Quantum Techniques for Stochastic Mechanics

Project Report

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By

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Abstract

The mathematics underlying the formalisms of 'chemical reaction networks'– which describes the interaction of molecules in a stochastic rather than quantum way – and that of 'stochastic Petri nets' – used to describe collections of randomly interacting entities – is very much like that used in the quantum theory of interacting particles—but modified to use probabilities instead of complex amplitudes. The report draws a a detailed analogy between quantum mechanics and the theory of random processes. To heighten the analogy, the latter is called 'stochastic mechanics'.

To illustrate the analogy, a notation which is similar to that used in Quantum Mechanics is used. This helps in emphasizing both similarities and distinction. The language developed enables us to borrow tools from quantum mechanics into stochastic mechanics. This can be used to express electrical circuits, models from population biology among others. This is a powerful tool which can be used to solve problems, whose solutions may not be easily available in the existing framework of stochastic mechanics.

Acknowledgements

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I would also like to thank my peers, discussions with whom, helped me understand the concepts better.

Contents

Introduction

There is an inherent difference between random processes and quantum mechanics. Events in quantum mechanics are dependant on the "measurement". In stochastic mechanics an observable has no impact on the evolution of the system. There is no uncertainty principle. However, there are many similarities between the two, which could be tapped to use the tools from quantum mechanics in stochastic mechanics.

A language of stochastic mechanics is developed, which highlights the analogy between quantum and stochastic mechanics. The report gives a general recipe to describe any stochastic process as 'petri net' (which is analogous to Feynman's diagrams). Construction of a Hamiltonian using ladder operators from the petri-net is also demonstrated.

A major results in the theory of chemical reaction networks, the 'Anderson–Craciun–Kurtz theorem' is explained using this analogy. The 'Anderson–Craciun–Kurtz theorem' gives conditions under which equilibrium exists when the number of molecules of each kind are treated as discrete, varying in a random way. This is done using a tool borrowed from quantum mechanics: coherent states.

Finally, the analogy is used to draw a parallel between stochastic and quantum mechanics, providing an insight into the differences and the similarities with respect to time evolution, symmetries and conservation laws. This analogy can be used to demystify quantum mechanics theory a bit, and all ideas from quantum mechanics can be applied to biology and chemistry!

Chapter 1

Introduction to Random Processes

1.1 Stochastic Processes

A stochastic process is simply a collection of random variables indexed by time. A discrete time stochastic process $X = \{X_n, n = 0, 1, 2, ...\}$ is a countable collection of random variables indexed by the non-negative integers, and a continuous time stochastic process $X = \{X_t, 0 \leq t < \infty\}$ is an uncountable collection of random variables indexed by the non-negative real numbers.

1.1.1 Examples

Bernoulli process is a sequence of independent and identically distributed random variables, where each random variable takes either the value one or zero, say one with probability p and zero with probability $1-p$. In other words, a Bernoulli process is a sequence of Bernoulli random variables, where each coin flip, probability of head being p, is an example of a Bernoulli trial.

Markov Process is a stochastic process x(t) is called Markov if for every n and $t_1 < t_2 ... < t_n$, we have $P\left(x\left(t_n\right) \leq x_n | x\left(t_{n-1}\right), \ldots, x\left(t_1\right)\right) = P\left(x\left(t_n\right) \leq x_n | x\left(t_{n-1}\right)\right)$, i.e. the current state alone determines the next state.

1.1.2 Formal Definition

Probability Space: A probability space $(\Omega, \mathcal{F}, P)$ is defined as:

- A sample space, Ω, which is the set of all possible outcomes.
- A set of events $\mathcal{F}$, where each event is a set containing zero or more outcomes.
- The assignment of probabilities to the events; that is, a function P from events to probabilities.

Stochastic Process: For a given probability space $(\Omega, \mathcal{F}, P)$, and measurable space (S, Σ) a stochastic process is a collection of S-valued random variables, which can be written as $\{X(t, \omega) : t \in T, \omega \in \Omega \}$

Remark We will always assume that the cardinality of T is infinite, either countable or uncountable. If $T = Z^+$, then we called X a discrete time stochastic process, and if T = $[0, \infty)$, then X is said to be a continuous time stochastic processes.

1.2 Rate Equation

This says how the *expected number* of things of each species changes with time. If we consider large numbers of things, we obtain this simplified deterministic model. Consider an example of the following couples differential equations. These are a special case of the Lotka-Voltera prey predator model.

$$\frac{dx}{dt} = \beta x - \gamma xy$$
$$\frac{dy}{dt} = \gamma xy - \delta y$$

In the above equations, let x(t) be the number of rabbits and let y(t) be the number of wolves at time t.

- We get a term βx in the equation for rabbits, because rabbits are born at a rate equal to the number of rabbits times the birth rate constant β.
- We get a term δy in the equation for wolves, because wolves die at a rate equal to the number of wolves times the death rate constant δ.

- We get a term γxy in the equation for rabbits, because rabbits die at a rate equal to the number of rabbits times the number of wolves times the predation rate constant γ .
- We also get a term γxy in the equation for wolves, because wolves are born at a rate equal to the number of rabbits times the number of wolves times γ.

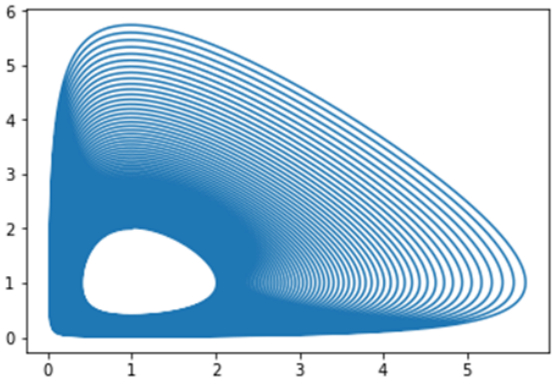

FIGURE 1.1: Simulation of Lotka-Voltera Model for $\beta = \gamma = \delta = 0.1$

Note: In the rate equation, we assume the number of things varies continuously and is known precisely (this matches with the expectation of the species).

1.3 Diagrammatic Representation using a petri net

A stochastic Petri net describes in a very general way how collections of things of different kinds can randomly interact and turn into other things.They are a convenient diagrammatic representations to study complex systems. They are used in molecular biology, population biology and queuing theory amongst others.

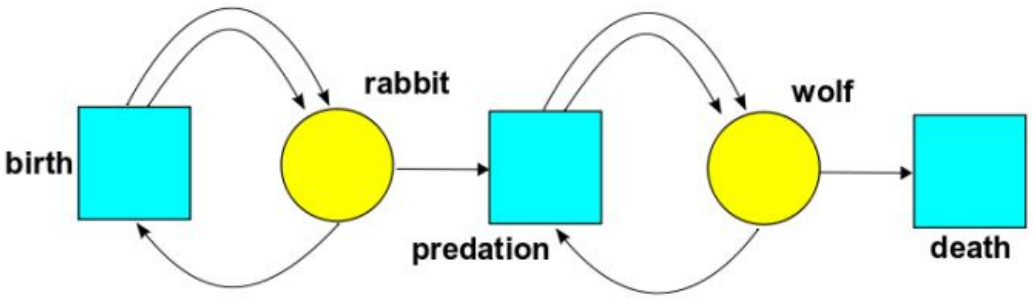

FIGURE 1.2: An example of a Petri net

The above Petri net describes three processes, representing the same rate equation describe previously:

- **Birth:** One rabbit comes in and two go out. This is a caricature of reality: these bunnies reproduce asexually, splitting in two like amoebas.
- **Predation:** One wolf and one rabbit come in and two wolves go out.This is a caricature of how predators need to eat prey to reproduce.
- **Death:** One wolf comes in and nothing goes out (assuming rabbits don't die unless they're eaten by wolves.) This Petri net is a special case of the Lotka-Voltera Prey Predator Model.

1.3.1 Formal Definition

Definition 1 A Petri net is defined by a set S of species and a set T of transitions, together with a function

$$i : S \times T \to \mathbb{N}$$

saying how many copies of each species shows up as input for each transition, and a function

$$o : S \times T \to \mathbb{N}$$

saying how many times it shows up as output.

Definition 2: A stochastic Petri net is a Petri net together with a function

$$r : T \to \mathbb{N}$$

giving a rate constant for each transition

1.3.2 Constructing a Rate Equation

Suppose we have a stochastic Petri net with k species. Let x_i be the number of things of the ith species, then the rate equation is

$$\frac{dx_i}{dt} = \sum_{r \in T} r\,(n_i - m_i)\, x_1^{m_1} \cdots x_k^{m_k}$$

Here the summation is over all the transitions. Similarly, from the rate equation, we can construct the Petri net by drawing one transition per element.

Let us define a vector,

$$x = (x_1, \ldots, x_k)$$

where x_i denote the expectation value of the i^th species at the given time. Similarly, we define an input vector m, and an output vector n as

$$m = (m_1, \ldots, m_k)$$
$$n = (n_1, \ldots, n_k)$$

Furthermore, we define $x^m = x_1^{m_1} \cdots x_k^{m_k}$ which helps us right the rate equation as:

$$\frac{dx}{dt} = \sum_{\tau \in T} r(\tau)(n(\tau) - m(\tau))x^{m(\tau)}$$

where $n(\tau)$ and $m(\tau)$ are the input and output vectors of the transition τ.

Chapter 2

A New Language for Stochastic Mechanics

2.1 Master Equation

While the rate equation served well to give the expectation values, it does not give the information of the probability of say the number of each of the species being $\ell_1, \ldots, \ell_k$. Let us define a k -tuple of natural numbers $\ell = (\ell_1, \ldots, \ell_k)$, giving the *number* of each species. This is different from the state vector in rate equation which merely gave us the expectation values.Let $\psi_\ell(t)$ be the probability that the labelling is ℓ at time t. Then the master equation is given by:

$$\frac{d}{dt}\psi_{\ell'}(t) = \sum_{\ell} H_{\ell'\ell}\psi_\ell(t)$$

for some matrix of real numbers $H_{\ell'\ell}$. called the Hamiltonian. **Note:**In the master equation, we assume the number of things varies discretely and is known only.

2.1.1 The state

Let there be a stochastic Petri net with k different species. Let $\psi_{n_1,\ldots,n_k}$ be the probability that there are n_1 things of the first species, n_2 of the second species, and so on. The following

notation is used – A vector is given as

$$n = (n_1, \ldots, n_k) \in \mathbb{N}^k$$

and

$$\psi_n = \psi_{n_1,\ldots,n_k}$$

. We also define, for any variables z,

$$z^n = z_1^{n_1} \cdots z_k^{n_k}$$

Then any formal power series in these variables will be

$$\Psi = \sum_{n \in \mathbb{N}^k} \psi_n z^n$$

Finally, Ψ a state if the probabilities sum to 1

$$\sum_n \psi_n = 1$$

An example of a state is a monomial:

$$z^n = z_1^{n_1} \cdots z_k^{n_k}$$

This is a state with we are 100% chances that there are n_1 things of the first species, n_2 of the second species, and so on. Hence, this is called a **pure state**. In general the state is mixed.

Master Equation The master equation describes how the probability of having various numbers of species changes with time. In the master equation ψ describes probabilities, so it's a vector in a real vector space. The master equation says how a state evolves in time:

$$\frac{d}{dt}\Psi(t) = H\Psi(t)$$

2.2 Constructing the Hamiltonian

The Hamiltonian is built a linear operator from special operators that annihilate and create things of various species.

2.2.1 Annihilation and Creation Operators

For each state $1 \leq i \leq k$ we have a annihilation operator:

$$a_i \Psi = \frac{d}{dz_i} \Psi$$

and a creation operator:

$$a_i^\dagger \Psi = z_i \Psi$$

Say, if at some time we're 100% sure we have n rabbit, we have so applying the creation operator gives $a^\dagger \Psi = z^{n+1}$. One more rabbit! Now, if we start out with n rabbits: $\Psi = z^n$ and then apply the annihilation operator, we obtain $a\Psi = nz^{n-1}$. The z^{n-1} means we have one fewer rabbit than before. The factor of n means there are n different ways to remove a rabbit. The annihilation operator reduces the number of species by 1, while the creation operator increases by one, for a pure state.
The creation and annihilation operators don't commute:

$$\left(aa^\dagger - a^\dagger a\right) \Psi = \frac{d}{dz}(z\Psi) - z\frac{d}{dz}\Psi = \Psi$$

Hence, if the commutator $[A, B]$ is defined as $AB - BA$,

$$aa^\dagger - a^\dagger a = 1 \implies \left[a, a^\dagger\right] = 1$$

This just means that just says that there's one more way to put a rabbit in a cage of rabbits, and then take one out, than to take one out and then put one in.

2.2.2 Formal Procedure

Given a stochastic Petri net whose set of transitions is T. Now, $r(\tau)$ gives the rate constant of the transition $\tau \in T$,. Let $n(\tau)$ and $m(\tau)$ be the input and output vectors of this transition. Then:

$$H = \sum_{\tau \in T} r(\tau) \left({a^\dagger}^{n(\tau)} - {a^\dagger}^{m}(\tau) \right) a^{m(\tau)}$$

Here, the following shorthand notations have been used:

$$a^{m(\tau)} = a_1^{m_1(\tau)} \cdots a_k^{m_k(\tau)}$$
$$a^{\dagger m(\tau)} = a_1^{\dagger m_1(\tau)} \cdots a_k^{\dagger m_k(\tau)}$$

We can understand the formula as follows: resume=,

- Each transition τ contributes to the Hamiltonian. Each term in the summation corresponds to the contribution from a transition
- Each term is proportional to the rate constant. This is intuitive, since the change in the number of species should be proportional to the rate of change of a process that eats up or produces the given species.
- The term: $a^{\dagger(\tau)} a^{m(\tau)}$ describes how $m_i(\tau)$ things of the ith species get annihilated, and $n_i(\tau)$ things of the ith species get created, for every transition
- The term: $-a^{\dagger m(\tau)} a^{m(\tau)}$ says how the probability that nothing happens - that we remain in the same pure state decreases as time passes. It is a factor added to conserve the sum of probabilities to one.

2.3 Expectation of an Observable

2.3.1 Number Operator

We define the number operator as $N = a^\dagger a$. This is an *observable* which amounts to multiplication by n, the number of species:

$$N z^n = z \frac{d}{dz} z^n = n z^n$$

Rule 1 : For any formal power series Φ

$$\sum a^\dagger \Phi = z\ \Phi|_{z=1} = \Phi|_{z=1} = \sum \Phi$$

Rule 2 : For any formal power series Φ

$$\sum N\Phi = \sum a^\dagger a\Phi = \sum a\Phi$$

These rules are used together with the commutation relation $\left[a, a^\dagger\right] = 1$ and its consequences $[a, N] = a, \quad \left[a^\dagger, N\right] = -a^\dagger$

The expected value of an observable O in the probability distribution Ψ is $\sum O\Psi$, and using the master equation:

$$\frac{d}{dt}\sum O\Psi(t) = \sum O\frac{d}{dt}\Psi(t) = \sum OH\Psi(t)$$

Example: For the Hamiltonian $H = a - N$, and any initial conditions, the master equation predicts that the expected number decays exponentially. This is seen as following: $\frac{d}{dt}\sum N\Psi = \sum NH\Psi = \sum N(a-N)\Psi$ The commutation relation $[a, N] = a$ implies that $Na = aN - a$. So:

$$\sum N(a-N)\Psi = \sum \left(aN - N - N^2\right)\Psi$$

From rule 2:

$$\sum \left(aN - N - N^2\right)\Psi = \sum \left(N^2 - N - N^2\right)\Psi = -\sum N\Psi$$

Hence,

$$\frac{d}{dt}\sum N\Psi = -\sum N\Psi$$

This implies that the expected number decreases exponentially:

$$\sum N\Psi(t) = ce^{-t}$$

2.4 Feynman Diagrams

The solution of the master equation for a state vector Ψ

$$\frac{d}{dt}\Psi(t) = H\Psi(t)$$

is given by

$$\Psi(t) = e^{tH}\Psi(0)$$

Now, assuming the series converges, we can write:

$$e^{tH} = 1 + tH + \frac{(tH)^2}{2!} + \cdots$$

$$\Psi(t) = \Psi(0) + tH\Psi(0) + \frac{t^2}{2!}H^2\Psi(0) + \cdots$$

This can be represented as a sum over Petri nets (Feynman Diagrams). The transitions are represented by a node, and the species by a line. Each term is given as a product of annihilation and creation operators. The Petri net can be constructed as follows: For each transition, draw number of input lines corresponding to the power of annihilation operator and draw output lines corresponding to the power of creation operator.

So, the sum over diagrams represented a sum over histories, each diagram representing a possible history. This idea of sum over histories is borrowed from quantum mechanics.

2.5 Example from Biology

Let's look at an example from population biology: **Amoeba fission and competition** Consider the number of amoebae be given by P, rate of fission be given by α and the rate of competition be given by β. The **rate equation** for the Petri net is given by :

$$\frac{dP}{dt} = \alpha P - \beta P^2$$

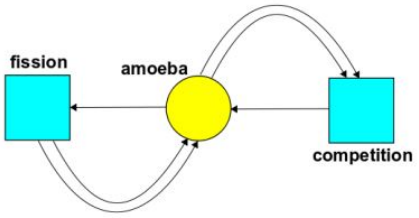

FIGURE 2.1: Petri net for the Model

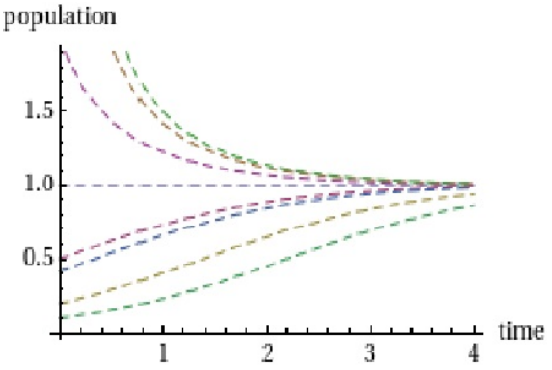

FIGURE 2.2: Population growth in the logistic model

For $\alpha = \beta = 1$, various initial states give the following solution given by the logistic equation (see figure).

The **Master Equation** says:

$$\frac{d}{dt}\Psi(t) = H\Psi(t)$$

where H is an operator on formal power series called the Hamiltonian. We arrive at the following Hamiltonian:

$$H = \alpha\left(a^\dagger a^\dagger a - N\right) + \beta\left(a^\dagger aa - N(N-1)\right)$$

Here, $N = a^\dagger a$ is the number operator.The term containing N is obtained to conserve probability.

FIGURE 2.3: Petri net corresponding to fission and competition respectively

We solve for the **Time evolution**: it's equivalent to $\frac{d}{dt}\left(e^{-tH}\Psi(t)\right) = 0$ so that $e^{-tH}\Psi(t)$ is constant, and so $\Psi(t) = e^{tH}\Psi(0)$

The **Feynman's diagrams** can be obtained as follows:

$$\begin{aligned} e^{tH} &= \sum_{n=0}^{\infty} \frac{1}{n!} t^n H^n \\ &= 1 + tH + \frac{1}{2} t^2 H^2 + \cdots \end{aligned}$$

The first-order terms correspond to the Hamiltonian acting once. These are proportional to either α or β. The second-order terms correspond to the Hamiltonian acting twice. These are proportional to either α^2, $\alpha\beta$ or β^2 and so on. An example of a second order Feynman diagram is as follows– Start with a lone amoeba $\Psi(0) = z$ which then reproduces and splits into two. The resulting amoebas compete and one dies. This is represented by the following term:

$$\frac{\alpha\beta}{2} \left(a^\dagger aa\right) \left(a^\dagger a^\dagger a\right) z$$

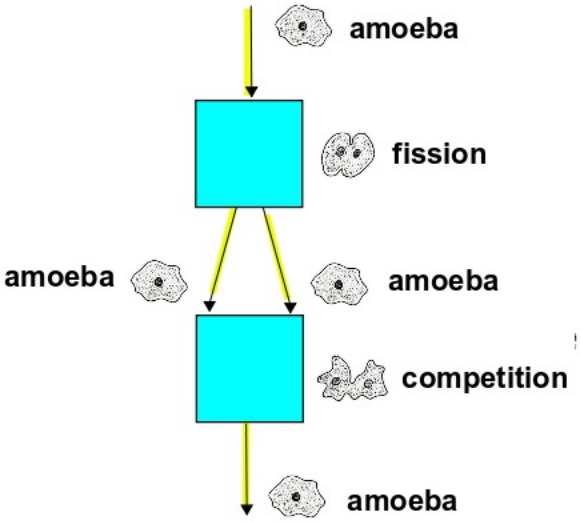

FIGURE 2.4: A typical history (Feynman's diagram)

Chapter 3

Using the Toolkit

With the toolkit we have developed, we put it to test by using it to prove an important result in Stochastic Mechanics– Anderson-Cracuin-Kurtz theorem. This is done using an important concept of quantum mechanics– coherent states. We also prove a stochastic analogue of an important result in quantum mechanics–Noether's theorem

3.1 Anderson-Craciun-Kurtz Theorem

Theorem: Suppose $c \in [0,\infty)^k$ is a **complex balanced equilibrium solution** of the rate equation. Then

$$H\Psi_c = 0$$

The theorem hence gives a way to find equilibrium solutions.

3.1.1 Complex Balance

For our Petri net, the set of complexes is the set $\mathbb{N}^k$, and the complexes of particular interest are the input complex $m(\tau)$ and the output complex $n(\tau)$ of each transition τ. We say a classical state $c \in [0,\infty)^k$ is complex balanced if for all complexes $\kappa \in \mathbb{N}^k$ we have

$$\sum_{\{\tau : m(\tau)=\kappa\}} r(\tau)c^{m(\tau)} = \sum_{\{\tau : n(\tau)=\kappa\}} r(\tau)c^{m(\tau)}$$

Hence, the net rate of production of the complex κ is zero in the classical state c.
If a classical state c is complex balanced, and we set $x(t) = c$ for all t, then $x(t)$ is a solution of the rate equation. Since x(t) doesn't change with time, it is the complex balanced equilibrium solution.

3.2 Proof of Anderson–Craciun–Kurtz Theorem

3.2.1 Coherent States

The uncertainty principle says that$\Delta p \Delta q \geq \hbar/2$ where Δp is the uncertainty in the momentum and Δq is the uncertainty in position. Coherent state is defined as the one in which ΔpΔq is minimum and also Δp=Δq.
For the quantum harmonic oscillator, quantum states can be written as formal power series:

$$\Psi = \sum_{n=0}^{\infty} \psi_n z^n$$

where ψ_n is the amplitude for having n quanta of energy. A coherent state is then given by:

$$\Psi = e^{cz} = \sum_{n=0}^{\infty} \frac{c^n}{n!} z^n$$

where c can be any complex number. The coherent state can be also used for classical stochastic states like amoebas. The coefficient of z^n gives the probability of having n number of the species. Hence, c should be real, and the probabilities should sum to one.

$$\Psi = \frac{e^{cz}}{e^c} = e^{-c} \sum_{n=0}^{\infty} \frac{c^n}{n!} z^n$$

This stochastic coherent state is in fact the Poisson distribution. For any $c \in [0, \infty)^k$ there is a stochastic state called a coherent state, defined by

$$\Psi_c = \frac{e^{cz}}{e^c}$$

Part one of proof

If a classical state c is complex balanced, and we set x(t) = c for all t, then x(t) is a solution of the rate equation

Proof: Assuming c is complex balanced,

$$\begin{aligned}
\sum_{\pi\in T} r(\tau)m(\tau)c^{m(\tau)} &= \sum_{\kappa}\sum_{\tau:m(\tau)=\kappa} r(\tau)m(\tau)c^{m(\tau)} \\
&= \sum_{\kappa}\sum_{\tau:m(\tau)=\kappa} r(\tau)\kappa c^{m(\tau)} \\
&= \sum_{\kappa}\sum_{\tau:n(\tau)=\kappa} r(\tau)\kappa c^{m(\tau)} \\
&= \sum_{\kappa}\sum_{\tau:n(\tau)=\kappa} r(\tau)\kappa c^{m(\tau)} \\
&= \sum_{\kappa}\sum_{\tau:n(\tau)=\kappa} r(\tau)n(\tau)c^{m(\tau)} \\
&= \sum_{\tau\in T} r(\tau)n(\tau)c^{m(\tau)}
\end{aligned}$$

So we have,

$$\sum_{\tau\in T} r(\tau)(n(\tau)-m(\tau))c^{m(\tau)} = 0$$

and thus if x(t) = c for all t, then x(t) is a solution of the rate equation:

$$\frac{dx}{dt} = 0 = \sum_{\tau\in T} r(\tau)(n(\tau)-m(\tau))x^{m(\tau)}$$

Part two of Proof

If we take $\Psi(t) = \Psi_c$ for all times t, the master equation holds: $\frac{d}{dt}\Psi(t) = H\Psi(t)$ So, We just need to show that H $\Psi_c = 0$.Since Ψ_c is a constant times e^{cz} it suffices to show $He^{cz} = 0$.

$$He^{cz} = \sum_{\tau\in T} r(\tau)\left(a^{\dagger n(\tau)} - a^{\dagger m(\tau)}\right)a^{m(\tau)}e^{cz}$$

Since the annihilation operator a_i is given by differentiation with respect to z_i, while the creation operator $a_i^\dagger$ is just multiplying by z_i, we have:

$$He^{cz} = \sum_{\tau \in T} r(\tau) c^{m(\tau)} \left(z^{n(\tau)} - z^{m(\tau)} \right) e^{cz}$$

Expanding out e^{cz}, we get:

$$He^{cz} = \sum_{i \in \mathbb{N}^k} \sum_{\tau \in T} r(\tau) c^{m(\tau)} \left(\frac{c^{i-n(\tau)}}{(i-n(\tau))!} z^i - \frac{c^{i-m(\tau)}}{(i-m(\tau))!} z^i \right)$$

Splitting the sum over T according to output and then input complexes, making use of the complex balanced condition:

$$\begin{aligned}
\sum_{i \in \mathbb{N}^k} \sum_{\kappa \in \mathbb{N}^k} \sum_{\tau : n(\tau) = \kappa} r(\tau) c^{m(\tau)} \frac{c^{i-n(\tau)}}{(i-n(\tau))!} z^i &= \sum_{i \in \mathbb{N}^k} \sum_{\kappa \in \mathbb{N}^k} \frac{c^{i-\kappa}}{(i-\kappa)!} z^i \sum_{\tau : n(\tau) = \kappa} r(\tau) c^{m(\tau)} \\
&= \sum_{i \in \mathbb{N}^k} \sum_{\kappa \in \mathbb{N}^k} \frac{c^{i-\kappa}}{(i-\kappa)!} z^i \sum_{\tau : m(\tau) = \kappa} r(\tau) c^{m(\tau)} \\
&= \sum_{i \in \mathbb{N}^k} \sum_{\kappa \in \mathbb{N}^k} \sum_{\tau : m(\tau) = \kappa} r(\tau) c^{m(\tau)} \frac{c^{i-m(\tau)}}{(i-m(\tau))!} z^i
\end{aligned}$$

Hence proven.

3.3 Noether's Theorem

3.3.1 Noether's Theorem for Quantum Mechanics

Let X be a finite set. Suppose H is a self-adjoint operator on $L^2(X)$, and let O be an observable. Then

$$[O, H] = 0$$

if and only if for all states $\psi(t)$ obeying Schrodinger's equation $\frac{d}{dt}\psi(t) = -iH\psi(t)$ the expected value of O in the state $\psi(t)$ does not change with t.

3.3.2 Markov Processes

Definition: Definition 4. Given a finite set X, a matrix of real numbers

$$H = (H_{ij})_{i,j \in X}$$

is infinitesimal stochastic if $i \neq j \Rightarrow H_{ij} \geq 0$ and

$$\sum_{i \in X} H_{ij} = 0$$

for all $j \in X$. From master equation:

$$\psi(t) = \exp(tH)\psi(0)$$

If H is an infinitesimal stochastic operator, we will call exp (tH) a Markov process, and H its Hamiltonian.

For an infinitesimally stochastic operator H,

$$\int HO\psi(t) = 0$$

and

$$\frac{d}{dt} \int O\psi(t) = \int OH\psi(t)$$

This gives the following **lemma** for any observable O and infinitesimally stochastic operator H:

$$\frac{d}{dt} \int O\psi(t) = \int [O, H]\psi(t)$$

3.3.3 Stochastic Analogue of Noether's Theorem

Suppose H is an infinitesimal stochastic operator and O is an observable. Then

$$[O, H] = 0$$

if and only if

$$\frac{d}{dt}\int O\psi(t) = 0$$

and

$$\frac{d}{dt}\int O^2\psi(t) = 0$$

and for all $\Psi(t)$ obeying the master equation. That is the expected values of O and O^2 in the state $\psi(t)$ do not change with t. Intuitively, an additional condition is that if the system can move from state j to state i, then the observable takes the same value on these two states.

3.4 Proof of Stochastic Noether's Theorem

Forward direction follows trivially from the lemma. For the Backward direction, we assume that

$$\frac{d}{dt}\int O\psi(t) = \frac{d}{dt}\int O^2\psi(t) = 0$$

for all solutions $\psi(t)$ of the master equation. This implies

$$\int OH\psi(t) = \int O^2H\psi(t) = 0$$

or since this holds for all solutions,

$$\sum_{i\in X} O_iH_{ij} = \sum_{i\in X} O_i^2H_{ij} = 0$$

To show that $[O, H] = 0$. O is defined as a diagonal matrix with:

$$O_{ij} = \begin{cases} O_i & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases}$$

So,

$$[O, H]_{ij} = \sum_{k\in X} (O_{ik}H_{kj} - H_{ik}O_{kj}) = O_iH_{ij} - H_{ij}O_j = (O_i - O_j)\, H_{ij}$$

To show this is zero for each pair of elements $i, j \in X$, it suffices to show that when $H_{ij} \neq 0$, then $O_j = O_i$. That is for any $j \in X$

$$\sum_{i \in X} (O_j - O_i)^2 H_{ij} = 0$$

When $i = j, O_j - O_i = 0$, so that term in the sum vanishes. But when $i \neq j, (O_j - O_i)^2$ and H_{ij} are both non-negative − the latter because H is infinitesimal stochastic. So if they sum to zero, they must each be individually zero. Thus for all $i \neq j$, we have $(O_j - O_i)^2 H_{ij} = 0$. But this means that either $O_i = O_j$ or $H_{ij} = 0$, which is what we need to show.

$$\begin{aligned}\sum_{i \in X} (O_j - O_i)^2 H_{ij} &= \sum_i \left(O_j^2 H_{ij} - 2 O_j O_i H_{ij} + O_i^2 H_{ij}\right) \\ &= O_j^2 \sum_i H_{ij} - 2 O_j \sum_i O_i H_{ij} + \sum_i O_i^2 H_{ij}\end{aligned}$$

The three terms here are each zero: the first because H is infinitesimal stochastic, and the latter two by the assumption. Hence proven.

Chapter 4

Parallel Between Quantum Mechanics and Stochastic Mechanics

Quantum and Stochastic Mechanics are inherently different. In stochastic mechanics, there is no uncertainty at play, neither is there a special status for measurement. We look in detail the parallels between the two.

4.1 Probabilities v/s Amplitudes

- In a probabilistic model, we may instead say that the system has a probability $\Psi(x)$ of being in any state $x \in X$. These probabilities are non negative real numbers with

$$\sum_{x \in X} \psi(x) = 1$$

- In a quantum model, we may instead say that the system has an amplitude $\Psi(x)$ of being in any state $x \in X$. These amplitudes are complex numbers with

$$\sum_{x \in X} |\psi(x)|^2 = 1$$

If we replace the sums with integrals, by replacing the set X my a measure space:

- In a probabilistic model, the system has a probability distribution$\psi : X \to \mathbb{R}$ which obeys $\psi \geq 0$ and

$$\int_X \psi(x)dx = 1$$

- In a quantum model, the system has a wave-function $\psi : X \to \mathbb{C}$, which obeys

$$\int_X |\psi(x)|^2 dx = 1$$

4.2 States

- In probability theory, the probability distribution ψ is a vector in the space

$$L^1(X) = \left\{ \psi : X \to \mathbb{C} : \int_X |\psi(x)|dx < \infty \right\}$$

- In quantum theory, the wave-function ψ is a vector in the space

$$L^2(X) = \left\{ \psi : X \to \mathbb{C} : \int_Y |\psi(x)|^2 dx < \infty \right\}$$

- In quantum mechanics we often use this abbreviation:

$$\langle \phi, \psi \rangle = \int \overline{\phi}\psi$$

so that a quantum state has

$$\langle \psi, \psi \rangle = 1$$

- Similarly, we could introduce this notation in stochastic mechanics:

$$\langle \psi \rangle = \int \psi$$

so that a stochastic state has

$$\langle \psi \rangle = 1$$

- In quantum mechanics, $\langle \phi, \psi \rangle$ is well-defined whenever both ϕ and ψ live in the vector space

$$L^2(X) = \left\{ \psi : X \to \mathbb{C} : \int |\psi|^2 < \infty \right\}$$

- In stochastic mechanics, $\langle \psi \rangle$ is well-defined whenever ψ lives in the vector space

$$L^1(X) = \left\{ \psi : X \to \mathbb{R} : \int |\psi| < \infty \right\}$$

4.3 Observables

- In quantum mechanics, an observable is a self-adjoint operator A on $L^2(x)$. In the case where X is a finite set, a self-adjoint operator on $L^2(x)$ is just one with

$$\langle \psi, A\phi \rangle = \langle A\psi, \phi \rangle$$

for all $\psi, \phi \in L^2(X)$. The expected value of an observable A in the state ψ is

$$\langle \psi, A\psi \rangle = \int \overline{\psi} A\psi$$

- In stochastic mechanics, an observable is a real-valued function A on X. The expected value of A in the state ψ is

$$\langle A\psi \rangle = \int A\psi$$

4.4 Time Evolution

- In stochastic mechanics, a stochastic operator is a linear map $U : L^1(X) \to L^1(X) \to L^1(X)$ such that

$$\int U\psi = \int \psi$$

and

$$\psi \geq 0 \Rightarrow U\psi \geq 0$$

for all $\psi \in L^1(X)$. If U is stochastic and ψ is a stochastic state, then $U\psi$ is again a stochastic state.

- In quantum mechanics, an isometry is a linear map $U : L^2(X) \to L^2(X)$ such that

$$\langle U\phi, U\psi \rangle = \langle \phi, \psi \rangle$$

for all $\psi, \phi \in L^2(X)$. If U is an isometry and ψ is a quantum state, then $U\psi$ is again a quantum state.

- In quantum mechanics we are mainly interested in invertible isometries, which are called unitary operators. However time evolution in stochastic mechanics is rarely invertible.

4.5 Infinitesimal stochastic versus self-adjoint operators

- In probability theory we often describe time evolution using a differential equation called the master equation

$$\frac{d}{dt}\psi(t) = H\psi(t)$$

whose solution is

$$\psi(t) = \exp(tH)\psi(0)$$

- In quantum theory we often describe time evolution using a differential equation called Schrodinger's equation

$$i\frac{d}{dt}\psi(t) = H\psi(t)$$

whose solution is

$$\psi(t) = \exp(-itH)\psi(0)$$

In both cases, we call the operator H the Hamiltonian

- In quantum mechanics, H is self adjoint, that is it has the following property

$$\langle H\psi, \phi \rangle = \langle \psi, H\phi \rangle$$

This comes from the condition that $exp(-itH)$ is unitary for all t.

- In stochastic mechanics $exp(tH)$ is stochastic, that is it has the following property

$$\int \exp(tH)\psi = \int \psi$$

and

$$\psi \geq 0 \Rightarrow \exp(tH)\psi \geq 0$$

The two conditions give that H is infinitesimally stochastic. That is:

$$\sum_{i \in X} H_{ij} = 0$$

and

$$H_{ij} \geq 0 \text{ if } i \neq j$$

So, H is infinitesimal stochastic if its columns sum to zero and its off-diagonal entries are non-negative. The idea is that any infinitesimal stochastic operator should be the infinitesimal generator of a stochastic process. This is the major difference between generators of a quantum process and a stochastic process.

Scope of the Project

We have been able to draw a detailed analogy between quantum and stochastic mechanics. A powerful tool to study random processes–Petri nets– have been explored. A more fundamental master equation for the stochastic process has been used, to explain results relating to conserved quantities and equilibrium solutions in stochastic mechanics.

While, a preliminary review of the two concepts of quantum and stochastic mechanics have been done, it has lead to a lot of scope for work. The study suggests a different way to view Quantum and stochastic mechanics. The traditional idea is that quantum theory generalizes classical probability theory by considering observables that don't commute. Instead of looking at quantum mechanics as a super-set of probability theory, which is the the typical view of how quantum mechanics and probability theory come into contact, a possible view could be such that quantum theory does not subsume probability theory, but they intersect. An interesting intersection of the Quantum and stochastic Mechanics lies in Network theory– of electrical circuits! (or in general any graph with positive edges) It would be interesting to explore what new solutions to problems and new insights helping us demystify quantum mechanics are offered by this new point of view.

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