order, hence decreasing, convex and twice differentiable. \square

The family F_Γ , $|\Gamma| < \infty$. Call $F_{\Gamma,t}$ the function F constructed in Proposition 3.2. The statement of Corollary 3.4 can then be expressed as weak convergence in $L^2(\Gamma)$ of $F_{\Gamma,t}$, as $t \rightarrow \infty$. Call the limit function F_Γ . Then the properties (3.9) carry over to F_Γ and we get:

PROPOSITION A.2 (Properties of F_Γ).

- (i) F_Γ is \mathcal{F}_Γ -measurable,
- (ii) $0 \leq F_\Gamma(x^k) - F_\Gamma(x) \leq a$,
- (A.5) (iii) $\int g F_\Gamma \, d\mu = E(g, f)$ for all $g \in \mathcal{D}(\Gamma)$,
- (iv) $\int F_\Gamma \, d\mu = 0$,
- (v) $F_\Gamma = \mathcal{L}(F_{\Gamma'} | \mathcal{F}_\Gamma)$ for $\Gamma \subset \Gamma'$.

(Notice that (v) follows directly from (i) and (iii)).

The Liapounov argument.

PROPOSITION A.3. If $g \in \mathcal{D}$ and $LG \in \mathcal{D}(\Gamma)$,

$$(A.6) \quad \int Lg \cdot F_\Gamma d\mu = 0.$$

PROOF. From Proposition A.1 one has

$$\int Lg \cdot F_{\Gamma,t} d\mu = \frac{d}{dt} E_t(g, f);$$

the r.h.s. goes to zero as derivative of a difference of bounded, decreasing, convex functions. \square

We introduce the operator

$$(A.7) \quad \Delta^{\dot{y}}h(x) := h(x^{\dot{y}}) - h(x);$$

the generator L then reads as

$$Lh(x) = \sum_j \sum_{|k-j|=1} c(x_j) \Delta^{jk}h(x).$$

Denote by $\Lambda(n)$ the cube of length $2n$, centered at 0; we write F_n for $F_{\Lambda(n)}$.

PROPOSITION A.4. For fixed m and $j, k \in \Lambda(m)$ we have

$$(A.8) \quad \int c(x_j) \cdot (\Delta^{jk}F_m)^2 d\mu = 0.$$

PROOF. It suffices to consider $|j - k| = 1$. We choose $n > m$ and start from

$$(A.9) \quad \int LF_n \cdot F_{n+1} d\mu = 0,$$

which follows from Proposition A.3. Using a familiar identity for reversible processes

$$(A.10) \quad \int g \cdot Lh d\mu = -\frac{1}{2} \int \sum_{|j-k|=1} c(x_j) \cdot \Delta^{jk}g \cdot \Delta^{jk}h d\mu$$

we obtain from (A.9)

$$(A.11) \quad \int \sum_{(j,k)} c(x_j) (\Delta^{jk}F_n) \cdot (\Delta^{jk}F_{n+1}) d\mu = 0,$$

where the summation goes over all bonds (j, k) with at least one of its vertices in $\Lambda(n)$. Since μ is a product measure, we have by (A.5v)

$$(A.12) \quad \mathcal{E}(\Delta^{jk}F_{n+1} | \mathcal{F}_{\Lambda(n)}) = \Delta^{jk}F_n$$

on the set $\{x_j > 0\}$, if $j, k \in \Lambda(n)$. So we can split the l.h.s. of (A.11) in two parts

$$(A.13a) \quad \sum_{j,k \in \Lambda(n)} \int c(x_j)(\Delta^{jk}F_n)^2 d\mu$$

and

$$(A.13b) \quad \sum_{j \in \Lambda(n), k \notin \Lambda(n)} \int c(x_j)(\Delta^{jk}F_n)(\Delta^{jk}F_{n-1}) d\mu.$$

The latter expression is for fixed m of the order $O(n^{d-1})$, because F_n and F_{n+1} have bounded increments. Each term in the first expression can be minorized in the form

$$(A.14) \quad \int c(x_j)(\Delta^{jk}F_n)^2 d\mu \geq \int c(x_j)(\Delta^{jk}F_\Gamma)^2 d\mu$$

whenever $\Gamma \subset \Lambda(n)$ and $j, k \in \Gamma$. ((A.12) plus Jensen's inequality.) We take as Γ now a cube of sidelength $2m$ and sum (A.14) over all those cubes contained in $\Lambda(n)$ and all bonds (j, k) contained in Γ . Due to shift invariance, we get

$$(A.15) \quad \begin{aligned} (2m + 1)^{d-1} \cdot 2m \sum_{(j,k) \subset \Lambda(n)} \int c(x_j)(\Delta^{jk}F_n)^2 d\mu \\ \geq (2n - 2m + 1)^d \cdot \sum_{(j,k) \subset \Lambda(m)} \int c(x_j)(\Delta^{jk}F_m)^2 d\mu. \end{aligned}$$

By (A.11) and (A.13) the l.h.s. is also $O(n^{d-1})$ for n large; hence the expression at the r.h.s.

$$(A.16) \quad \sum_{(j,k) \subset \Lambda(m)} \int c(x_j)(\Delta^{jk}F_m)^2 d\mu$$

must be zero. That proves (A.8). \square

Final computations. By Proposition A.4, to each cube Γ there exists a function D_Γ such that

$$(A.17) \quad D_\Gamma(x) = F_\Gamma(x^k) - F_\Gamma(x)$$

whenever $k \in \Gamma$. By (A.5ii), D is bounded; further, as in (A.12),

$$(A.18) \quad \mathcal{L}(D_\Gamma | \mathcal{F}_\Gamma) = D_\Gamma \quad \text{for } \Gamma \subset \Gamma'.$$

By a martingale argument we find a D , also bounded, such that

$$(A.19) \quad D_\Gamma = \mathcal{L}(D | \mathcal{F}_\Gamma) \quad \text{for all } \Gamma.$$

Since obviously $S_j D_\Gamma = D_{\Gamma+j}$ and $D = \lim_\Gamma D_\Gamma = \lim_\Gamma D_{\Gamma+j}$ (in L^1 -sense), we conclude that $D = S_j D$. The spatial ergodicity of μ implies that D , and hence all D_Γ , are equal to a constant, say α .

Going back to F , we get from (A.17) and (A.5iv)

$$(A.20) \quad F_{\Gamma}(x) = \sum_{j \in \Gamma} \alpha \cdot (x_j - \rho);$$

hence, for all $g \in \mathcal{D}(\Gamma)$

$$(A.21) \quad E(g, f) = \int g F_{\Gamma} d\mu = \alpha \cdot \sum_{j \in \Gamma} \int g \cdot (x_j - \rho) d\mu = \alpha \cdot E_0(g, f_0).$$

This proves the theorem: the coefficient α in (A.21) is computed by setting $g = f_0$ and applying Proposition 3.4; the result is

$$(A.22) \quad \alpha = \chi^{-1} \cdot E_0(f_0, f)$$

as stated in (3.22).

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