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 ρ. The distribution is the Bernoulli distribution μ_ρ 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

$$\mathcal{A}_1 = \frac{1}{2} \sum_{x,y \neq 0} \pi(y-x)[f(\eta^{x,y}) - f(\eta)] \tag{5.1}$$

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

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

contributing to the generator the term

$$\mathcal{A}_2 = \sum_z \pi(z)(1-\eta(z))[f(T_z\eta) - f(\eta)] \tag{5.2}$$

The full generator is therefore

$$\begin{aligned}(\mathcal{A}f)(\eta) &= \frac{1}{2} \sum_{x,y \neq 0} \pi(y-x)[f(\eta^{x,y}) - f(\eta)] \\ &\qquad + \sum_z \pi(z)(1-\eta(z))[f(T_z\eta) - f(\eta)] \\ &= (\mathcal{A}_1 f)(\eta) + (\mathcal{A}_2 f)(\eta)\end{aligned} \tag{5.3}$$

It is not difficult to check that the probability distribution μ_ρ on $\mathbb{Z}^d - \{0\}$ is a reversible invariant distribution for $\mathcal{A}$ given by 5.3. The jumps $x \to y$ and $y \to x$ as well as T_z and T_{-z} provide pairs with detail balance. The rates are same in either direction and μ_ρ 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 $\mathcal{A}$ and a reversible ergodic invariant measure μ for $\mathcal{A}$ 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 $\mathcal{A}$ is the self adjoint generator of the process $-\mathcal{A}$ has a spectral resolution $-\mathcal{A} = \int_0^\infty \sigma E(d\sigma)$. We have the Dirichlet form $\mathcal{D}(f) = \langle -\mathcal{A}f, f\rangle_{L_2(\mu)}$ associated with $\mathcal{A}$. The space $\mathcal{H}_1$ 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 $\mathcal{A}$, ensuring the finiteness of $\mathcal{D}(f)$. The completion will be an abstract space $\mathcal{H}_1$. There will be a dual H_{-1} to $\mathcal{H}_1$ relative to the inner product of $\mathcal{H}_0 = L_2(\mu)$. Formally $\|u\|_{-1} = \langle (-\mathcal{A})^{-1}u, u\rangle$ and

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

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*

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

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 limi theorem follows. Moreover

$$P[\sup_{0\le t\le T} |a(t) \ge c\sqrt{T}] \to 0$$

for every $c > 0$ implying the functional CLT.

For the proof of the theorem we need two lemmas.

Lemma 5.1.2. *Let P be a reversible stationary Markov process with invariant measure μ and generator $\mathcal{A}$. Let $u \in L_2[\mu]$ with $\mathcal{D}(u) = \langle -\mathcal{A}u, u\rangle < \infty$. Then*

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

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

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

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_σ satisfies

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

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 $\sigma = T^{-1}$,

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

We obtain the estimate

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

□

This lemma quantifies the statement that set of singularities of a function u on $\mathbb{R}^d$ that is in the Sobolev space $W_2^1(\mathbb{R}^d)$ 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 $c > 0$*

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

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

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

and

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

and δ 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

$$\begin{aligned}\frac{1}{t}E^P[|\int_0^t f(x(s))ds|^2] &= \frac{1}{t}E^P[\int_0^t\int_0^t f(x(s))f(x(s'))dsds'] \\ &= \frac{2}{t}\int_{0\le s\le s'\le t}\langle T_{s'-s}f,f\rangle dsds' \\ &= 2\int_0^t(1-\frac{s}{t})\langle T_sf,f\rangle ds \\ &\simeq 2\int_0^\infty\langle T_sf,f\rangle ds \\ &= 2\langle(-\mathcal{A})^{-1}f,f\rangle \\ &= 2\sigma^2\end{aligned}$$

Since $\langle T_tf,f\rangle\ge 0$, the convergence has to be absolute. Let us solve the resolvent equation

$$\lambda u_\lambda - \mathcal{A}u_\lambda = f$$

Then $\mathcal{A}u_\lambda = \lambda u_\lambda - f$ 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

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

An easy computation shows that $(\sigma+\lambda)^{-1}\to\sigma^{-1}$ and is dominated by σ^{-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 $\frac{1-e^{-t\sigma}}{t}\le\sigma$ 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 $\lambda = T^{-1}$,

$$\xi_T = \sup_{0\le t\le 1} |\frac{1}{\sqrt{T}}\int_0^{tT} \lambda u_\lambda(s)ds| \le \frac{1}{T}\int_0^T \sqrt{\lambda}|u_\lambda(x(s))|ds$$

and $E[|\xi_T|^2] \to 0$ as $t \to \infty$. To complete the proof we need to show that, with $\lambda = T^{-1}$

$$P[\sup_{0\le t\le T} |u_{\frac{1}{T}}(x(s))| \ge c\sqrt{T}] \to 0$$

We can represent $u_{\frac{1}{T}}$ as $u_\delta + (u_{\frac{1}{T}} - u_\delta)$. By lemma 5.1.3, we have for any $\delta > 0$,

$$\limsup_{T\to\infty} P[\sup_{0\le s\le T} |u_\delta(x(s))| \ge c\sqrt{T}] = 0$$

Moreover

$$\lim_{T\to\infty} \frac{1}{T}\|u_{\frac{1}{T}} - u_\delta\|_2^2 = 0$$

and

$$\lim_{\substack{T\to\infty\\ \delta\to 0}} D(u_{\frac{1}{T}} - u_\delta) = 0$$

They imply that

$$\limsup_{\delta\to 0}\limsup_{T\to\infty} P[\sup_{0\le t\le T} |u_{\frac{1}{T}}(x(s)) - u_\delta(x(s))| \ge c\sqrt{T}] = 0$$

□

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 $w(t) \in Z^d$ and $\eta(\cdot) \in \{0,1\}^{\mathbb{Z}^d - \{0\}}$ is

$$(\tilde{\mathcal{A}}f)(\eta) = \sum_z \pi(z)(1-\eta(z))[f(w+z, T_z\eta) - f(w,\eta)] + (\mathcal{A}f)(w,\eta) \tag{5.4}$$

with $\mathcal{A}$ acting only on η for each w. The $\eta(t,\cdot)$ part is a Markov process by itself and is in equilibrium at density ρ, the distribution being μ_ρ. 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

$$M(t) = \sum_z zM_z(t)$$

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*

$$\langle S(\rho)\xi,\xi\rangle = \inf_f \left[\int [\sum_z \pi(z)(1-\eta(z))(\tau_z f - f - \langle \xi, z\rangle)^2 + \frac{1}{2}\sum_{x,y}\pi(y-x)(f(\eta^{x,y}) - f(\eta))^2]d\mu_\rho\right]$$

First we need to prove, for each vector $\xi \in \mathbb{R}^d$, a bound of the form

$$|\int \sum_z \langle z,\xi\rangle(1-\eta(z))\pi(z)f(\eta)d\mu_\rho| \le \sqrt{C(\xi)}\sqrt{D_\rho(f)}$$

We can rewrite, after combining the z and $-z$ terms and symmetrizing

$$\begin{aligned}
&E^{\mu_\rho}\Big[\sum_z \langle z,\xi\rangle(1-\eta(z))\pi(z)f(\eta)\Big] \\
&\quad=\frac{1}{2}E^{\mu_\rho}\Big[\sum_z \langle z,\xi\rangle[(1-\eta(z))-(1-\eta(-z))]\pi(z)f(\eta)\Big] \\
&\quad=\frac{1}{2}E^{\mu_\rho}\Big[\sum_z \langle z,\xi\rangle[1-\eta(z))]\pi(z)[f(\eta)-f(T_z\eta)]\Big] \\
&\quad\le\frac{1}{2}\Big[E^{\mu_\rho}\Big[\sum_z |\langle z,\xi\rangle|^2[1-\eta(z))]\pi(z)\Big]\Big]^{\frac{1}{2}}\Big[E^{\mu_\rho}\Big[\sum_z [1-\eta(z))]\pi(z)[f(\eta)-f(T_z\eta))]^2\Big]\Big]^{\frac{1}{2}} \\
&\quad\le \sqrt{C(\xi)}\sqrt{\mathcal{D}_\rho(f)}
\end{aligned}$$

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 $\eta(x)\ne\eta(y)$ 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

$$E^{\mu_\rho}[\sum_z \pi(z)(1-\eta(z))[g_z(\eta)-\langle\xi,z\rangle][f(\tau_z\eta)-f(\eta)]] + \frac{1}{2}E^{\mu_\rho}[\sum_{x,y}\pi(y-x)g^{x,y}(\eta)[f(\eta^{x,y})-f(\eta)]]=0$$

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

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

with

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

Therefore

$$\begin{aligned}\langle \xi, w(t)\rangle &= \int_0^t \sum_z [\langle z, \xi\rangle - g_z(\eta(s))] dM_z(s) \\ &\qquad - \int_0^t \sum_{x,y} g_{x,y}(\eta(s)) dN_{x,y}(s) + a(t) \\ &= M(t) + a(t)\end{aligned}$$

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

$$E^{\mu_\rho}[(\eta(z) - \eta(-z)) f(\eta)] \le C\sqrt{\mathcal{D}_2(f)}$$

in terms of the Dirichlet form

$$\mathcal{D}_1(u) = \langle -\mathcal{A}_1 u, u\rangle = \frac{1}{4} E^{\mu_\rho}[\sum_{x,y} \pi(y-x)[f(\eta^{x,y}) - f(\eta)]^2]$$

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

$$E^{\mu_\rho}[(\eta(z) - \eta(-z)) f(\eta)] \le C(z)\big[E^{\mu_\rho} \sum_{x,y} [\pi(y-x)[f(\eta^{x,y}) - f(\eta)]^2]\big]^{\frac{1}{2}} \qquad (5.5)$$

We can estimate, for any $a > 0$,

$$\begin{aligned}\langle(\lambda I - \mathcal{A})^{-1}\langle V,\xi\rangle,\langle V,\xi\rangle\rangle &\le \sqrt{\langle(-\mathcal{A}_1(\lambda I - \mathcal{A})^{-1}\langle V,\xi\rangle,(\lambda I - \mathcal{A})^{-1}\langle V,\xi\rangle\rangle}\sqrt{\langle(-\mathcal{A}_1)^{-1}\langle V,\xi\rangle,\langle V,\xi\rangle\rangle}\\ &\le \frac{a}{2}\langle(-\mathcal{A}_1(\lambda I - \mathcal{A})^{-1}\langle V,\xi\rangle,(\lambda I - \mathcal{A})^{-1}\langle V,\xi\rangle\rangle + \frac{1}{2a}\langle(-\mathcal{A}_1)^{-1}\langle V,\xi\rangle,\langle V,\xi\rangle\rangle\end{aligned}$$

Letting $\lambda \to 0$,

$$\langle S(\rho)\xi,\xi\rangle \ge \langle(-\mathcal{A}_1(-\mathcal{A})^{-1}\langle V,\xi\rangle,(-\mathcal{A})^{-1}\langle V,\xi\rangle\rangle \ge \frac{2}{a}\langle(-\mathcal{A})^{-1}\langle V,\xi\rangle,\langle V,\xi\rangle\rangle - \frac{1}{a^2}\langle(-\mathcal{A}_1)^{-1}\langle V,\xi\rangle,\langle V,\xi\rangle\rangle$$

We can obtain a lower bound for the first quadratic form on the right form the variational formula

$$\langle(-\mathcal{A})^{-1}g,g\rangle = \sup_f \big[2\langle g,f\rangle - \langle -\mathcal{A}f,f\rangle\big]$$

and an upper bound for the second one from (5.5). Picking a large will do it.