Chapter 5

Self diffusion.

5.1 Motion of a tagged particle.

Let us look at the simple exclusion process in equilibrium on $\mathbb{Z}^d$ at density $\rho$. The distribution is the Bernoulli distribution $\mu_\rho$ defined by $\mu_\rho[\eta(x) = 1] = \rho$ with $\{\eta(x) : x \in \mathbb{Z}^d\}$ being independent. Let us suppose that at time 0, there is a particle at 0 which is tagged and observed. It is convenient to move the origin with that particle. The simple exclusion process now acts only on $\mathbb{Z}^d - \{0\}$ and is the environment as seen by the particle. The environment changes in two different ways. When one of the other particles currently at $x$ moves to $y$. The generator for this part is

$$A_1 = \frac{1}{2} \sum_{x,y \neq 0} \pi(y - x)[f(\eta^{x,y}) - f(\eta)]$$

(5.1)

Or the tagged particle moves from 0 to $z$ and then the origin is shifted to $z$. This is a transformation $T_z$ that acts when $\eta(z) = 0$ and the new configuration on $\mathbb{Z}^d - \{0\}$ is given by

$$(T_z \eta)(x) = \eta(x + z) \quad \text{if} \ x \neq -z, 0; \ (T_z \eta)(-z) = 0$$

contributing to the generator the term

$$A_2 = \sum_z \pi(z)(1 - \eta(z))[f(T_z \eta) - f(\eta)]$$

(5.2)

The full generator is therefore

$$(Af)(\eta) = \frac{1}{2} \sum_{x,y \neq 0} \pi(y - x)[f(\eta^{x,y}) - f(\eta)]$$

$$+ \sum_z \pi(z)(1 - \eta(z))[f(T_z \eta) - f(\eta)]$$

(5.3)

$$= (A_1 f)(\eta) + (A_2 f)(\eta)$$

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It is not difficult to check that the probability distribution \( \mu_\rho \) on \( \mathbb{Z}^d - \{0\} \) is a reversible invariant distribution for \( A \) given by 5.3. The jumps \( x \rightarrow y \) and \( y \rightarrow x \) as well as \( T_z \) and \( T_{-z} \) provide pairs with detail balance. The rates are same in either direction and \( \mu_\rho \) is invariant under the transitions.

Our main tool is a central limit theorem for additive functions of a reversible Markov process. Given a real valued function \( f \) on a space \( \mathcal{X} \), a Markov process on that space with generator \( A \) and a reversible ergodic invariant measure \( \mu \) for \( A \) satisfying with \( E^\mu[f(x)] = 0 \) under suitable conditions we will show that

\[
\int_0^t f(x(s))ds = M(t) + a(t)
\]

where \( M(t) \) is a square integrable Martingale with stationary increments and \( a(t) \) is negligible. If \( A \) is the self adjoint generator of the process \( -A \) has a spectral resolution \( -A = \int_0^\infty \sigma E(d\sigma) \). We have the Dirichlet form \( D(f) = \langle -Af, f \rangle_{L^2(\mu)} \) associated with \( A \). The space \( H_1 \) is the abstract Hilbert space obtained by completing the space of square integrals functions with respect to the Dirichlet inner product. One might start with functions \( u \) in the domain of \( A \), ensuring the finiteness of \( D(f) \). The completion will be an abstract space \( H_1 \). There will be a dual \( H_{-1} \) to \( H_1 \) relative to the inner product of \( H_0 = L^2(\mu) \).

Formally \( \|u\|_{-1} = \langle (-A)^{-1}u, u \rangle \) and

\[
\|u\|_{-1}^2 = \sup_f 2\langle u, f \rangle - D(f)
\]

We have the following theorem.

**Theorem 5.1.1.** If \( f \) is in \( L^2 \) with spectral resolution \( \langle E(d\sigma)f, f \rangle \), and

\[
\langle (-A)^{-1}f, f \rangle = \int_0^\infty \sigma^{-1}\langle E(d\sigma)f, f \rangle < \infty = \sigma^2 < \infty
\]

there is a square integrable Martingale \( M(t) \) with stationary increments such that \( E^P[M(t)^2] = 2\sigma^2 t \) and

\[
\int_0^t f(x(s))ds = M(t) + a(t)
\]

with \( E[|a(t)|^2] = o(t) \) as \( t \to \infty \). The central limit theorem follows. Moreover

\[
P[\sup_{0 \leq t \leq T} |a(t)| \geq c\sqrt{T}] \to 0
\]

for every \( c > 0 \) implying the functional CLT.

For the proof of the theorem we need two lemmas.
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Lemma 5.1.2. Let $P$ be a reversible stationary Markov process with invariant measure $\mu$ and generator $A$. Let $u \in L^2(\mu)$ with $\mathcal{D}(u) = \langle -Au, u \rangle < \infty$. Then

$$P[\sup_{0 \leq t \leq T} |u(x(t))| \geq \ell] \leq \frac{e}{\ell} \sqrt{T\mathcal{D}(u) + \|u\|^2_2}$$

Proof. Since $\mathcal{D}(|u|) \leq \mathcal{D}(u)$ we can assume that $u \geq 0$. If $x(t)$ is a Markov process and $\tau$ is the exit time from $G$, then $E_x[e^{-\sigma \tau}] = v(\sigma, x)$ is the solution of

$$\sigma v(x) - (Av)(x) = 0 \quad \text{for } x \in G; \quad v = 1 \text{ on } G^c$$

The function $v$ is also the minimizer of

$$\sigma \|v\|^2_2 + \mathcal{D}(v)$$

over $v$ such that $v = 1$ on $G^c$. Therefore the solution $v_\sigma$ satisfies

$$\sigma \|v_\sigma\|^2_2 \leq \inf_{v \equiv 1 \text{ on } G^c} [\sigma \|v\|^2_2 + \mathcal{D}(v)]$$

If we take for $G$ the set $u(x) < \ell$, the function $v = \frac{u \wedge \ell}{\ell}$ is an admissible choice for $v$. Therefore with $\sigma = T^{-1}$,

$$\|v_\sigma\|_1 \leq \frac{1}{\ell} \sqrt{\|u\|^2_2 + T\mathcal{D}(u)}$$

We obtain the estimate

$$\int P_x[\tau < T] d\mu \leq e^\sigma T \int E_x[e^{-\sigma \tau}] d\mu = e \|v_\sigma\|_1 \leq \frac{e}{\ell} \sqrt{\|u\|^2_2 + T\mathcal{D}(u)}$$

This lemma quantifies the statement that set of singularities of a function $u$ on $\mathbb{R}^d$ that is in the Sobolev space $W^{1,2}(\mathbb{R}^d)$ has capacity 0. In other words even if $u$ has singularities, a Brownian path will not see it, i.e. $u(\beta(t))$ is almost surely continuous.

Lemma 5.1.3. Let $\|u\|_2$ and $\mathcal{D}(u)$ be finite. Then for any $c > 0$

$$\limsup_{T \to \infty} P[\sup_{0 \leq t \leq T} |u(x(t))| \geq c\sqrt{T}] = 0$$

Proof. For any given $\delta > 0$ find $u' \in L_\infty$ such that $\|u - u'\|^2_2 \leq \delta$ and $\mathcal{D}(u - u') \leq \delta$. Clearly

$$\limsup_{T \to \infty} P[\sup_{0 \leq t \leq T} |u'(x(t))| \geq c\sqrt{T}] = 0$$

and

$$\limsup_{T \to \infty} P[\sup_{0 \leq t \leq T} |(u - u')(x(t))| \geq c\sqrt{T}] \leq \frac{c\sqrt{\delta}}{c}$$

and $\delta$ can be made arbitrarily small the lemma is proved.
Proof. Now we return to complete the proof of Theorem 5.1.1. First let us note that the condition is natural. An elementary calculation shows that

\[
\frac{1}{t} E_P \left[ \int_0^t f(x(s)) ds \right]^2 = \frac{1}{t} E_P \left[ \int_0^t \int_0^t f(x(s)) f(x(s')) ds ds' \right]
\]

\[
= \frac{2}{t} \int_{0 \leq s \leq s' \leq t} (T_{s'-s} f, f) ds ds'
\]

\[
= 2 \int_0^t (1 - \frac{s}{t}) (T_s f, f) ds
\]

\[
\approx 2 \int_0^\infty (T_s f, f) ds
\]

\[
= 2 \langle (-A)^{-1} f, f \rangle
\]

\[
= 2 \sigma^2
\]

Since \( (T_t f, f) \geq 0 \), the convergence has to be absolute. Let us solve the resolvent equation

\[
\lambda u_\lambda - A u_\lambda = f
\]

Then \( A u_\lambda = \lambda u_\lambda - f \) and

\[
u_\lambda(x(t)) - u_\lambda(x(0)) - \int_0^t \lambda u_\lambda(x(s)) ds + \int_0^t f(x(s)) ds = M_\lambda(t)
\]

where \( M_\lambda(t) \) is a martingale with

\[
\frac{1}{t} E \left[ |M_\lambda(t)|^2 \right] = 2 \mathcal{D}(u_\lambda) = 2 \langle -A u_\lambda, u_\lambda \rangle = 2 \int_0^\infty \frac{2 \sigma}{(\lambda + \sigma)^2} \langle E(d\sigma) f, f \rangle
\]

An easy computation shows that \( (\sigma + \lambda)^{-1} \to \sigma^{-1} \) and is dominated by \( \sigma^{-1} \) which is integrable with respect to \( \langle E(d\sigma) f, f \rangle \). The martingales \( M_\lambda(t) \) have a limit in \( L_2(P) \). \( \lambda u_\lambda \to 0 \) in \( L_2(\mu) \). Therefore \( a_\lambda(t) = u_\lambda(x(0)) - u_\lambda(x(t)) \) has a limit \( a(t) \) and

\[
\int_0^t f(x(s)) ds = M(t) + a(t)
\]

We will show that \( E[|a(t)|^2] = o(t) \). Then martingale CLT will imply our result. This is again a spectral calculation.

\[
E_P [|a(t)|^2] = 2 \lim_{\lambda \to 0} \int_0^\infty \frac{1 - e^{-t\sigma}}{(\lambda + \sigma)^2} \langle E(d\sigma) f, f \rangle = 2 \int_0^\infty \frac{1 - e^{-t\sigma}}{\sigma^2} \langle E(d\sigma) f, f \rangle
\]

Since \( \frac{1 - e^{-t\sigma}}{t} \leq \sigma \) and \( \int_0^\infty \frac{1}{\sigma} \langle E(d\sigma) f, f \rangle < \infty \), the dominated convergence theorem implies that

\[
\lim_{t \to \infty} \frac{1}{t} E_P [|a(t)|^2] = 0
\]
To prove the functional CLT, we need to consider
\[ \frac{1}{\sqrt{T}} \int_0^{tT} f(x(s))ds = \frac{1}{\sqrt{T}} M_\lambda(Tt) + \frac{1}{\sqrt{T}} \int_0^{tT} \lambda u_\lambda(s)ds - \frac{1}{\sqrt{T}} [u_\lambda(x(tT)) - u_\lambda(x(0))] \]

The functional CLT holds for \( \frac{1}{\sqrt{T}} M_\lambda(tT) \) and uniformly so as \( \lambda \to 0 \) because \( M_\lambda(t) \to M(t) \) in mean square. We note that with the help of the dominated convergence theorem,
\[
\lambda \|u_\lambda\|^2 = \int_0^\infty \frac{\lambda}{(\lambda + \sigma)^2} \langle E(d\sigma)f, f \rangle \to 0
\]
as \( \lambda \to 0 \). Clearly with the choice of \( \lambda = T^{-1} \),
\[
\xi_T = \sup_{0 \leq t \leq 1} |\frac{1}{\sqrt{T}} \int_0^{tT} \lambda u_\lambda(s)ds| \leq \frac{1}{T} \int_0^T \sqrt{\lambda} |u_\lambda(x(s))|ds
\]
and \( E[|\xi_T|^2] \to 0 \) as \( t \to \infty \). To complete the proof we need to show that, with \( \lambda = T^{-1} \)
\[ P[ \sup_{0 \leq t \leq T} |u_\perp(x(s))| \geq c\sqrt{T}] \to 0 \]
We can represent \( u_\perp \) as \( u_\perp + (u_\perp - u_\delta) \). By lemma 5.1.3, we have for any \( \delta > 0 \),
\[
\limsup_{T \to \infty} P[ \sup_{0 \leq s \leq T} |u_\delta(x(s))| \geq c\sqrt{T}] = 0
\]
Moreover
\[
\lim_{T \to \infty} \frac{1}{T} \|u_\perp - u_\delta\|_2^2 = 0
\]
and
\[
\lim_{\delta \to 0} D(u_\perp - u_\delta) = 0
\]
They imply that
\[
\limsup_{\delta \to 0} \limsup_{T \to \infty} P[ \sup_{0 \leq t \leq T} |u_\perp(x(s)) - u_\delta(x(s))| \geq c\sqrt{T}] = 0
\]
We now return to the motion of the tagged particle. We need to keep track of its motion as well as the changing environment seen by it. If \( w \in \mathbb{Z}^d \) is the location of the tagged particle in the original reference frame, then jointly the generator for \( w(t) \in \mathbb{Z}^d \) and \( \eta(\cdot) \in \{0, 1\}^{Z^d - \{0\}} \) is
\[
(\tilde{A}f)(\eta) = \sum_z \pi(z)(1 - \eta(z))[f(w + z,Tz\eta) - f(w,\eta)] + (Af)(w,\eta) \quad (5.4)
\]
with $A$ acting only on $\eta$ for each $w$. The $\eta(t, \cdot)$ part is a Markov process by itself and is in equilibrium at density $\rho$, the distribution being $\mu_\rho$. We are interested in establishing a central limit theorem for $w(t)$. We note that

$$w(t) - w(0) = \int_0^t \sum_z z \pi(z)(1 - \eta(s, z))ds + M(t)$$

where $M(t)$ is a Martingale with the decomposition

$$M(t) = \sum_z z M_z(t)$$

and

$$M_z(t) = N_z(t) - \pi(z) \int_0^t (1 - \eta(s, z))ds$$

The quantity

$$V(\eta(\cdot)) = \sum_z z \pi(z)(1 - \eta(z))$$

has mean 0 in equilibrium and one may expect a CLT for

$$\int_0^t V(\eta(s, \cdot))ds$$

We will prove a decomposition of the form

$$\int_0^t V(\eta(s, \cdot))ds = N(t) + a(t)$$

where $N(t)$ is a martingale and $a(t)$ is negligible. Then

$$w(t) - w(0) = M(t) + N(t) + a(t)$$

and since central limit theorems for martingales are automatic the result will follow. The quantities here are vectors and the equations are for each component or they are interpreted as

$$\langle w(t) - w(0), \xi \rangle = \langle M(t), \xi \rangle + \langle N(t), \xi \rangle + \langle a(t), \xi \rangle$$

for $\xi \in \mathbb{R}^d$. We have now the main theorem.

**Theorem 5.1.4.** The position $w(t)$ of the tagged particle satisfies a functional CLT, with positive definite covariance matrix $S(\rho)$ given by

$$\langle S(\rho)\xi, \xi \rangle = \inf_f \left[ \int \left[ \sum_z \pi(z)(1 - \eta(z))(\tau_z f - f - \langle \xi, z \rangle)^2 + \frac{1}{2} \sum_{x,y} \pi(y-x)(f(y^x,y) - f(\eta))^2 \right] d\mu_{\rho} \right]$$
First we need to prove, for each vector $\xi \in \mathbb{R}^d$, a bound of the form
\[
| \int \sum_z \langle z, \xi \rangle (1 - \eta(z))\pi(z)f(\eta)d\mu_\rho | \leq \sqrt{C(\xi)}\sqrt{D_\rho(f)}
\]
We can rewrite, after combining the $z$ and $-z$ terms and symmetrizing
\[
E^{\mu_\rho} \left[ \sum_z \langle z, \xi \rangle (1 - \eta(z))\pi(z)f(\eta) \right]
= \frac{1}{2} E^{\mu_\rho} \left[ \sum_z \langle z, \xi \rangle [(1 - \eta(z)) - (1 - \eta(-z))]\pi(z)f(\eta) \right]
= \frac{1}{2} E^{\mu_\rho} \left[ \sum_z \langle z, \xi \rangle [1 - \eta(z)]\pi(z)[f(\eta) - f(T_z\eta)] \right]
\]
\[
\leq \frac{1}{2} \left[ E^{\mu_\rho} \left[ \sum_z |\langle z, \xi \rangle|^2[1 - \eta(z)]\pi(z) \right] \right]^{\frac{1}{2}} \left[ E^{\mu_\rho} \left[ \sum_z [1 - \eta(z)]\pi(z)[f(\eta) - f(T_z\eta)]^2 \right] \right]^{\frac{1}{2}}
\leq \sqrt{C(\xi)}\sqrt{D_\rho(f)}
\]
with
\[
C(\xi) = \frac{1 - \rho}{4} \sum_z |\langle z, \xi \rangle|^2\pi(z)
\]
This proves the validity of functional CLT for $w(t)$ with an upper bound on the variance.

The next step is to establish the formula and a lower bound for it. Let us compute $\langle S(\rho)\xi, \xi \rangle$. The minimizer $f = f_\xi$ may not exist. The space $H_1$ of functions $u \in L_2$, with the Dirichlet inner product, when completed, will admit objects that are not in $L_2(\mu_\rho)$. There is no Poincaré inequality available. Abstractly the space consists of collections of functions $\{g^{x,y}(\eta)\}, \{g_z\}$, that are the limits in $H_1$ of $\{f(\eta^{x,y}) - f(\eta)\}, (1 - \eta(z))[f(T_z\eta) - f(\eta)]$. The functions $g^{x,y}(\eta), g_z$ satisfy identities. $g^{x,y}$ is 0 unless $\eta(x) \neq \eta(y)$ and satisfies $\eta^{x,y} + \eta^{y,x} = 0$. Similarly $g_z$ is nonzero only when $\eta(z) = 0$ and $(1 - \eta(z))g_z(\eta) + (1 - \eta(-z))g_{-z}(T_{-z}\eta) = 0$. The Euler equation for the variational problem is
\[
E^{\mu_\rho} \left[ \sum_z \pi(z)(1 - \eta(z))[g_z(\eta) - \langle \xi, z \rangle][f(T_z\eta) - f(\eta)] \right]
+ \frac{1}{2} E^{\mu_\rho} \left[ \sum_{x,y} \pi(y - x)g^{x,y}(\eta)[f(\eta^{x,y}) - f(\eta)] \right] = 0
\]
for all $f$, which after a bit of calculation, takes the form
\[
V(\eta) + \frac{1}{2} \sum \pi(y - x)g^{x,y} + \sum_z \pi(z)(1 - \eta(z))g_z = 0
\]
w(t) now has the representation

\[
\langle \xi, w(t) \rangle = \int_0^t \langle \xi, V(\eta(s)) \rangle ds + \sum_z \int_0^t \langle \xi, z \rangle (1 - \eta(z))dM_z(t)
\]

with

\[
\int_0^t \langle \xi, V(\eta(s)) \rangle ds = a(t) + N(t)
\]

and

\[
N(t) = \sum_z \int_0^t g_z(\eta(s))dM_z(s) + \sum_{x,y} \int_0^t g^{x,y}(\eta(s))dM_{x,y}(t)
\]

with

\[
M_{x,y}(t) = N_{x,y}(t) - \int_0^t \pi(y - x)\eta(s, x)(1 - \eta(y, s))ds
\]

Therefore

\[
\langle \xi, w(t) \rangle = \int_0^t \sum_z \left[ \langle z, \xi \rangle - g_z(\eta(s)) \right]dM_z(s)
\]

\[
- \int_0^t \sum_{x,y} g_{x,y}(\eta(s))dN_{x,y}(s) + a(t)
\]

\[
= M(t) + a(t)
\]

Computing the quadratic variation of the martingale M(t) proves the formula. Finally we will prove the non degeneracy of the quadratic form \( \langle S(\rho)\xi, \xi \rangle \). We have to exclude the one dimensional nearest neighbor case, where \( S(\rho) \equiv 0 \). The proof depends on the following fact. We can obtain an estimate of the form

\[
E^{\mu}[\eta(z) - \eta(-z)f(\eta)] \leq C\sqrt{D_2(f)}
\]

in terms of the Dirichlet form

\[
D_1(u) = \langle -A_1u, u \rangle = \frac{1}{4} E^{\mu}[\sum_{x,y} \pi(y - x)[f(\eta^{x,y}) - f(\eta)]^2]
\]

It is possible to shift a particle from \( z \) to \( -z \) without touching the tagged particle at 0. Jump over it or go around it. This provides an estimate of the form

\[
E^{\mu}[\eta(z) - \eta(-z)f(\eta)] \leq C(z) \left[ E^{\mu}[\sum_{x,y} \pi(y - x)[f(\eta^{x,y}) - f(\eta)]^2] \right]^\frac{1}{2} \tag{5.5}
\]
We can estimate, for any \( a > 0 \),
\[
\langle (\lambda I - \mathcal{A})^{-1} (V, \xi), (V, \xi) \rangle \leq \sqrt{\langle (-\mathcal{A}_1 (\lambda I - \mathcal{A})^{-1} (V, \xi), (\lambda I - \mathcal{A})^{-1} (V, \xi) \rangle} \sqrt{\langle (-\mathcal{A}_1)^{-1} (V, \xi), (V, \xi) \rangle}
\]
\[
\leq \frac{a}{2} \langle (-\mathcal{A}_1 (\lambda I - \mathcal{A})^{-1} (V, \xi), (\lambda I - \mathcal{A})^{-1} (V, \xi) \rangle + \frac{1}{2a} \langle (-\mathcal{A}_1)^{-1} (V, \xi), (V, \xi) \rangle
\]

Letting \( \lambda \to 0 \),
\[
\langle S(\rho) \xi, \xi \rangle \geq \langle (-\mathcal{A}_1)^{-1} (V, \xi), (-\mathcal{A})^{-1} (V, \xi) \rangle \geq \frac{2}{a} \langle (-\mathcal{A})^{-1} (V, \xi), (V, \xi) \rangle - \frac{1}{a^2} \langle (-\mathcal{A}_1)^{-1} (V, \xi), (V, \xi) \rangle
\]

We can obtain a lower bound for the first quadratic form on the right form the variational formula
\[
\langle (-\mathcal{A})^{-1} g, g \rangle = \sup_f \left[ 2 \langle g, f \rangle - \langle -\mathcal{A} f, f \rangle \right]
\]
and an upper bound for the second one from (5.5). Picking \( a \) large will do it.