Stochastic (classical) representations of quantum Hamiltonians

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1 Introduction

Given a Hamiltonian H, we wish to find a corresponding stochastic process whose statistics reveal information about the physics of H. With this correspondence in hand, we have all tools of probability at our disposal to apply to our problem.

To illustrate this technique, our running example will be the ferromagnetic Heisenberg model with a field h on a graph $G = (V, E)$, whose Hamiltonian can be written as

$$H = -\sum_{e\in E} \vec{S}_e - hM^{(3)}, \tag{1.1}$$

where we define, for $e = (i, j) \in E$,

$$\vec{S}_e := 2\vec{S}_i \cdot \vec{S}_j, \qquad M^{(3)} := \sum_{i\in V} S_i^{(3)}. \tag{1.2}$$

$\vec{S}_i, S_i^{(\alpha)}$ for $i \in [|V|], \alpha \in \{0, 1, 2, 3\}$ are the usual spin operators and $M^{(3)}$ represents the magnetization in the z-direction. In terms of the usual Pauli matrices, we can write

$$H = -\frac{1}{2} \sum_{(i,j)\in E} (X_i X_j + Y_i Y_j + Z_i Z_j) - \frac{h}{2} \sum_{i\in V} Z_i. \tag{1.3}$$

It will be useful to write H in yet another way:

$$H = -\sum_{(i,j)\in E} \mathrm{SWAP}_{ij} + \frac{|E|}{2}\mathbb{I} - hM^{(3)}. \tag{1.4}$$

This follows from the identity $X_iX_j + Y_iY_j + Z_iZ_j = 2\,\mathrm{SWAP}_{ij} - \mathbb{I}$.

As an intentional nonsequitor, we describe the Interchange Process, a Markov chain on the symmetric group S_n. Given a graph $G(V,E)$, where the vertices are identified with $1,2,\dots,n = |V|$, the transitions are given as follows: at each time step, pick an edge uniformly at random and apply the corresponding transposition. Let π be the stationary distribution, and consider the slightly modified distribution $\pi'_\theta(\sigma) \propto \theta^{|\sigma|}\pi(\sigma)$, where $|\sigma|$ represents the size of the largest cycle in the cycle decomposition of $\sigma \in S_n$.

Although they are objects from completely separate contexts in physics and math, the Heisenberg model and the Interchange Process are intimately related:[1]

Theorem 1 (Heisenberg - Interchange Process correspondence [Tót93, GUW11])**.** *Let the thermal average of the operator O on the Heisenberg model at inverse temperature β be denoted by*

$$\langle O \rangle := \frac{\mathrm{Tr}\left[Oe^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H}\right]}. \tag{1.5}$$

Then, when $h = 0$,

$$\langle S_i^{(3)} S_j^{(3)} \rangle = \frac{1}{4}\mathbb{P}_{\pi'_2}[i,j \text{ in the same cycle}]. \tag{1.6}$$

This remarkable result shows that knowledge about this simple-to-describe and well-studied classical Markov chain carries information about a noncommuting, highly complex physical system. Namely, the existence of large cycles in π'_2 implies high magnetic ordering in the Heisenberg model. A few other references the reader might find useful include [AN94, Iof09, Uel13, Bjö16, Pou22, Bjö15].

2 The connection from quantum to classical-stochastic

To see how stochastic processes come about, we will need a few lemmas.

Lemma 2.1 (Duhamel's identity)**.** *Let A, B be square matrices and $t \geq 0$. Then*

$$e^{(A+B)t} = e^{tA} + \int_0^t e^{sA} B e^{(t-s)(A+B)}\, \mathrm{d}s. \tag{2.1}$$

Corollary 2.2 (Duhamel infinite series expansion)**.** *Let A, B be square matrices and $t \geq 0$. We have the following series expansion:*

$$e^{(A+B)t} = e^{tA} + \sum_{k=1}^{\infty} \int_{0<t_1<\cdots<t_k<t} \mathrm{d}t_1 \cdots \mathrm{d}t_k e^{t_1 A} B e^{(t_2-t_1)A} B \cdots B e^{(t-t_k)A}. \tag{2.2}$$

The proof of Lemma 2.1 and Corollary 2.2 can be found in Appendix A.1.

Remark 2.3. We will compactify the notation and write

$$e^{(A+B)t} = \sum_{k=0}^{\infty} \int_{0<t_1<\cdots<t_k<t} \mathrm{d}t_1 \cdots \mathrm{d}t_k e^{t_1 A} B e^{(t_2-t_1)A} B \cdots B e^{(t-t_k)A}, \tag{2.3}$$

with the appropriate convention for the $k = 0$ term.

To illustrate our technique, let's compute the partition function

$$\mathrm{Tr}\, e^{-\beta H} = e^{-\frac{\beta |E|}{2}}\, \mathrm{Tr}\, e^{\beta \sum_{e\in E} \mathrm{SWAP}_e + \beta h M^{(3)}}. \tag{2.4}$$

[1] I have swept a few technical details under the rug, for instance the distinction between discrete- and continuous-time Interchange Process.

We apply Corollary 2.2 to the exponential with $A = hM^{(3)}$, $B = \sum_{e\in E} \mathrm{SWAP}_e$ and $t = \beta$ get

$$e^{-\beta H} = e^{-\frac{\beta|E|}{2}} \sum_{k=0}^{\infty} \int_{0<t_1<\cdots<t_k<\beta} e^{t_1 hM^{(3)}} \left(\sum_{e\in E} \mathrm{SWAP}_e\right) e^{(t_2-t_1)hM^{(3)}} \left(\sum_{e\in E} \mathrm{SWAP}_e\right) \cdots$$
$$\cdots \times \left(\sum_{e\in E} \mathrm{SWAP}_e\right) e^{(\beta-t_k)hM^{(3)}} \, \mathrm{d}t_1 \cdots \mathrm{d}t_k \tag{2.5}$$
$$= e^{-\frac{\beta|E|}{2}} \sum_{k=0}^{\infty} \sum_{e_1,\dots,e_k\in E} \int_{0<t_1<\cdots<t_k<\beta} e^{t_1 hM^{(3)}} \mathrm{SWAP}_{e_1} e^{(t_2-t_1)hM^{(3)}} \mathrm{SWAP}_{e_2} \cdots \mathrm{SWAP}_{e_k} e^{(\beta-t_k)hM^{(3)}} \, \mathrm{d}t_1 \cdots \mathrm{d}t_k. \tag{2.6}$$

Here comes the crux of the technique. We ask ourselves:

Can we interpret this sum as the expectation of some random variable?

It turns out that this expression can be seen as coming from an appropriate collection of Poisson point process. (For the basics on PPPs, see Appendix B.) Namely, for each edge $e \in E$, we instantiate a PPP N_e on $[0, \beta]$ of intensity $\lambda = 1$. For a given $e \in E$, we can interpret the discontinuities of N_e as ticks of a Poisson clock. Taking all instantiations of the PPPs on all edges, we get a collection of edges and times

$$\omega = \{(e_1, t_1), \dots, (e_k, t_k)\}. \tag{2.7}$$

For instance, if edge e_1 clicked at times t_1, t_3, e_2 at t_4 and e_3 at t_2, t_5, then the instance is

$$\omega = \{(e_1, t_1), (e_3, t_2), (e_1, t_3), (e_2, t_4), (e_3, t_5)\}. \tag{2.8}$$

In the literature, an instance is often represented by a space-time diagram $V \times [0, \beta]$, with time on the vertical axis, vertices on the horizontal axis, and the top and bottom identified. We can then decompose the vertices into disjoint, closed paths also called cycles[2], by following along the vertical lines and traversing the edges. For a technically precise definition, see [GUW11, Section 3.1]. For an illustration, see Fig. 1.

We define $C(\omega)$ as the set of all cycles, and given a cycle $\gamma \in C(\omega)$, we define $L(\gamma)$ as its length. Note that $L(\gamma) \in \beta\mathbb{Z}_{\geq 0}$ since every vertical edge is traversed an integer number of times. Additionally, let $\rho(\omega)$ be the measure on the set of edge-time tuples induced by the collection of PPPs $\{N_e : e \in E\}$. Integration against $\rho(\omega)$ can be done as follows.

Proposition 2.4 (Average under the collection of PPPs)**.** *Given a function $f : 2^{E\times[0,\beta]} \to \mathbb{R}$, its average under the collection of PPPs is given by*

$$\mathbb{E}_\omega[f(\omega)] = \sum_{k\geq 0} e^{-\beta|E|} \frac{(\beta|E|)^k}{k!} \mathop{\mathbb{E}}_{e_1,\dots,e_k\sim E} \int_{[0,1]^k} f(\{(e_{\ell_1}, t_1), \dots, (e_{\ell_k}, t_k)\}) \, \mathrm{d}t_1 \cdots \mathrm{d}t_k. \tag{2.9}$$

where we denoted $\omega = \{(e_1, t_1), \dots, (e_k, t_k)\}$.

Proof. Conditioning on $|\omega|$, where $|\omega| \sim \mathrm{Poi}(\beta|E|)$ by Lemma B.2,

$$\mathbb{E}_\omega[f(\omega)] = \sum_{k\geq 0} \mathbb{E}[f(\omega)||\omega| = k] \, \mathbb{P}[|\omega| = k] \tag{2.10}$$
$$= \sum_{k\geq 0} \mathbb{E}[f(\omega)||\omega| = k] e^{-\beta|E|} \frac{(\beta|E|)^k}{k!} \tag{2.11}$$
$$= \sum_{k\geq 0} e^{-\beta|E|} \frac{(\beta|E|)^k}{k!} \mathop{\mathbb{E}}_{e_1,\dots,e_k\sim E} \int_{[0,1]^k} f(\{(e_{\ell_1}, t_1), \dots, (e_{\ell_k}, t_k)\}) \, \mathrm{d}t_1 \cdots \mathrm{d}t_k, \tag{2.12}$$

where we applied Lemma B.3. ☐

[2] Note the overloading of this word. This notion of cycles is slightly different than the cycles from the cycle decomposition of a permutation.

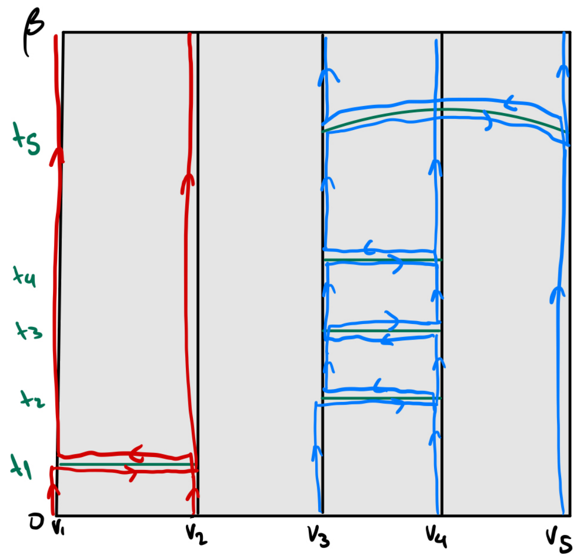

Figure 1: Loop diagram for the instance $\omega = \{((v_1, v_2), t_1), ((v_3, v_4), t_2), ((v_3, v_4), t_3), ((v_3, v_4), t_4), ((v_3, v_5), t_5)\}$. There are two cycles in $C(\omega)$ given by the red and blue paths.

This already looks similar to Eq. (2.6). To see how it is really the same average, we rescale the right-hand side of Eq. (2.6) to write

$$e^{-\beta H} = e^{-\frac{\beta|E|}{2}} \sum_{k=0}^{\infty} |E|^k \mathop{\mathbb{E}}_{e_1,\ldots,e_k \sim E} \int_{0<t_1<\cdots<t_k<\beta} e^{t_1 hM^{(3)}} \mathrm{SWAP}_{e_1} \cdots \mathrm{SWAP}_{e_k} e^{(\beta - t_k)hM^{(3)}} \,\mathrm{d}t_1 \cdots \mathrm{d}t_k. \quad (2.13)$$

Next, we change the integration from the k-hypercube to the k-simplex[3] which picks up a factor of $k!$, followed by a rescaling $t_i \to t_i\beta$, which introduces a factor of β^k:

$$= e^{-\frac{\beta|E|}{2}} \sum_{k=0}^{\infty} \frac{|E|^k}{k!} \mathop{\mathbb{E}}_{e_1,\ldots,e_k \sim E} \int_{[0,\beta]^k} e^{t_1 hM^{(3)}} \mathrm{SWAP}_{e_1} \cdots \mathrm{SWAP}_{e_k} e^{(\beta - t_k)hM^{(3)}} \,\mathrm{d}t_1 \cdots \mathrm{d}t_k \quad (2.14)$$

$$= e^{\frac{\beta|E|}{2}} \sum_{k=0}^{\infty} e^{-\beta|E|} \frac{(\beta|E|)^k}{k!} \mathop{\mathbb{E}}_{e_1,\ldots,e_k \sim E} \int_{[0,1]^k} e^{\beta t_1 hM^{(3)}} \mathrm{SWAP}_{e_1} \cdots \mathrm{SWAP}_{e_k} e^{\beta(1 - t_k)hM^{(3)}} \,\mathrm{d}t_1 \cdots \mathrm{d}t_k. \quad (2.15)$$

By Proposition 2.4, this is exactly the expectation of the collection of PPPs! Hence we may write

$$e^{-\beta H} = e^{\frac{\beta|E|}{2}} \int \mathrm{d}\rho(\omega) e^{\beta t_1 hM^{(3)}} \mathrm{SWAP}_{e_1} \cdots \mathrm{SWAP}_{e_k} e^{\beta(1-t_k)hM^{(3)}}, \quad (2.16)$$

with the same identification in Eq. (2.7).

[3]For this to be valid, f needs to be invariant under permutation of arguments. It is unclear to me why this is true, even looking ahead at Eq. (3.4). However this is the only way I could reproduce the derivation in [GUW11]. Let me know if you see what I'm missing.

3 Stochastic representation of the partition function

With our stochastic representation in hand, we start by computing the partition function. Letting $\{|z\rangle : z \in \{\pm 1\}^n\}$ be the computational basis, we write

$$\operatorname{Tr} e^{-\beta H} = e^{\frac{\beta|E|}{2}} \sum_z \int \mathrm{d}\rho(\omega) \langle z| e^{\beta t_1 h M^{(3)}} \mathrm{SWAP}_{e_1} \cdots \mathrm{SWAP}_{e_k} e^{\beta(1-t_k)hM^{(3)}} |z\rangle \tag{3.1}$$

$$= e^{\frac{\beta|E|}{2}} \sum_z \int \mathrm{d}\rho(\omega) e^{\beta t_1 h M^{(3)}(z)} \langle z^{e_1}| e^{\beta(t_2-t_1)hM^{(3)}} \mathrm{SWAP}_{e_2} \cdots \mathrm{SWAP}_{e_k} e^{\beta(1-t_k)hM^{(3)}} |z\rangle , \tag{3.2}$$

where we used the fact that $|z\rangle$ is an eigenvector of $M^{(3)}$ and denoted by $|z^{e_1}\rangle$ the bitstring z after the permutation of indices given by the transposition corresponding to e_1. Proceeding in this fashion from left to write, we end up with

$$= e^{\frac{\beta|E|}{2}} \sum_z \int \mathrm{d}\rho(\omega) \exp\left[\beta h \sum_{i=1}^n (t_1 z_i + (t_2 - t_1) z_i^{e_1} + \cdots + (1-t_k) z_i^{e_1 \cdots e_k})\right] \langle z^{e_1\cdots e_k}|z\rangle \tag{3.3}$$

$$= e^{\frac{\beta|E|}{2}} \sum_z \int \mathrm{d}\rho(\omega) \exp\left[\beta h \sum_{i=1}^n (t_1 z_i + (t_2 - t_1) z_i^{e_1} + \cdots + (1-t_k) z_i^{e_1 \cdots e_k})\right] \mathbf{1}\{\text{spin constant on cycles}\}, \tag{3.4}$$

where the indicator ensures that each cycle $\gamma \in C(\omega)$ has the same bit ± 1, which we denote $z(\gamma)$. With that constraint, we may do the sum in the exponent cycle by cycle, where all bits are the same, and the telescoping sum is the length of the cycle $L(\gamma)$:

$$\operatorname{Tr} e^{-\beta H} = e^{\frac{\beta|E|}{2}} \sum_z \int \mathrm{d}\rho(\omega) \exp\left[\beta h \sum_{\gamma \in C(\omega)} z(\gamma) L(\gamma)\right] \tag{3.5}$$

$$= e^{\frac{\beta|E|}{2}} \int \mathrm{d}\rho(\omega) 2^{|C(\omega)|} \prod_{\gamma \in C(\omega)} \cosh\left(\beta h L(\gamma)\right). \tag{3.6}$$

4 Proof of Theorem 1

We now have the tools to prove the theorem. Assuming $h = 0$, the partition function Eq. (3.6) simplifies to

$$\operatorname{Tr} e^{-\beta H} = e^{\frac{\beta|E|}{2}} \int \mathrm{d}\rho(\omega) 2^{|C(\omega)|}. \tag{4.1}$$

To compute $\operatorname{Tr}\left[S_i^{(3)} S_j^{(3)} e^{-\beta H}\right]$, we return to Eq. (3.4). The only modifications are that the exponential goes away since $h = 0$, and that we have a factor of $z_i z_j/4$ due to inserting $S_i^{(3)} S_j^{(3)}$ between $\langle z|$ and $e^{\beta t_1 h M^{(3)}}$ in Eq. (3.1):

$$\operatorname{Tr}\left[S_i^{(3)} S_j^{(3)} e^{-\beta H}\right] = \frac{e^{\frac{\beta|E|}{2}}}{4} \sum_z \int \mathrm{d}\rho(\omega) z_i z_j \mathbf{1}\{\text{spin constant on cycles}\}. \tag{4.2}$$

Let γ_i represent the cycle $\gamma \in C(\omega)$ to which the bit i belongs. If $\gamma_i \neq \gamma_j$, the cancellation from the sum over z will lead to zero. Otherwise, $z_i z_j = z_i^2 = 1$, and the sum over z is just the assignment of one of two bits to each cycle:

$$= \frac{e^{\frac{\beta|E|}{2}}}{4} \int \mathrm{d}\rho(\omega) 2^{|C(\omega)|} \mathbf{1}\{\gamma_i = \gamma_j\}. \tag{4.3}$$

Combining these, we get

$$\langle S_i^{(3)} S_j^{(3)} \rangle = \frac{\frac{1}{4}\int \mathrm{d}\rho(\omega) 2^{|C(\omega)|}\mathbf{1}\{\gamma_i = \gamma_j\}}{\int \mathrm{d}\rho(\omega) 2^{|C(\omega)|}} \tag{4.4}$$

$$= \frac{1}{4}\mathbb{P}_{\rho'}[\gamma_i = \gamma_j], \tag{4.5}$$

where the measure ρ' is ρ tilted by the $2^{|C(\omega)|}$ factor.

A Proofs of Duhamel expansions

A.1 Proof 1 of Lemma 2.1

Both sides satisfy the differential equation

$$\frac{\mathrm{d}C(t)}{\mathrm{d}t} = (A+B)C \tag{A.1}$$

with the initial condition $C(0) = \mathbb{I}$.

A.2 Proof 2 of Lemma 2.1

Define $f(s) = e^{(t-s)A}e^{s(A+B)}$. By the Fundamental Theorem of Calculus,

$$e^{t(A+B)} - e^{tA} = f(t) - f(0) \tag{A.2}$$

$$= \int_0^t f'(s)\,\mathrm{d}s \tag{A.3}$$

$$= \int_0^t \left(e^{(t-s)A}(A+B)e^{s(A+B)} - Ae^{(t-s)A}e^{s(A+B)}\right)\mathrm{d}s \tag{A.4}$$

$$= \int_0^t \left(e^{(t-s)A}(A+B)e^{s(A+B)} - e^{(t-s)A}Ae^{s(A+B)}\right)\mathrm{d}s \tag{A.5}$$

$$= \int_0^t e^{(t-s)A}Be^{s(A+B)}\,\mathrm{d}s. \tag{A.6}$$

Setting $s \to s - t$ and rearranging concludes the proof.

A.3 Proof of Corollary 2.2

We may reapply Lemma 2.1 to the right-hand side of Eq. (2.1) to get

$$e^{(A+B)t} = e^{tA} + \int_0^t \mathrm{d}s\, e^{sA}B\left(e^{(t-s)A} + \int_0^{s-t}\mathrm{d}r\, e^{rA}Be^{t-s-r}\right) \tag{A.7}$$

$$= e^{tA} + \int_0^t \mathrm{d}s\, e^{sA}Be^{(t-s)A} + \int_0^t \mathrm{d}s\int_s^t \mathrm{d}r\, e^{sA}Be^{(r-s)A}Be^{(t-r)(A+B)}, \tag{A.8}$$

where we set $r \to r - s$. With N more steps of induction, we get

$$e^{(A+B)t} = e^{tA} + \sum_{k=1}^N \int_{0<t_1<\cdots<t_k<t} \mathrm{d}t_1\cdots\mathrm{d}t_k e^{t_1A}Be^{(t_2-t_1)A}B\cdots Be^{(t-t_k)A}$$
$$+ \int_{0<t_1<\cdots<t_{N+1}<t}\mathrm{d}t_1\cdots\mathrm{d}t_{N+1}e^{t_1A}Be^{(t_2-t_1)A}B\cdots Be^{(t-t_{N+1})(A+B)}. \tag{A.9}$$

The series in the first line is absolutely convergent because the norm of each term is upper-bounded by

$$\left\|\int_{0<t_1<\cdots<t_k<t} \mathrm{d}t_1 \cdots \mathrm{d}t_k e^{t_1 A} B e^{(t_2-t_1)A} B \cdots B e^{(t-t_k)A}\right\| \leq \left|\int_{0<t_1<\cdots<t_k<t} \mathrm{d}t_1 \cdots \mathrm{d}t_k\right| \|B\|^k e^{t\|A\|} \tag{A.10}$$

$$= \frac{\|B\|^k t^k}{k!} e^{t\|A\|}, \tag{A.11}$$

where we used the triangle inequality and the fact that $\left\|e^A\right\| \leq e^{\|A\|}$, also by the triangle inequality. Comparison to the exponential series shows convergence. Finally, the term on the second line is similarly upper-bounded by $\frac{\|B\|^{N+1} t^{N+1}}{(N+1)!} e^{t\|A+B\|}$, which goes to zero as $N \to \infty$.

B Poisson point processes (PPPs)

We recall some basic facts about PPPs. See [DD12] for an introduction or [LP18] for a more rigorous, measure-theoretic exposition.

Definition B.1 (Poisson Point Process)**.** *A* Poisson Point Process *on $X \subseteq \mathbb{R}_{\geq 0}$ with parameter λ is a random function $N\colon X \to \mathbb{Z}_{\geq 0}$ satisfying*

1. *$N(0) = 0$,*
2. *$N(t+s) - N(t) \sim \mathrm{Poi}(\lambda s)$,*
3. *If $0 < t_1 < \cdots < t_k$, then $N(t_2 - t_1), N(t_3 - t_2), \ldots, N(t_k - t_{k-1})$ are independent.*

$\mathrm{Poi}(\lambda)$ *stands for the Poisson distribution with intensity λ.*

This definition is indeed not vacuous since such a process can be constructed by taking exponentially-distributed increments. A useful interpretation is that $N(t)$ represents how many ticks of a Poisson clock happened up to time t, so the discontinuities of N are precisely those times.

Below are some useful facts about Poisson distributions:

Lemma B.2 (Sum of Poissons is Poisson)**.** *Let $X_i \sim \mathrm{Poi}(\lambda_i)$ for $i \in [k]$ independently. Then*

$$\sum_{i=1}^{k} X_i \sim \mathrm{Poi}\left(\sum_{i=1}^{k} \lambda_i\right). \tag{B.1}$$

Proof. It suffices to check the $k = 2$ case. Convolving X_1, X_2, we get

$$\mathbb{P}[X_1 + X_2 = k] = \sum_{m=0}^{\infty} \mathbb{P}[X_1 = m]\mathbb{P}[X_2 = k - m] \tag{B.2}$$

$$= \sum_{m=0}^{\infty} e^{-\lambda_1} \frac{\lambda_1^m}{m!} e^{-\lambda_2} \frac{\lambda_2^{k-m}}{(k-m)!} \tag{B.3}$$

$$= \frac{e^{-(\lambda_1+\lambda_2)}}{k!} \sum_{m=0}^{k} \binom{k}{m} \lambda_1^m \lambda_2^{k-m} \tag{B.4}$$

$$= \frac{e^{-(\lambda_1+\lambda_2)}}{k!} (\lambda_1 + \lambda_2)^k, \tag{B.5}$$

by the Binomial Theorem.

□

Lemma B.3 (Conditioning of Poisson)**.** *If we condition on $N(t) = n$, the clock ticks $t_1, \ldots, t_n$ are uniformly distributed.*

The proof of this lemma relies on the construction of the PPP so we refer the reader to [DD12, Theorem 2.14].

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