Self Diffusion in Simple Models:

Systems with Long Range Jumps.

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Abstract

We review some exact results for the motion of a tagged particle in simple models. Then, we study the density dependence of the self diffusion coefficient, $D_N(\rho)$, in lattice systems with simple symmetric exclusion in which the particles can jump, with equal rates, to a set of N neighboring sites. We obtain positive upper and lower bounds on $F_N(\rho) = N((1-\rho) - [D_N(\rho)/D_N(0)])/(\rho(1-\rho))$ for $\rho \in [0,1]$. Computer simulations for the square, triangular and one dimensional lattice suggest that F_N becomes effectively independent of N for $N \geq 20$.

1. Introduction

Many properties of macroscopic systems are universal, retaining their qualitative features under drastic simplifications of the underlying microscopic structures. Thus, lattice gas models have greatly enhanced our understanding of phase transition phenomena in equilibrium systems. Their dynamical behavior, currently an active area of research, promises to be similarly fruitful for understanding nonequilibrium properties of macroscopic systems.

This article explores some aspects of self-diffusion in lattice models. After a brief overview of some rigorous results, we derive new results for systems with long range jumps. It is dedicated to Matthieu H. Ernst, a leader in the field of kinetic theory and lattice gases, on the occasion of his sixtieth birthday.

We shall be concerned here with the motion of a tagged particle in an infinite interacting particle system. A tagged particle is *exactly* like any other particle in the system, its 'tag' permits us to follow its trajectory $X(t)$. This yields a relatively simple probe of time correlations in a system of interacting particles in an overall stationary state.

The self-diffusion coefficient D_s is defined, in an infinite stationary system without drift, as [1]

$$D_s = \frac{1}{2d} \lim_{t\to\infty} \frac{1}{t} \langle [X(t) - X(0)]^2 \rangle, \tag{1.1}$$

where d is the spatial dimension of the system and the average $\langle\rangle$ is over the stationary measure. We expect that in a real fluid the limit (1.1) will exist, be positive, and be given by the Einstein-Green-Kubo formula

$$D_s = \frac{1}{d} \lim_{t\to\infty} \int_0^t \langle v(\tau) \cdot v(0) \rangle d\tau, \tag{1.2}$$

where $\langle v(\tau) \cdot v(0) \rangle$ is the velocity autocorrelation function [1]: A simple computation gives $\langle (X(t) - X(0))^2 \rangle = 2\int_0^t (t-\tau) \langle v(\tau) \cdot v(0) \rangle d\tau$, so (1.2) reduces to (1.1) when $\langle v(\tau) \cdot v(0) \rangle$ decays sufficiently rapidly.

The self-diffusion coefficient is a global dynamical parameter associated with macroscopic system in equilibrium, i.e. spacially uniform. Therefore, it is generally different from the bulk diffusion coefficient D_b, which relates to the evolution of a nonuniform density in a non-stationary system. D_s can be thought of as a color diffusion coefficient by considering the evolution of the relative density of two components of a system which differ only by a property, say color, that plays no role in the dynamics, while the overall system, ignoring color, is in a uniform state [1, 2]. An approximate experimental realization of such a situation occurs when the components are isotopes of He^3 atoms whose spins are polarized in different directions.

Going beyond (1.1) and (1.2), we can introduce a "scaling" parameter ϵ and define $X_\epsilon(t)$ as $\epsilon[X(t/\epsilon^2;\cdot) - X(0)]$, where the $\cdot$ indicates the dependence of the trajectory on the coordinates and velocities of *all* the particles at $t = 0$ [1,2]. Typically, we expect that in the long time limit, $\epsilon \to 0$, the process $\{X_\epsilon(t),\ t \in I\!R\}$ converges in probability -after subtracting out any drift- to the law of a Brownian motion $\{W_{D_s}(t),\ t \in I\!R\}$ with diffusion coefficient D_s given by (1.1)[1,2]. We summarize this by

$$\lim_{\epsilon \to 0} X_\epsilon(t) = W_{D_s}(t). \tag{1.3}$$

The behavior (1.1)-(1.3) has been proven for the one component, one dimensional system of hard rods with diameter a [1, 3, 4]. For this idealized system D_s can be computed exactly,

$$D_s(\rho) = \frac{(1-\rho a)}{\rho}\langle|v|\rangle, \quad \text{and} \quad \langle|v|\rangle = \int_{-\infty}^{\infty} |v|h(v)dv. \tag{1.4}$$

Here $h(v) = h(-v)$ is the one particle velocity distribution function; this need not be Maxwellian, since collisions in this system merely exchange velocities. Noting that $(1/\rho - a)$ is the mean free path in this system, the interpretation of (1.4) is very simple. On the other hand, the velocity autocorrelation function $\langle v(\tau)v(0)\rangle$ depends non-trivially on $h(v)$: it decays like an exponential when $h(v)$ vanishes near $v = 0$, and like t^{-3} when $h(v)$ is Maxwellian [5].

The only other continuum system for which the existence of the limits (1.1)-(1.3) has been proven is a system of interacting Brownian particles ([6,7]) which models suspensions of polymers or even of small macroscopic balls in a fluid. Actually, one needs to assume ergodicity of the dynamics, and formula (1.2) has to be modified because instantaneous velocities are no longer well defined [1].

In $d = 1$, stochastic models in which the particles cannot cross each other behave differently from the mechanical model which yields (1.4): $\langle X^2(t)\rangle \sim \sqrt{t}$ so $D_s = 0$ [1,8]. Interestingly, however, $\sqrt{\epsilon}X(t/\epsilon^2;\cdot)$ still goes to a Gaussian process; see [4] for a simple derivation of the one dimensional results.

2. Lattice Models

a) General Dynamics

We consider now systems with one type of particles whose total number is the only quantity conserved by the dynamics. We expect however that much of our discussion will remain valid also for models where momentum is also conserved [7, 9]. The stochastic dynamics of these systems consists of particles "jumping" between lattice sites. The jump from a site x to a site y on the lattice occurs with a rate $c(x, y; \eta)$, where η is the configuration of the system just prior to the jump: $\eta = \{\eta(z)\}$, with $\eta(z) = 0, 1, 2, ..$, specifying the number of particles at site z. We shall generally consider the d-dimensional (simple) cubic lattice $\mathbb{Z}^d$.

The system will be in a stationary state with measure ν whenever

$$\sum_{x,y} c(x, y; \eta)\nu(\eta) = \sum_{x,y} c(x, y; \eta^{x,y})\nu(\eta^{x,y}), \tag{2.1}$$

where $\eta^{x,y}$ is the configuration which arises from η after a particle has jumped from x to y. A simple way to satisfy (2.1) is to have the equality hold for each term in the sum. The rates are then said to satisfy detailed balance with respect to ν. In such cases ν can be written in the form of a Gibbs measure, $\nu_{eq}(\eta) \sim \exp[-\beta H(\eta)]$, where $H(\eta)$ is the energy of a configuration η, and β is the reciprocal temperature: see [10] for a detailed discussion of Gibbs measures. Detailed balance then corresponds to

$$c(x,y;\eta)/c(y,x;\eta^{x,y}) = \exp\{-\beta[H(\eta^{x,y}) - H(\eta)]\}. \tag{2.2}$$

In the probability literature a stationary process whose rates satisfy detailed balance is called reversible: a film of the system in the stationary state would look the same if run backwards.

The trajectory $X(t)$ now takes values on the lattice. However, after scaling with ϵ and letting $\epsilon \to 0$, as in (1.3), the limit will again be a continuous process.

b) Models without Exclusion

One of the simplest dynamics for a system of particles on a lattice is the so called "zero-range" process [11]. This corresponds to the jump rates $c(x,y;\eta)$ depending only on $\eta(x)$, the number of particles at site x,

$$c(x,y;\eta) = \lambda g(\eta(x)) p(y-x). \tag{2.3}$$

Here λ is a constant, $\lambda > 0$, while g and p satisfy the conditions

$$g(0) = 0, \qquad g(k) > 0, \qquad for \quad k > 0, \tag{2.4}$$

$$p(0) = 0, \qquad p(r) \geq 0, \qquad \sum_{r \in \mathbb{Z}^d} p(r) = 1. \tag{2.5}$$

The stationary measures for this dynamics in the macroscopic (infinite volume) limit, are a translation invariant family of product measures, ν_ρ, parametrized by the average density ρ[11]. The probability of having exactly j particles at any given site is

$$W_j = \frac{b^j}{G(j)} W_0, \qquad j = 0, 1, 2, ... \tag{2.6}$$

where

$$G(0) = 1, \qquad G(j) = \Pi_{l=1}^{j} g(l), \qquad j \geq 1, \tag{2.7}$$

and the parameters b and W_0 are determined by the normalization and the specified average density, $\rho \geq 0$, i.e.

$$\sum_{j=0}^{\infty} W_j = 1, \qquad \text{and} \qquad \sum_{j=0}^{\infty} j W_j = \rho. \tag{2.8}$$

An easy check shows that these measures satisfy the detailed balance condition (2.2), with $\beta H(\eta)$ a sum of single site energies equal to $-\log W_j$, if and only if $p(r) = p(-r)$.

Two particular cases of the zero range process deserve mention. When $g(l) = l$ the dynamics corresponds to that of independent particles. This gives rise to the Poisson distribution

$$W_j = (\rho^j / j!) e^{-\rho}, \tag{2.9}$$

Taking $g(l) = 1 - \delta_{0,l}$, corresponding to only the 'top' particle jumping, yields a geometric stationary distribution

$$W_j = \frac{1}{1+\rho}(\frac{\rho}{1+\rho})^j. \tag{2.10}$$

The stationary measure seen from the tagged particle is the 'Palm measure'

$$\hat{\nu}_\rho(\eta) = \frac{\eta(0)}{\rho}\nu_\rho.$$

As the "waiting time" of the tagged particle depends on the number of particles at the same site, its average jump rate is given by

$$\bar{\lambda} = \sum_{k=1}^{\infty} \frac{\lambda_k}{\rho} W_k, \qquad \text{with} \qquad \lambda_k = \lambda g(k). \tag{2.11}$$

Let the displacement, after K steps, of the random walk specified by transition probability $p(r)$ be X_K. Assuming for simplicity that there is no drift,

$$\sum rp(r) = 0, \tag{2.12}$$

we have

$$\langle X_{K+1}^2 \rangle = \langle (X_K + Y_K)^2 \rangle = \langle X_K^2 \rangle + \langle Y_K^2 \rangle, \tag{2.13}$$

where Y_k is the displacement of the particle at the $(K+1)$ step. Clearly,

$$\langle Y_K^2 \rangle = \sum r^2 p(r) \equiv 2\tilde{D}_0, \tag{2.14}$$

and

$$\langle X_K^2 \rangle = 2\tilde{D}_0 K. \tag{2.15}$$

A little thought shows that for the zero range process, the trajectory of the tag will look the same as the trajectory of a single particle performing a random walk on the lattice with transition probabilities $p(\mathbf{r})$. The only difference is that the "waiting time" at any site will generally depend on the number of particles there. In fact [9], As soon as the process is ergodic, the scaled trajectory $X_\epsilon(t)$ satisfies (1.3) with

$$D(\rho) = \bar{\lambda}(\rho)\tilde{D}_0.$$

Ergodicity is easy to show for $g(k) = k$, and was shown in the case $g(k) = 1 - \delta_{k,0}$ in [12]. In fact, (1.3) is proven in [13] for all $g(k)$.

For the case of independent particles, $\bar{\lambda}$ is independent of ρ and equal to λ, while for $g(k) = 1 - \delta_{k,0}$,

$$\bar{\lambda}(\rho) = \frac{\lambda}{1+\rho},$$

so that $D(\rho)$ decreases with density for this case. The opposite behavior is clearly also possible.

Looking back on our arguments leading to (2.15) we see that the main ingredients are the independence of the step Y_K from the past history of the process (e.g. X_k

is a martingale). This means that (2.15) should remain valid whenever

$$c(x,y;\eta) = h(\eta;x)p(y-x), \tag{2.16}$$

i.e. as long as $c(x,x+r;\eta)/c(x,x+r';\eta)$ is independent of η (and by translation invariance of x).

A particular example of (2.16) is (a generalization of) a model due to van Beijeren [14], in which

$$c(x,y;\eta) = \sum_{i=1}^{k} \lambda_i g_i(\eta(x)) p_i(y-x),$$

with the g_i and p_i satisfying the conditions (2.4), (2.5) and (2.12). The stationary measure is now not known in general. In fact we expect that it will have very long range correlations [14], yet (1.1) and (1.3) should still be valid with

$$\tilde{D}(\rho) = \frac{1}{2}\bar{\lambda}(\rho) \sum_i r^2 p_i(r)$$

where $\bar{\lambda}(\rho)$ is the average rate in the stationary measure.

Remark: It is clear that the diffusion constants D and $\tilde{D}_0$ are, for anisotropic $p(r)$, the traces of the corresponding positive-definite diffusion tensors D and D_0. When (2.12) holds and $p(r)$ is isotropic with respect to the lattice directions then D is diagonal.

c) Models with Exclusion

We consider now the case where there is a hard core interaction between the particles, forbidding the presence of more than one particle at any lattice site. The configurations of the system are now given by $\eta = \{\eta(x)\}$ with $\eta(x) = 0$ or 1 and $c(x, y; \eta) = 0$ when $\eta(y) = 1$. The simplest dynamics for these systems correspond to the so called simple exclusion processes, in which the jump rate from a site x to a site y is independent of the configuration at other sites of the lattice,

$$c(x, y; \eta) = \lambda \eta(x)(1 - \eta(y))p(y - x),$$

with $p(r)$ satisfying (2.5).

The translation invariant stationary measures ν_ρ, with $0 \leq \rho \leq 1$, will again be product measure with

$$W_0 = 1 - \rho, \qquad W_1 = \rho, \qquad W_j = 0 \quad for \quad j \geq 2.$$

The ν_ρ will, like before, satisfy detailed balance if and only if the jump rates are symmetric, $p(r) = p(-r)$.

The behavior of a tag trajectory $X(t)$ is now considerably more complicated than in the zero range process. In particular, knowledge of the past history of $X(t)$ will influence the probabilities that certain sites are empty and hence the future position of the trajectory.

The proof that (1.1)-(1.3) hold for these models was given by Kipnis and Varadhan [5] for the reversible case: if $d \geq 2$, then $D(\rho) > 0$ when $\rho < 1$; if $d = 1$, then

$D(\rho) = 0$ unless $p(r) > 0$ for $|r| > 1$. For the non-reversible case satisfying (2.12) the result is due to Varadhan [15]. As already mentioned, in $d = 1$, with jumps limited to nearest neighbor sites, $p(1) = p(-1) = \frac{1}{2}$, the mean square displacement only grows like $\sqrt{t}$ [8].

In the asymmetric case, with $p(1) = p, \quad p(-1) = 1 - p$, $p > \frac{1}{2}$, (1.1) still holds after subtraction of the drift, i.e. for $\hat{X}(t) = X(t) - vt$, where the velocity v is given by, $v = (2p - 1)(1 - \rho)$. This was proven for $d = 1$ by Kipnis [16] and for $d \geq 3$ by Varadhan and Yau [17] who also prove (1.3) (there is no proof for $d = 2$). Somewhat surprisingly the diffusion constant for $\hat{X}(t)$ in $d = 1$ is equal to the drift $D(\rho) = (1 - \rho)(2p - 1)$ [16].

The dependence of D on ρ is not known even for the simple exclusion process. It is intuitively clear that $D(\rho) \to 0$ as $\rho \to 1$. Varadhan [18] proved that the so-called "correlation factor" $D(\rho)/[1 - \rho]$ is a decreasing function of ρ bounded away from zero as $\rho \to 1$. This confirms the behavior found in numerical results for nearest neighbor jumps [19]. He also showed that $D(\rho)$ is continuous in all dimensions and that for $d \geq 3$, $D(\rho)$ is Lipshitz, e.g. $|D(\rho) - D(\rho')| < c|\rho - \rho'|$.

Remark: We remark here for completeness that many authors (beginning with Einstein) have studied situations where there is a special particle with a different dynamics than the other particles of the system: in particular, the case where an external field acts only on the special particle (see [1]). Though we will not discuss this problem here in any detail, we want to mention that recently, Landim, Olla and Volchan [20] have studied a one dimensional system where the special particle jumps with probability $p > 1/2$ to the right and $1-p$ to the left -with an exclusion rule- while all the other particles follow a symmetric dynamics with $p = 1/2$ (recall that the self diffusion constant is 0 in this system [8]). They showed that $X_\epsilon(t)$ converges in probability to a number $v(t)$ which solves a differential equation and depends on the initial macroscopic density profile. Their result holds for a large class of initial profiles. For instance, when the initial measure is a product Bernouilli measure of density ρ, they showed that

$$v(t) = (2p-1)\frac{1-\rho}{\rho}\sqrt{\frac{2}{\pi}}\sqrt{t}.$$

3. Long Range Jumps

We discuss now the situation where particles make jumps to a symmetric neighborhood U, containing N sites, with equal probability, $p(r) = N^{-1}$ for $r \in U$, $p(r) = 0$ otherwise. We shall be interested in the behavior of the diffusion constant $D_N(\rho)$ and the suitably scaled trajectory $X^N(t)$ when N becomes large. Intuitively, as N increases the tag is less likely to revisit, during a fixed number of jumps, a previously occupied site and hence there will be less and less memory left of previous jumps. The only effect of the hard core exclusion will then be to slow down the jump rates by a factor $(1-\rho)$, the fraction of attempted jumps which are unsuccessful due to the target site being occupied. Intuitively this will lead to a density independent correlation factor, $D_N(\rho)/(D_N(0)(1-\rho))$, in the limit $N\to\infty$: this limit is analogous to the van der Waals or mean field limit in equilibrium systems when the particles interact via a long range Kac potential [21].

Since our dynamics is reversible the result of Kipnis and Varadhan [6] applies, so that for each N

$$\lim_{\epsilon\to 0}\frac{\epsilon X^N(t\epsilon^{-2})}{\sqrt{D_N(\rho)}}=W_1(t), \tag{3.1}$$

and one expects that

$$\lim_{N\to\infty}\frac{D_N(\rho)}{D_N(0)}=1-\rho. \tag{3.2}$$

Actually, we show more:

Proposition. Set $C_N(\rho)=D_N(0)(1-\rho)-D_N(\rho)$. Then there are positive constants c_1 and c_2 such that

$$c_1\le F_N(\rho)=\frac{NC_N(\rho)}{\rho(1-\rho)D_N(0)}\le c_2, \qquad \forall\rho\in[0,1]. \tag{3.3}$$

The proof of the proposition is given in the Appendix.

In order to determine the behaviour of $D_N(\rho)$, we have performed numerical simulations in one and two dimensions with periodic boundary conditions at different densities. The average of $[X^N(t)]^2$ over many realizations (from 100 to 1000) was plotted against t and fit to a straight line passing through the origin. The fitted slope is then taken for the diffusion coefficient.

The one dimensional lattice had 2000 sites. Typically, 200 realizations were run for 1000 time steps. The maximum N considered was 100. In two dimensions, square and triangular lattices were used, with 200×200 lattice sites. 300 realizations were run for about 500 time steps and $N \leq 90$. Simulations with larger N were also run, but the statistical accuracy was not enough to extract any information beyond the zero order one. In Fig. 1 we plot $F_N(\rho)$ vs. ρ for the square, triangular, and one dimensional lattices for different values of N: the set U to which the particle jumps being the N closest neighbors as measured by the number of bonds required to reach the site. It appears that $F_N(\rho)$ varies linearly in ρ with a slope independent of dimensions.

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Appendix. Proof of the Proposition

We will work in the moving frame of the tag particle and for simplicity write the proof for cubic lattices. Thus, $U = \{y \neq 0\colon ||y|| \leq n\}$ and $N = (2n+1)^d - 1$. The generator of this process is $-A$ with

$$Af(\eta) = \sum_{y \in U} \frac{1}{N}(1 - \eta(y))(f(\eta) - f(\tau_y \eta)) + \frac{1}{2} \sum_{x \in Z^d \setminus \{0\}} \sum_{y \in x+U} \frac{1}{N}(f(\eta) - f(T_{xy}\eta)),$$

where $T_{xy}\eta = \eta^{x,y}$, $\tilde{\tau}_y$ shifts the configuration by a vector y, and we have denoted $\tilde{\tau}_y(T_{0y})$ by τ_y. The process seen from the tag particle is reversible with respect to $\hat{\nu}_\rho(\eta) = \nu_\rho(\eta | \eta(0) = 1)$ with ρ in $[0,1]$. The expectation with respect to $\hat{\nu}_\rho$ is denoted by E^ρ.

It is well known, see [1], that if S_t is the semigroup generated by A

$$D_N(\rho) = D_N(0)(1-\rho) - \int_0^\infty (S_t w, w)dt,$$

$$D_N(0) = \frac{1}{N} \sum_{||y|| \leq n} y_1^2 \sim n^2 \qquad \text{and} \qquad w(\eta) = \frac{1}{N} \sum_{||y|| \leq n, y_1 > 0} y_1(\eta(\overline{y}) - \eta(y)),$$

where $y = (y_1, \ldots, y_d)$, $\overline{y} = (-y_1, y_2, \ldots, y_d)$ and because the diffusion matrix is diagonal, we chose w to be the current in the e_1 direction. Note that $C_N(\rho) = -\int (S_t w, w)dt$.

We introduce the normalized variables

$$r_y = \frac{(\eta(y) - \rho)}{\sqrt{\rho(1-\rho)}} \qquad \text{such that} \qquad E^\rho[r_x r_y] = \delta_{x,y} \qquad \forall x, y \in Z^d \backslash \{0\}.$$

a) $C_N(\rho) \leq \overline{c}\rho(1-\rho)\frac{n^2}{n^d}$.

Recalling a variational formula used in [17]

$$C_N(\rho) = \sup_{f \ local} \frac{E^\rho[wf]^2}{E^\rho[fAf]},$$

we just need to show that for any local function f,

$$E^\rho[wf]^2 \leq \overline{c}\rho(1-\rho)\frac{n^2}{n^d} E^\rho[fAf].$$

Now,

$$E^\rho[wf] = \frac{\sqrt{\rho(1-\rho)}}{N} \sum_{||y|| \leq n, y_1 > 0} y_1 E^\rho[(r_{\overline{y}} - r_y)f]$$

$$= \frac{\sqrt{\rho(1-\rho)}}{N} \sum_{||y|| \leq n, y_1 > 0} y_1 E^\rho[r_y(T_{\overline{y},y} f - f)].$$

First, we fix $(y_2^o, \ldots, y_n^o)$ and work on the line $y = (y_1, y_2^o, \ldots, y_n^o)$ for $y_1 \in [-n, n]$. For each $y_1 > 1$, there are $y_1 - 1$ different ways of joining $\overline{y}$ and y in three steps $(\overline{y}, ke_1 + \overline{y}, (k, y_2^o, \ldots, y_n^o), y)$ with $k = 1, \ldots, y_1 - 1$ while remaining on the line joining y and $\overline{y}$. It is important to note that $ke_1 + \overline{y}$ is at y_1 units from $(k, y_2^o, \ldots, y_n^o)$, and thus as y_1 ranges from 2 to n, a given pair of sites on the same line will be used at most once. Now, with the notations $k_1 = ke_1 + \overline{y}$ and $k_2 = (k, y_2^o, \dots, y_n^o)$

$$T_{\overline{y},y} - I = T_{\overline{y},k_1} T_{k_1,k_2} T_{k_2,y} T_{k_1,k_2} T_{\overline{y},k_1} - T_0$$

$$= T_1 T_2 T_3 T_4 T_5 - T_0 = \sum_{m=1}^{5} [T_0 \dots T_{m-1}](T_m - T_0).$$

Also, the product measure being invariant under exchanges

$$\forall m \in [1,5] \qquad E^\rho r_y [T_0 T_1 \dots T_{m-1}](T_m f - f) = E^\rho r_{y_m}(T_m f - f),$$

where y_m belongs to $\{\overline{y}, k_1, k_2, y\}$.

Now, if y_1, y_2 belong to a line parallel to e_1, we want to 'split' T_{y_1,y_2} -which arose in our previous decomposition- into $T_{y_1,z}$ and T_{z,y_2} where z is a common neighbor. y_1 and y_2 will have of the order of n^d common neighbors if $||y_1 - y_2|| \leq n$. However, for each neighbor, say z, the pair (y_1, z) will be used at most $2n$ times because in our line, y_1 has $2n$ neighbors at most. Thus, we end up with

$$\sum_{||y|| \leq n, y_1 > 0} y_1 E^\rho |r_y (T_{\overline{y},y} f - f)| \leq \frac{\overline{a}}{n^{d-1}} \sum_{\substack{||x-y|| \leq n \\ ||y|| \leq n}} E^\rho |r_\gamma (T_{x,y} f - f)|$$

where $\overline{a}$ depends just on the dimension d, and γ is an inocuous index different for each pair (x, y).

Denoting by T_m a generic exchange operator and γ an arbitrary index and using the Cauchy inequality

$$|E^\rho[r_\gamma(T_m f - f)]| \leq (E^\rho[r_\gamma^2]E^\rho[(T_m f - f)^2])^{1/2} = \sqrt{E^\rho[(T_m f - f)^2]}.$$

gives

$$E^\rho[wf]^2 \leq [\overline{a}\frac{\sqrt{\rho(1-\rho)}}{N} \sum_{\substack{||x-y||\leq n \\ ||y||\leq n}} \frac{1}{n^{d-1}} \sqrt{E^\rho[(T_{x,y}f - f)^2]}]^2$$

$$\leq \rho(1-\rho)\overline{a}^2 \frac{1}{N^2}[\frac{1}{n^{d-1}}]^2 (n^d)^2 \sum_{\substack{|x-y|\leq n \\ x,y\neq 0}} E^\rho[(T_{x,y}f - f)^2]$$

$$\leq \overline{c}\frac{n^2}{N}\rho(1-\rho)E^\rho[fAf],$$

and the first inequality follows.

b) $C_N(\rho) \geq \underline{c}\rho(1-\rho)\frac{n^2}{n^d}$.

Choose $f = \sum_{||y||\leq n, y_1>0} r_y$, and write

$$E^\rho[fAf] \leq \frac{1}{N}[\sum_{0<||y||\leq n} E^\rho[(\tau_y f - f)^2] + \frac{1}{2} \sum_{\substack{||x-y||\leq n \\ x,y\neq 0}} E^\rho[(T_{x,y}f - f)^2]].$$

The reason to choose such an f is that

$$E^\rho[wf]^2 = \frac{\rho(1-\rho)}{N^2}[(2n)^{d-1}\sum_{y_1=1}^{n} y_1]^2 \geq \frac{n^2\rho(1-\rho)}{8},$$

Now, $\tau_x r_y$ is equal to r_{x+y} if $y \neq -x$ and to r_x if $y = -x$, so, for any y, it is easy to see that

$$E^\rho[(\tau_y f - f)^2] \leq N.$$

Thus,

$$\sum_{0<||y||\leq n} E^\rho[(\tau_y f - f)^2] \leq N^2.$$

Now, it is also easy to see that

$$\sum_{\substack{||x-y||\leq n \\ x,y\neq 0}} E^\rho[(T_{x,y} f - f)^2] \leq N^2,$$

and thus

$$C_N(\rho) \geq \frac{n^2}{N}\rho(1-\rho)\frac{1}{16}.$$

which completes the proof. □

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Fig.1 Simulation results of the quantity $F_N(\rho)$ versus the density ρ. Results of simulations in one dimensional lattices are represented by circles, in a square lattice by squares and in the triangular lattices by triangles. The number of neighbours is shown in the legend. The slope of $F_N(\rho)$ as a function of ρ appears to be independent of the dimension or the type of lattice. The intercept, on the contrary, appears to depend on the dimension but not on the lattice structure.