Complete proof of Proposition 4.2 in Information Loss in Coarse Graining of Polymer Configurations via Contact Matrices

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December 3, 2002

Consider simple random walks on $\mathbb{Z}^n$ (SRW) and define the contact matrix $\mathcal{C}$ of a SRW ω by

$$\mathcal{C}_{ij}(\omega) = \begin{cases} 1 & \text{for } |\omega(i) - \omega(j)| = 0, i \neq j \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

Let $\mathbf{C}$ be the set of contact matrices of SRW of length N. Then the number of contact matrices are given by

$$W(N) = |\mathbf{C}| = \sum_{\omega \in \Omega} 1/\deg \mathcal{C}(\omega) = |\Omega| \mathbb{E}(\deg \mathcal{C})^{-1}, \tag{2}$$

where $\mathbb{E}$ is the expectation value with respect to the relevant uniform distribution.

We define the growth factor of the number of contact matrices by

$$\gamma_N = \frac{\ln |\mathbf{C}|}{\ln |\Omega|}. \tag{3}$$

In *Information Loss in Coarse Graining of Polymer Configurations via Contact Matrices* we proved that $\gamma_N \to 1$ as $N \to \infty$. An upper bound for large but finite size system is given in the following proposition.

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Proposition 1. *For all fixed $\varepsilon > 0$, there exists a constant $\kappa' > 0$ such that for N large enough,*

$$\gamma_N \leq 1 - \kappa' \frac{|\ln \mathbb{P}(R_N/N \leq \varepsilon)|}{N}. \tag{4}$$

Let $I_N = N+1-R_N$ be the number of intersections. Consider an interval $J = [k_0, k_1]$ and the subset of random walk with intersection ratio $I_N/N \in J$:

$$\Lambda_N(J) = \{\omega \in \Omega_N \text{ s.t. } I_N(\omega)/N \in J\}. \tag{5}$$

Definition 2. *The mean degeneracy on the subset $\Lambda_N(J)$ is defined by*

$$\langle \deg \mathcal{C} \rangle_J = \frac{|\{\omega \ s.t. \ I_N(\omega)/N \in J\}|}{|\{\mathcal{C}(\omega) \ s.t. \ I_N(\omega)/N \in J\}|} \equiv \frac{|\Lambda_N(J)|}{W(N)_J}, \tag{6}$$

where $W(N)_J$ is the number of contact matrices of random walks with $I_N/N \in J$.

Definition 3. *Let $J = [k_0, k_1]$. We define*

$$d(J) = \liminf_{N \to \infty} \frac{1}{N} \ln \langle \deg \mathcal{C} \rangle_J. \tag{7}$$

The main result of this section is that, for $k_0 < \pi' \equiv \lim_{N\to\infty} \mathbb{E}(I_N)/N$, and $k_0 < k_1 < 1$, the mean degeneracy increases exponentially in N.

Proposition 4. *For SRW on $\mathbb{Z}^n$, $n \geq 2$,*

$$d([k_0, k_1]) > 0 \textit{ for all } k_0 < \pi' \textit{ and } k_0 < k_1 < 1. \tag{8}$$

In order to prove Proposition 4 we need the following proposition. First let us introduce some notations. We divide $\mathbb{Z}^n$ into disjoint n-cubes of edge length 4. For a $\omega \in \Omega_N$, $F(\omega)$ is defined to be the number of free-4-loops (loops of length 4 which are not intersected by the remaining of ω, see configuration P in Figure 1 in the proof of Proposition 5).

Proposition 5. *For SRW on $\mathbb{Z}^n$ and $J = [k_0, k_1]$ with $k_0 < \pi'$ and $k_1 \in (k_0, 1)$, there exists an $\alpha_J > 0$ such that*

$$\beta_J = \liminf_{N\to\infty} -\frac{1}{N} \ln \mathbb{P}\{\omega \in \Lambda_N(J) \ s.t. \ F(\omega) \leq \alpha_J N\} > 0. \tag{9}$$

Assuming Proposition 5 we prove Proposition 4.

Proof of Proposition 4. Let us consider $k_0 < \pi'$ and $k_1 \in (k_0, 1)$.

$$\begin{aligned} \frac{W(N)_J}{|\Lambda_N(J)|} &\leq \mathbb{P}\{\omega \in \Lambda_N(J) \text{ s.t. } F(\omega) \leq \alpha_J N\} + \\ + \quad & 2^{-\alpha_J N}\mathbb{P}\{\omega \in \Lambda_N(J) \text{ s.t. } F(\omega) > \alpha_J N\} \leq 2\exp(-\min\{\beta_J, \alpha_J \ln 2\}N) \end{aligned} \tag{10}$$

since the contact matrix of a random walk contains M free-4-loops is at least 2^M times degenerate. But $d(J) = \liminf_{N\to\infty} -\frac{1}{N}\ln(W(N)_J/|\Lambda_N(J)|)$, then by Proposition 5, $d(J) \geq \min\{\beta_J, \alpha_J \ln 2\} > 0$. □

Proof of Proposition 5. It is known that $\mathbb{P}(\omega(n) \neq 0, \forall\, n \geq 1) \simeq \tilde{\pi} = \lim_{N\to\infty} R_N/N$ with $\tilde{\pi} \in (0,1)$ for $n \geq 3$. Hamana and Kesten in [1] proved, for SRW of $\mathbb{Z}^n$, that $\psi(x) = \lim_{N\to\infty} -\ln \mathbb{P}(R_N \geq Nx)/N$ exists for all x. $0 < \psi(x) < \infty$ for $\tilde{\pi} < x \leq 1$ and $\psi(x)$ is increasing and convex on $[\tilde{\pi}, 1]$. For $0 \leq x \leq \tilde{\pi}$, $\psi(x) = 0$. Since we work with intersection instead of the range of the support, we use the following notations: $\psi'(x) = \psi(1-x)$ and $\pi' = 1 - \tilde{\pi}$.

We consider k_0, k_1 fixed with $k_0 < \pi'$, $k_1 \in (k_0, 1)$ and let $J = [k_0, k_1]$. In what follows we consider only the cubes visited by the random walk. Since $I_N/N \in J$, $R_N/N \geq 1 - k_1 > 0$ and each cube contains 4^n points, therefore there are *at least* $aN = \frac{1-k_1}{4^n}N$ visited cubes for each $\omega \in \Lambda_N(J)$. It is easy to see that *at least* $\frac{a}{2}N$ of these cubes are occupied *at most* by $b = \frac{2}{a} < \infty$ steps.

Consider the set $\Lambda_N^{\alpha N}(J) = \{\omega \in \Lambda_N(J) \text{ s.t. } F(\omega) \leq \alpha N\}$, $\alpha \ll 1$. We do two successive operations one these random walks.

Operation 1: Let $\omega \in \Lambda_N^{\alpha N}(J)$, then $0 < \frac{F(\omega)}{N} = \beta \leq \alpha$. If $\beta = 0$ we do not have to do this operation. At each of these βN occurrences we eliminate the free-4-loop replacing P with L (see Figure 1). We therefore obtain a random walk $\widetilde{\omega}$ of length N with $F(\widetilde{\omega}) = 0$. The intersection

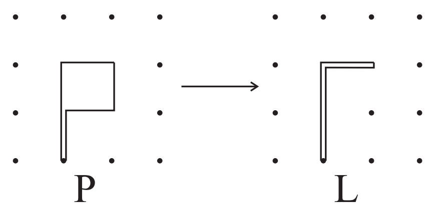

Figure 1: The transformation from the configuration P to L.

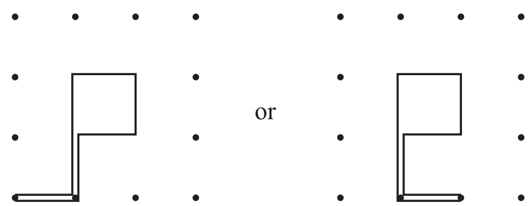

Figure 2: The transformation which adds a 4-loop.

number is changed to $I_N(\widetilde{\omega})/N \in [k_0, k_1+\alpha]$. $\widetilde{\omega}$ is degenerate because can be obtained by different random walks. Two random walks ω_1 and ω_2 change to the same one, i.e. $\widetilde{\omega}_1 = \widetilde{\omega}_2$, if they differs only by the change of some P by L configurations. Let $\gamma N = \#(\text{P in } \omega_1) + \#(\text{L in } \omega_1)$, obviously $\beta \leq \gamma \leq 1$. There are $\binom{\gamma N}{\beta N}$ possible ω changed to the same $\widetilde{\omega}$. By Stirling's formula $\binom{\gamma N}{\beta N} \simeq e^{A(\gamma,\beta)N}$ with $A(\gamma,\beta) = \gamma \ln\gamma - \beta\ln\beta - (\gamma-\beta)\ln(\gamma-\beta)$ and $0 \leq \beta \leq \alpha$, $\beta \leq \gamma \leq 1$. $A(\gamma,\beta)$ remains bounded by $-\beta\ln\beta + \mathcal{O}(\beta) \leq -\frac{3}{2}\beta\ln\beta \leq -\frac{3}{2}\alpha\ln\alpha$, and for $\beta \leq \alpha \ll 1$, therefore the resulting random walk do not have free-4-loops and are *at most* $e^{-N\frac{3}{2}\alpha\ln\alpha}$ degenerate. Thus we have constructed *at least* $|\Lambda_N^{\alpha N}(J)|e^{N\frac{3}{2}\alpha\ln\alpha}$ random walks.

Operation 2: Consider a random walk $\widetilde{\omega}$ resulting from Operation 1. Consider the first $\frac{a}{2}N$ cubes with at most $b=\frac{2}{a}$ steps of $\widetilde{\omega}$ and choose $2\alpha N$ out of these (disjointed) cubes. This can be made in $\binom{\frac{a}{2}N}{2\alpha N}$ possibilities. The first time that $\widetilde{\omega}$ passes in one chosen cube, we add a 4-loop as in Figure 2. This uses 8 steps at each time, therefore $N \to N(1+16\alpha)$. $\widetilde{\omega}$ passes in a cube not more than b times and at each time we replace the path inside the chosen cubes by another one of length increased by 2 which remains on the boundary of the cube, leaving the enter and the exit points unchanged. Then $N(1+16\alpha) \to n \in N(1+16\alpha) + [2\cdot 2\alpha N, 2b\cdot 2\alpha N]$ and $I_n/n \leq k_1 + c_2\alpha$, $c_2 = 17+4b$. The resulting random walk, called $\widehat{\omega}$, has $2\alpha N$ free-4-loops in the center of the cubes and is also degenerate because $\widetilde{\omega}_1$ and $\widetilde{\omega}_2$ are modified to the same random walk, i.e. $\widehat{\omega}_1 = \widehat{\omega}_2$, if they differ only in the $2\alpha N$ cubes. Since each cube contains *at most* b steps of the random walk and for each step we have *at most* $2n$ possible places to occupy, then the new random walk are *at most* $C^{\alpha N}$ times degenerate, with $C = (2n)^{2b}$.

We have constructed *at least* $\binom{\frac{a}{2}N}{2\alpha N} C^{-\alpha N} |\Lambda_N^{\alpha N}(J)| e^{N\frac{3}{2}\alpha\ln\alpha}$ random walks of length $n \in [N(1+20\alpha), N(1+c_2\alpha)]$ and $\frac{I_n}{n} \leq k_1 + c_2\alpha$. Therefore

$$\binom{\frac{a}{2}N}{2\alpha N} C^{-\alpha N} |\Lambda_N^{\alpha N}(J)| e^{N\frac{3}{2}\alpha\ln\alpha} \leq \sum_{n=N}^{N(1+c_2\alpha)} |\Lambda_n(J')| \tag{11}$$

with $J' = [k_0, k_1 + c_2\alpha]$. Up to non exponential corrections,

$$|\Lambda_N(J)| \simeq |\Omega_N| (e^{-\psi'(k_1)N} - e^{-\psi'(k_0)N}). \tag{12}$$

But $\psi'(k)$ is convex and strictly increasing for $k < \pi'$ and $\psi'(k) = 0$ for $k \geq \pi'$, then

$$\psi'(k_1 + c_2\alpha) \geq \psi'(k_1) - c_2\alpha Z(k_1) \tag{13}$$

with $Z(k_1) = \frac{\psi'(0)-\psi'(k_1)}{k_1} < \infty$. Then $e^{-\psi'(k_1)N} - e^{-\psi'(k_0)N} \simeq e^{-\psi'(k_1)N}$ and

$$e^{-\psi'(k_1+\alpha c_2)N(1+\alpha c_2)} - e^{-\psi'(k_0)N(1+\alpha c_2)} \leq e^{-\psi'(k_1)N} e^{\alpha N B_1} \tag{14}$$

with $B_1 = c_2 Z(k_1) + c_2^2 \alpha Z(k_1)$. Consequently

$$RHS(11) \simeq (2n)^{N(1+c_2\alpha)} e^{-\psi'(k_1)N} e^{\alpha B_1 N} \text{ and} \tag{15}$$

$$LHS(11) = \binom{\frac{a}{2}N}{2\alpha N} \frac{(2n)^N e^{-\psi'(k_1)N} e^{N\frac{3}{2}\alpha\ln\alpha}}{C^{\alpha N}} \times \mathbb{P}\{\omega \in \Lambda_N(J) \text{ s.t. } F(\omega) \leq \alpha N\}. \tag{16}$$

Taking $\liminf_{N\to\infty} -\frac{\ln eqn(11)}{N}$, we obtain

$$P(\alpha) = \lim_{N\to\infty} -\frac{1}{N}\ln\binom{\frac{a}{2}N}{2\alpha N} + \beta_J - \frac{3}{2}\alpha\ln\alpha + \alpha\ln C - \alpha B \geq 0, \qquad (17)$$

with $B = c_2 \ln 2n - B_1$. Moreover

$$\lim_{N\to\infty} -\frac{1}{N}\ln\binom{\frac{a}{2}N}{2\alpha N} = -\frac{a}{2}\ln\frac{a}{2} + \left(\frac{a}{2} - 2\alpha\right)\ln\left(\frac{a}{2} - 2\alpha\right) + 2\alpha\ln 2\alpha. \quad (18)$$

For α small enough, the hypothesis $\beta_J = 0$ leads to a contradiction because $\lim_{\alpha\to 0} P(\alpha) = 0$ and $\lim_{\alpha\to 0} \frac{d}{d\alpha}P(\alpha) = -\infty$. Therefore $\beta_J > 0$. □

Proof of proposition 1. It is known that that $\mathbb{P}(R_N/N \leq \varepsilon)$ does not go to 0 exponentially fast in N (see e.g. [1]). Let $J_1 = [0, 1-\varepsilon)$ and $J_2 = [1-\varepsilon, 1]$. Then

$$W(N) = W(N)_{J_1} + W(N)_{J_2}. \qquad (19)$$

The terms in the sum are evaluated by

$$W(N)_{J_1} \simeq |\Omega_N| \mathbb{P}(I_N/N \in J_1) e^{-Nd(J_1)} \qquad (20)$$

and

$$W(N)_{J_2} \leq |\Omega_N| \mathbb{P}(R_N/N \leq \varepsilon). \qquad (21)$$

$W(N)_{J_1}/|\Omega_N|$ is exponentially small in N because $d(J_1) > 0$ by Proposition 4. Since $\mathbb{P}(R_N/N \leq \varepsilon)$ is not exponentially small in N, for N large enough,

$$\gamma_N \leq 1 - \frac{1}{2}\frac{\ln \mathbb{P}(R_N/N \leq \varepsilon)}{N \ln(2n)}. \qquad (22)$$

Consequently for N large enough we obtain the desired result with $\kappa' = 1/2\ln(2n)$. □

References

[1] Y. Hamana and H. Kesten, *A large deviation result for the range of random walk and for the Wiener sausage*, Probab Theory Relat Fields,