

Modelling Open Quantum Systems

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Fourth Year
MPhys Project

Dec 2020

Give a
More
Instructure
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Abstract

The aim of this project is to study open quantum systems: a quantum mechanical system which is contact with environmental degrees of freedom. The study of such a system is crucial as no real-world quantum systems are completely isolated from their surroundings. Ultimately, our goal is to determine the time evolution of these systems by solving their effective equations of motion, known as master equations, which govern the dynamics of a quantity named the density operator which contains all information about the system observables. Particularly, we study a numerical technique called the quantum jump method which allows for calculation of said density matrix as a stochastic average over many simulated trajectories of the systems wave-function with time. We consider the numerical accuracy and physical interpretation of such a method and apply it for two physical examples: the optical Bloch-equations and the spin-boson model. Finally, we consider entropy production rates for the quantum jump approach.

1. Introduction

All physical quantum systems are comprised of both the system itself and its surrounding environment. Naturally, interactions occur which significantly change the dynamics of the system. Thus, to obtain a complete understanding of real-world quantum systems, a different theoretical framework than that of unitary operators, used to treat closed systems, is required.

Open quantum systems, by ~~their~~ very nature, cannot be in a pure state, i.e a state that completely determines the statistical outcome of a measurement. This motivated the formalism of an object known as the density matrix, an idea initially developed by John von Neumann in 1927 [1], which can describe any state, pure or mixed. The time evolution of such an object is governed by master equations, which are often not soluble and require multiple approximations.

We begin by introducing the mathematical formalism required for studying open-quantum systems, including discussions of the density matrix, interaction picture and a heuristic derivation of the Markovian master equation. We will then go onto consider the numerical method of quantum trajectories originally developed by Dalibard, Castin and Mølmer in the early 1990s [2]. How to apply such a method as a first-order Monte-Carlo algorithm is outlined and demonstrated to be mathematically equivalent to the master equation. The statistical errors involved for the method as well as its physical interpretations will be discussed. The technique is then applied in the case of two illustrative examples, namely the optical Bloch equations and the spin-boson model. Finally, at the end of Section (3) we look at the rate of quantum entropy production which is a combination of the von Neumann entropy and the frequencies of quantum jumps occurring.

2. Theoretical Background

We will first review the theoretical background of unitary time evolution for open quantum systems and derive the Liouville-von Neumann equation in the interaction picture. We will then move onto deriving the master equation.

2.1. Unitary time evolution of closed quantum systems

Note that throughout ~~these notes~~ Plank's constant \hbar will be set to one. According to classical quantum mechanics, the state vector $|\psi(t)\rangle$, which mathematically describes the pure quantum state of an isolated quantum system, is described by a linear partial differential equation known as the Schrödinger equation [3] p; 1]

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \quad (2.1.1)$$

where $H(t)$ is the Hamiltonian of the system. Such an equation can be solved via means of the unitary time-evolution operator, $U(t, t_0)$, which transforms the initial state, $|\psi(t_0)\rangle$, at some initial time t_0 , to a state at time t , $|\psi(t)\rangle$, [4] p; 145]

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle. \quad (2.1.2)$$

For a closed system, the Hamiltonian is time-independent and thus equation (2.1.1) can be readily integrated to give,

$$U(t, t_0) = e^{-iH(t-t_0)}. \quad (2.1.3)$$

In intro could be a bit longer, physical examples?

Applications?

for open quantum systems
or Many-body Systems

textbook?

From this expression it is clear that $U(t, t_0)$ satisfies the condition

$$U(t, t_0)U(t, t_0)^\dagger = U(t, t_0)^\dagger U(t, t_0) = I, \quad (2.1.4)$$

where I is the identity matrix, and hence it is a unitary operator.

In the situation of a time-dependent Hamiltonian, the solution to equation (2.1.1) can be written [5] p; 3]

$$U(t, t_0) = T_{\leftarrow} \exp \left[-i \int_{t_0}^t ds H(s) \right], \quad (2.1.5)$$

where T_{\leftarrow} represents the chronological time ordering operator which orders products of time-dependent operators such that their time-arguments increase in the direction of the arrow, right to left in this case.

2.2. The density operator

An alternative formalism to the language of state vectors is to use what is known as the density operator or density matrix. This formulation is mathematically equivalent, and holds in the case of pure quantum states as above, but is particularly useful when dealing with mixed states, as any state can be represented by a single density matrix [6] p; 99].

The density operator for a system described by a pure state is defined by the equation,

$$\rho(t) \equiv |\psi_i(t)\rangle \langle \psi_i(t)|. \quad (2.2.1)$$

If instead the system is characterised by an ensemble of ~~of state~~ states $|\psi_i(t)\rangle$, the density operator takes its most general form [7] p; 111]

$$\rho(t) \equiv \sum_i \rho_i |\psi(t)\rangle \langle \psi(t)|, \quad (2.2.2)$$

where ρ_i is the probability that the system realises the pure quantum state $|\psi(t)\rangle$. Using equation (2.1.2), this can be re-written as

$$\rho(t) = \sum_i \rho_i U(t, t_0) |\psi(t_0)\rangle \langle \psi(t_0)| U^\dagger(t, t_0) \quad (2.2.3)$$

$$= U(t, t_0) \left[\sum_i \rho_i |\psi(t_0)\rangle \langle \psi(t_0)| \right] U^\dagger(t, t_0), \quad (2.2.4)$$

and thus the density operator evolves in time according to the unitary transformation

$$\rho(t) = U(t, t_0) \rho(t_0) U^\dagger(t, t_0). \quad (2.2.5)$$

Differentiating equation (2.2.5) with respect to time, we obtain an equation of motion for the density operator,

$$\frac{\partial}{\partial t} \rho = -i[H(t), \rho(t)], \quad (2.2.6)$$

which is known as the Liouville-von Neumann equation and governs the evolution of both pure and mixed state density operators for closed systems.

report

The density operator has several useful properties that we will exploit throughout this thesis. Firstly, it is a Hermitian operator, which can be readily seen from equation (2.2.2). It can also be easily shown that the expectation of any general operator, \hat{O} , is given by taking the trace of $\hat{O}\rho$, [5 p; 11]

$$\langle \hat{O} \rangle \equiv \text{Tr} (\hat{O}\rho) = \text{Tr} (\hat{O} |\psi\rangle\langle\psi|) \quad (2.2.7)$$

$$= \sum_n \langle n | \hat{O} |\psi\rangle \langle\psi| n \rangle = \langle\psi| \left(\sum_n |n\rangle\langle n| \right) \hat{O} |\psi\rangle \quad (2.2.8)$$

$$= \langle\psi| \hat{O} |\psi\rangle, \quad (2.2.9)$$

Mixed states?

which is the definition of the expectation of an operator \hat{O} .

2.3. The interaction picture

In the above formalism of the density operator we have worked in what is known as the Schrödinger picture, where we allow the state vectors to evolve with time but the operators are held constant with respect to time. The opposite formalism, where the operators incorporate a time-dependency but the states are time independent, is called the Heisenberg picture [8 pp; 80-81]. There exists an intermediate representation of these two pictures, known as the interaction or Dirac picture, which we will make frequent use of in our derivation of master equation S

To see why this is a useful tool, consider the partitioning of the full Hamiltonian, H ,

$$H = H_0 + H_I, \quad (2.3.1)$$

where H_0 is generally chosen to be simple and exactly soluble, while H_I contains more complex, perturbative terms. Note that H is taken to be time-independent for simplicity, but in general could contain explicit time dependence, for example if the quantum system interacts with a time-varying electric field. In such a case, we include the explicitly time-dependent terms in H_I . We will return to this idea in section REF.

In order for the interaction picture to be physically viable we require that the expectation of operators remains unchanged when changing pictures. Using equations (2.2.5) and (2.2.7) we first write

$$\langle \hat{O}(t) \rangle = \text{Tr} (\hat{O}\rho(t)) = \text{Tr} (\hat{O}U(t, t_0)\rho(t_0)U^\dagger(t, t_0)), \quad (2.3.2)$$

and then split the time-evolution operator as

$$U(t, t_0) \equiv U_0(t, t_0)U_I(t, t_0), \quad (2.3.3)$$

where these time-evolution operators are defined analogously to that of equation (2.1.3). Substituting equation (2.3.3) into equation (2.3.2) gives

$$\langle \hat{O} \rangle = U_0(t, t_0)U_I(t, t_0)\rho(t_0)U_I^\dagger(t, t_0)U_0^\dagger(t, t_0). \quad (2.3.4)$$

Using the following cyclic trace property [9]

$\text{Tr}(U_0^\dagger(t, t_0)U_I^\dagger(t, t_0)U_I(t, t_0)\rho(t_0)U_0(t, t_0))$

$$\text{Tr}(ABC) = \text{Tr}(CAB) = \text{Tr}(BCA), \quad (2.3.5)$$

and defining

$$\hat{O}_I(t) \equiv U_0^\dagger(t, t_0) \hat{O} U_0(t, t_0), \quad (2.3.6)$$

$$\rho_I(t) \equiv U_I(t, t_0) \rho(t_0) U_I^\dagger(t, t_0), \quad (2.3.7)$$

$$= U_0^\dagger(t, t_0) \rho(t) U_0(t, t_0), \quad (2.3.8)$$

we arrive at an equation for operators in the interaction picture

$$\hat{O}_I(t) = U_0^\dagger(t, t_0) \hat{O} U_0(t, t_0), \quad (2.3.9)$$

which evolves with the time-independent free Hamiltonian, H_0 . As in equation (2.2.6), the interaction picture density evolution has Liouville-von Neumann form

$$\frac{\partial \tilde{\rho}(t)}{\partial t} = -i[\tilde{H}(t), \tilde{\rho}(t)], \quad (2.3.10)$$

where we now switch to using the tilde notation to denote objects in the interaction picture. Again, with analogy to equation (2.1.5), if the Hamiltonian has time-dependence the unitary operator can be written

$$U(t, t_0) = T_{\leftarrow} \exp \left[-i \int_{t_0}^t ds \tilde{H}(s) \right]. \quad (2.3.11)$$

2.4. Open Quantum Systems

2.4.1 General Framework *link to previous sections*

In the case of open quantum systems, we consider a system, S , coupled to a large environment, E . In this setup, we partition the Hamiltonian in the following way

$$H = H_S + H_E + H_I, \quad (2.4.1)$$

where

H_S and H_E are the contributions of the system and environment respectively, and describe the coherent dynamics of their relative degrees of freedom. The interaction between the system and the reservoir is represented in H_I . Figure 1 illustrates this idea schematically.

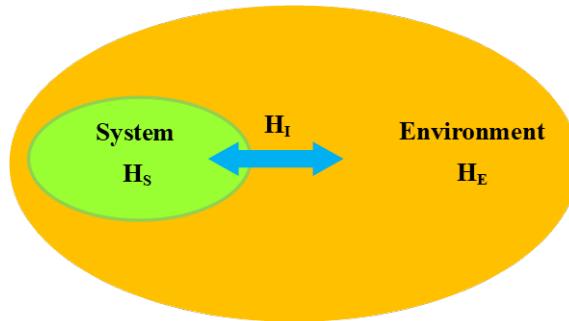


Figure 1: Image showing the general framework of an open quantum system. The open system, S , is the subsystem of a larger combined system, $S + E$, where E represents the environment. The dynamics of the system and environment degrees of freedom are described by their respective Hamiltonians, H_S and H_E , and H_I describes the interaction between the two. This image was created using tools in Microsoft Publisher.

*Caption
formatting*

In what follows we will use what is known as the reduced density operator

$$\rho_s(t) = \text{Tr}_E(\rho(t)), \quad (2.4.2)$$

where we have used the partial trace operation to "trace out" the environmental degrees of freedom. This is useful as ρ_S has dimensions much less than the full density operator while maintaining all information about the system, S . To see this, note that the system and environment are separate Hilbert spaces, thus any observable of our system can be written as a tensor product

$$\hat{O} = \hat{O}_S \otimes \mathbb{1}_E, \quad (2.4.3)$$

where $\mathbb{1}_E$ is the identity. Then using (2.3.2) we can write

$$\langle \hat{O} \rangle = \text{Tr}_{S+E}(\hat{O}_S \otimes \mathbb{1}_E \rho(t)) = \text{Tr}(\hat{O}_S \rho_S(t)), \quad (2.4.4)$$

i.e $\langle \hat{O} \rangle$ is fully described by $\rho_S(t)$.

2.4.2 Markovian master equations

Knowing that $\rho_S(t)$ is the object we wish to work with, we seek an equation that governs its dynamical evolution in order to determine the system's behaviour under the influence of the environment.

We begin by treating the H_0 term in equation (2.4.1) as a small perturbation and make the connection with equation (2.3.1) to identify $H_0 = H_S + H_E$. Equation (2.3.10) can be solved to give

$$\tilde{\rho}(t) = \rho(0) - i \int_0^t ds [\tilde{H}_I(s), \tilde{\rho}(s)], \quad (2.4.5)$$

and then substituting this back into equation (2.3.10) gives

$$\frac{\partial \tilde{\rho}(t)}{\partial t} = -i[\tilde{H}_I(t), \tilde{\rho}(0)] - \int_0^t ds [\tilde{H}_I(t), [\tilde{H}_I(s), \tilde{\rho}(s)]] . \quad (2.4.6)$$

Finally, as noted in section (2.4.1), we take the partial trace over the environment to give

$$\tilde{\rho}_S = \frac{\partial \tilde{\rho}(t)}{\partial t} = -i \text{Tr}_E [\tilde{H}_I(t), \tilde{\rho}(0)] - \int_0^t ds \text{Tr}_E [\tilde{H}_I(t), [\tilde{H}_I(s), \tilde{\rho}(s)]] . \quad (2.4.7)$$

Of course, this equation is still exact, but we can make a number of simplifying assumptions [10, pp; 12-13]:

1. Firstly, at the initial time $t = 0$, we assume that the system and environment can be separated as $\rho(0) = \rho_S(0) \otimes \rho_E(0)$, i.e there are no correlations between the system and the bath.
2. Ultimately, the first term can be taken to be zero by redefining the interaction and system Hamiltonian. *for a thermal environment and linear bosonic operators*
3. The Born approximation extends assumption 1 to all times, $\tilde{\rho}(t) \approx \tilde{\rho}(t) \otimes \rho_E(0)$. Due to the interaction Hamiltonian, some correlations are expected to appear. However, given that we are in the weak coupling regime, and that the environment is large relative to the system, so it is always thermal and decoupled, this approximation is valid.

not decoupled

l. $\text{Tr}(\alpha \rho_E) = 0 = \text{Tr}(\alpha^\dagger \rho_E)$

4. The Markov approximation allows us to replace $\rho_I(t)$ with $\rho_I(s)$, i.e we remove the density operators dependence on its past to make the equation memoryless. So long as the correlation time of the environment is much smaller than the typical time scale for system evolution this is a justified assumption. There remains a dependence on the initial state preparation of the system, but this can be removed via the substitution $s \rightarrow t - s$ and then extending the upper limit of integration to infinity without changing the outcome by means of our previous discussion of timescales.

Through these four approximations, equation (2.4.7) can be written in the form

$$\frac{\partial \tilde{\rho}_S(t)}{\partial t} = - \int_0^\infty ds Tr_E [\tilde{H}_I(t), [\tilde{H}_I(t-s), \tilde{\rho}_S(t) \otimes \rho_E]], \quad (2.4.8)$$

which is known as the weak-coupling Markovian master equation in the interaction picture.

Consider now an interaction Hamiltonian of the form [10, p; 14]

$$H_I = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}, \quad (2.4.9)$$

where A_{α} and B_{α} are the system and environment operators respectively. Again, using equation (2.3.9) we transform to the interaction picture

$$\tilde{H}_I(t) = \sum_{\alpha} A_{\alpha}(t) \otimes B_{\alpha}(t), \quad (2.4.10)$$

where $A_{\alpha}(t) = e^{iH_{St}} A_{\alpha} e^{-iH_{St}}$ and $B_{\alpha}(t) = e^{iH_{Et}} B_{\alpha} e^{-iH_{Et}}$. We also introduce environment correlation functions [5, p; 31],

$$C_{\alpha\beta} = \langle B_{\alpha}(t) B_{\beta}(s) \rangle_E = Tr(B_{\alpha}(t) B_{\beta}(s) \rho_E), \quad (2.4.11)$$

where we have again used equation (2.2.7) to write the expectation as a trace. In the case of a stationary environment, i.e $[H_E, \rho_E] = 0$, it can easily be shown with use of the cyclic trace property states in equation (2.3.5) that *True for Normal State*

$$C_{\alpha\beta} = Tr_E(B_{\alpha}(t-s) B_{\beta} \rho_E) \equiv C_{\alpha\beta}(t-s). \quad (2.4.12)$$

Now, expanding out the commutators in the master equation (2.4.8), substituting in the expression for the decomposed Hamiltonian, \tilde{H}_I , as stated in equation (2.4.10), and using the environment correlation functions in equation (2.4.12), we get

$$\frac{\partial \tilde{\rho}_S(t)}{\partial t} = - \sum_{\alpha\beta} \int_0^\infty d\tau ([A_{\alpha}(t), A_{\beta}(t-\tau) \tilde{\rho}(t)] C_{\alpha\beta} + [\tilde{\rho}_S(t) A_{\beta}(t-\tau), A_{\alpha}(t)] C_{\beta\alpha}(-\tau)), \quad (2.4.13)$$

where we have dropped the tensor direct products to lighten the notation.

To transform this equation back to the interaction picture we first note that, using equation (2.3.9), the density matrix for our system in the interaction picture is

$$\tilde{\rho}_S(t) = e^{iH_{St}} \rho_S(t) e^{-iH_{St}}. \quad (2.4.14)$$

Perhaps explain that trajectories are main focus,
but Master equation solutions useful for comparison

Rearranging this equation and then differentiating with respect to time we get a transformation from the interaction to Schrödinger picture for the evolution of system density matrix

$$\frac{\partial \rho_S(t)}{\partial t} = -i[H_S, \rho_S(t)] + e^{-iH_S t} \left(\frac{\partial \tilde{\rho}_S(t)}{\partial t} \right) e^{iH_S t}. \quad (2.4.15)$$

Finally, we use this equation to transform equation (2.4.13) back to the Schrödinger picture which gives what is known as the Schrödinger picture master equation

$$\begin{aligned} \frac{\partial \rho_S(t)}{\partial t} = & -i[H_S, \rho_S(t)] - \sum_{\alpha\beta} \int_0^{\infty} d\tau ([A_\alpha, A_\beta(-\tau)\rho_S(t)]C_{\alpha\beta}(\tau) \\ & + [\rho_S(t)A_\beta(-\tau), A_\alpha]C_{\beta\alpha}(-\tau)). \end{aligned} \quad (2.4.16)$$

The first term on the left hand generates unitary evolution due to H_S while the remaining terms describe the influence on the environment.

2.4.3 Illustrative examples

To take the Schrödinger picture Born-Markov master equation further we require specific models, unfortunately very few are exactly solvable. Ultimately, we seek to derive equations of Lindbladian form which can then be readily solved. We shall consider two specific examples, both of a two-level system, our system of interest S, interacting with a bath of harmonic oscillators in the first case and a bosonic bath in the second.

2.4.3.1 Optical Bloch equations

In this first model, we consider a driven two-level system interacting with a bath of harmonic oscillators. Physically this could represent for example a two-level atom interacting with a classical laser field. *+ me electromagnetic environment*

We consider partitioning the Hamiltonian as in equation (2.4.1) where the system Hamiltonian is taken to be

$$H_S = \frac{\epsilon}{2}\sigma_z = \frac{\epsilon}{2}(|e\rangle\langle e| - |g\rangle\langle g|), \quad \text{No driving here} \quad (2.4.17)$$

where ϵ is the energy splitting between the excited state, $|e\rangle$, and ground state, $|g\rangle$, of the system. The environment Hamiltonian is given by

$$H_E = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \quad (2.4.18)$$

which is essentially a bath of harmonic oscillators of frequency $\omega_{\mathbf{k}}$, with creation and annihilation operators $b_{\mathbf{k}}^\dagger$ and $b_{\mathbf{k}}$. Finally the interaction Hamiltonian is

$$H_I = \sum_{\mathbf{k}} (g_{\mathbf{k}}\sigma_+ b_{\mathbf{k}} + g_{\mathbf{k}}^*\sigma_- b_{\mathbf{k}}^\dagger), \quad (2.4.19)$$

where $g_{\mathbf{k}}$ and $g_{\mathbf{k}}^*$ are coupling constants.

The details of the derivation are not important, but the idea is to expand the commutators and evaluate the correlation functions of equation (2.4.16), subject to the Hamiltonian's written above. Ultimately, the final result, which is known as the optical master equation, is

$$\frac{\partial \rho_S}{\partial t} = -i \frac{\epsilon'}{2} [\sigma_z, \rho_S] + \Gamma(\epsilon)(N(\epsilon) + 1)(2\sigma_- \rho_S \sigma_+ - \{\sigma_+ \sigma_-, \rho_S\}) + \Gamma(\epsilon)N(\epsilon)(2\sigma_+ \rho_S \sigma_- - \{\sigma_- \sigma_+, \rho_S\}),$$

(2.4.20)

*? Perhaps rephrase this
for
could
neglect the shift?
Maybe
give
a step or
two*

where ϵ' is just a shifted energy scale known as the Lamb shift. $N(\epsilon)$ is the Bose-Einstein occupation number defined by

$$N(\epsilon) = \left(e^{\frac{\epsilon}{k_B T}} - 1 \right)^{-1},$$

(2.4.21)

where T is the bath temperature and k_B is the Boltzmann constant. $\Gamma(\epsilon)$ are rates, in this case defined to be $\Gamma(\epsilon) = J(\epsilon)$, where $J(\epsilon)$ is the spectral density defined by [11] p; 7]

2πJ(ε)?

$$J(\epsilon) = \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \delta(\epsilon - \epsilon_{\mathbf{k}}),$$

(2.4.22)

which describes the density of the bath modes weighted by the square of their individual coupling strength to the system.

The first term of equation (2.4.20) describes coherent system dynamics, the second term describes decay due to both spontaneous and stimulated emission, at rates proportional to $\Gamma(\epsilon)$ and $\Gamma(\epsilon)N(\epsilon)$ respectively, and the third term describes absorption at a rate proportional to $\Gamma(\epsilon)N(\epsilon)$. — *Show the solution or Bloch equations to highlight this.*

To extend this slightly further, we add a driving term to the system Hamiltonian so that it reads

$$H_S = \frac{\epsilon}{2} \sigma_z + \Omega \cos(\omega_l t) \sigma_x,$$

(2.4.23)

where ω_l is the frequency of oscillations and Ω is known as the Rabi frequency, effectively a measure of interaction strength [12]. In this case, we move to a rotating frame and use the rotating-wave approximation, allowing us to ignore fast-oscillating terms [13]. This leads to the optical master equation for a driven system in the rotating frame,

*driving
ignore shift?
to remove time
dependence*

$$\frac{\partial \rho'_S}{\partial t} = -i \frac{\nu'}{2} [\sigma_z, \rho'_S] - i \frac{\Omega}{2} [\sigma_x, \rho'_S] + \Gamma(\epsilon)(N(\epsilon) + 1)(2\sigma_- \rho'_S \sigma_+ - \{\sigma_+ \sigma_-, \rho'_S\}) + \Gamma(\epsilon)N(\epsilon)(2\sigma_+ \rho'_S \sigma_- - \{\sigma_- \sigma_+, \rho'_S\}),$$

(2.4.24)

where the ' notation indicates we are in the rotating frame and ν is the detuning of the driving frequency from resonance, $\nu = \epsilon - \omega_l$ [14] p; 104].

It is possible to cast equation (2.4.24) as the following matrix equation

$$\frac{d}{dt} \begin{pmatrix} \rho'_{ee} \\ \rho'_{ge} \\ \rho'_{eg} \\ \rho'_{gg} \end{pmatrix} = \begin{pmatrix} -2\Gamma(\epsilon)(1+N(\epsilon)) & i\frac{\Omega}{2} & -i\frac{\Omega}{2} & 2\Gamma(\epsilon)N(\epsilon) \\ i\frac{\Omega}{2} & -i\nu' - \Gamma(\epsilon)(2N(\epsilon)+1) & 0 & -i\frac{\Omega}{2} \\ -i\frac{\Omega}{2} & i\frac{\Omega}{2} & i\nu' - \Gamma(\epsilon)(2N(\epsilon)+1) & 0 \\ 2\Gamma(\epsilon)(N(\epsilon)+1) & -i\frac{\Omega}{2} & i\frac{\Omega}{2} & -2\Gamma(\epsilon)N(\epsilon) \end{pmatrix} \begin{pmatrix} \rho'_{ee} \\ \rho'_{ge} \\ \rho'_{eg} \\ \rho'_{gg} \end{pmatrix}.$$

(2.4.25)

In the steady-state case we can then solve ρ_{ee} exactly to be PLACE HOLDER

$$\rho_{ee} = \frac{\frac{1}{4}|\Omega|^2}{\Delta^2 + \frac{1}{4}\Gamma^2 + \frac{1}{2}|\Omega|^2}. \quad (2.4.26)$$

2.4.3.2 Spin-boson model

Now consider the case of a system coupled to a bosonic bath. The total Hamiltonian now reads [15 p; 3]

$$H_{\text{tot}} = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \sigma_z \sum_{\mathbf{k}} g_{\mathbf{k}}(b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}), \quad (2.4.27)$$

where Δ is the tunnelling matrix element.

We switch to the eigenbasis of H_S for convenience, which can be shown to be

$$|+\rangle = \sin\left(\frac{\theta}{2}\right)|g\rangle + \cos\left(\frac{\theta}{2}\right)|e\rangle, \quad (2.4.28)$$

$$|-\rangle = \cos\left(\frac{\theta}{2}\right)|g\rangle - \sin\left(\frac{\theta}{2}\right)|e\rangle, \quad (2.4.29)$$

where $|g\rangle$ and $|e\rangle$ are the z-basis eigenvectors we have previously been using and $\theta = \tan^{-1}\left(\frac{\Delta}{\epsilon}\right)$.

Again, we omit the derivation, which can be found here INSERT REFERENCE, but essentially we evaluate the commutators and correlation functions of equation (2.4.16) to get the master equation in Lindblad form

$$\begin{aligned} \frac{\partial \rho(t)}{\partial t} = & -i[H_s + H_{LS}] + \Gamma_0 \left(P_0 \rho_S(t) P_0 - \frac{1}{2} \{P_0^2, \rho_S(t)\} \right) \\ & + \Gamma(\eta)(1+N(\eta)) \left[P_\eta \rho_S(t) P_\eta^\dagger - \frac{1}{2} \{P_\eta^\dagger P_\eta, \rho_S(t)\} \right] \\ & + \Gamma(\eta)N(\eta) \left[P_\eta^\dagger \rho_S(t) P_\eta - \frac{1}{2} \{P_\eta P_\eta^\dagger, \rho_S(t)\} \right]. \end{aligned} \quad (2.4.30)$$

where $\eta = \sqrt{\epsilon^2 + \Delta^2}$. P_0 and P_η are operators defined in the following manner

$$P_0 = \frac{\epsilon}{\eta} (|+\rangle \langle +| - |-\rangle \langle -|), \quad (2.4.31)$$

$$P_\eta = \frac{\Delta}{\eta} |-\rangle \langle +|. \quad (2.4.32)$$

Γ_0 and $\Gamma\eta$ are the rates defined as

$$\Gamma_0 = 2\pi \lim_{\omega \rightarrow 0} J(\omega)(1+N(\omega)), \quad (2.4.33)$$

$$\Gamma_\eta = 2\pi J(\omega). \quad (2.4.34)$$

Analogously to the optical Bloch equation of (2.4.24), the first term of equation (2.4.30) is a combination of the system and Lamb-shift Hamiltonian's which give rise to coherent dynamics. The remaining terms cause dissipation and decoherence at their respective rates.

ignore?

Say abit more
about the forms?

3. Quantum Trajectories

Quantum trajectory techniques originated in quantum optics and provide a method of numerically solving dissipate dynamics for a system where the density operator is described by a master equation in Lindblad form [16]. The method involves re-writing the master equation as a stochastic average over individual trajectories, which are evolved in time using a numerical technique such as the Monte Carlo method. This has advantages over the alternative of propagating the full density matrix. Most notably, if the space you are working in has dimension N then evolving the full matrix involves evolving an object of size N^2 , whereas the quantum trajectory method requires propagation of the state vectors, which are only of size N . The main drawback is the need to average over multiple samples, but provided the number of samples is less than the size of the space this is still advantageous.

In Sub-section [2.4.3] we derived equations of Lindblad form for two specific cases, namely equations (2.4.24) and (2.4.30), but in general the Markovian master equation, working in natural units with $\hbar = 1$, has a Lindblad form [7]

$$\frac{\partial \rho_S(t)}{\partial t} = -i[H(t), \rho_S(t)] - \frac{1}{2} \sum_m \Gamma_m (c_m^\dagger c_m \rho_S(t) + \rho_S(t) c_m^\dagger - 2c_m \rho_S(t) c_m^\dagger), \quad (3.0.1)$$

where c_m are the Lindblad operators, or jump operators, that describe dissipative dynamics that occur at characteristic rates Γ_m . Equation (3.0.1) can be re-written in the form [17, p; 86],

$$\frac{\partial \rho_S(t)}{\partial t} = -i(H_{\text{eff}} \rho_S(t) - \rho_S(t) H_{\text{eff}}^\dagger) + \sum_m \Gamma_m c_m \rho_S(t) c_m^\dagger, \quad (3.0.2)$$

where the effective Hamiltonian, H_{eff} , is defined as [17, p; 86],

$$H_{\text{eff}} = H_S - \frac{i}{2} \sum_m \Gamma_m c_m^\dagger c_m. \quad (3.0.3)$$

It is this non-Hermitian effective Hamiltonian that we are interested in with regards to quantum trajectories.

3.1. Stochastic averages and quantum mechanical expectation values

stochastic?

An important distinction needs to be made between the stochastic average and the quantum mechanical expectation value of an operator \hat{A} . The expectation of an operator can be determined using the density matrix, ρ , as in equation (2.2.7). If the density matrix can be expanded in terms of pure states, as in equation (2.2.1), then the expectation of \hat{A} can be expanded as

$$\langle A \rangle = \text{Tr}(A\rho) = \sum_i p_i \langle \phi_i | A | \phi_i \rangle \equiv \sum_i p_i A_i \equiv \bar{A}_i, \quad (3.1.1)$$

where $\langle \phi_i | A | \phi_i \rangle$ is the quantum mechanical expectation value and the weighted sum of said value gives the statistical average. In what follows we denote the total expectation of \hat{A} using angled braces, $\langle A \rangle$, and the statistical average with an over-line, \bar{A} .

3.2. First-Order Monte Carlo wavefunction method

For simplicity, we will use a method that is first-order in the time-step, δt , but an equivalent higher order method is outlined in Sub-section (3.5). The algorithm proceeds as follows [17] pp; 88-89]:

1. Choose an initial state, $|\psi(t=0)\rangle$.
2. Take the initial state and propagate it under the effective Hamiltonian to find a candidate state at time $t + \delta t$,

$$|\psi^{(1)}(t + \delta t)\rangle = e^{-iH_{\text{eff}}\delta t} |\psi(t)\rangle \approx (1 - iH_{\text{eff}}\delta t) |\psi(t)\rangle. \quad (3.2.1)$$

3. Compute the norm of the candidate state,

$$\langle \psi^{(1)}(t = \delta t) | \psi^{(1)}(t + \delta t) \rangle = \langle \psi(t) | (1 + iH_{\text{eff}}^\dagger \delta t)(1 - iH_{\text{eff}}\delta t) |\psi(t)\rangle \quad (3.2.2)$$

$$\approx 1 - \delta t \langle \psi(t) | i(H_{\text{eff}} - H_{\text{eff}}^\dagger) |\psi(t)\rangle \quad (3.2.3)$$

$$\equiv 1 - \delta p. \quad (3.2.4)$$

Note that δp can arise from the action of different Lindblad operators, c_m ,

$$\delta p = \delta t \sum_m \langle \psi(t) | c_m^\dagger c_m | \psi(t) \rangle \quad (3.2.5)$$

$$\equiv \sum_m \delta p_m, \quad (3.2.6)$$

where δp_m is the probability that the operator c_m will act in this time-step.

4. Draw a random number, r_1 , between 0 and 1 from a uniform distribution. Then propagate the state statistically in the following way:

- (a) If $r_1 > \delta p$, no jump occurs, and we propagate the state under H_{eff} ,

$$|\psi(t + \delta t)\rangle = \frac{|\psi^{(1)}(t + \delta t)\rangle}{\sqrt{1 - \delta p}}. \quad (3.2.7)$$

This ‘no jump’ situation occurs with probability $1 - \delta p$.

- (b) If $r_1 < \delta p$, a jump occurs, and we choose the particular jump operator to apply by means of the following:

- i. Associate each m with an interval of size proportional to δp_m , normalised to total length one so that each m uniquely corresponds to a range between 0 and 1.
- ii. Draw a second random number, r_2 , again uniformly distributed between 0 and 1.
- iii. Choose the associated c_m for which its assigned interval contains r_2 . The probability to choose such an operator would be

$$\Pi_m = \frac{\delta p_m}{\delta p}. \quad (3.2.8)$$

iv. Apply the chosen operator to propagate the state as

$$|\psi(t + \delta t)\rangle = \frac{c_m |\psi(t)\rangle}{\sqrt{\frac{\delta p_m}{\delta t}}}. \quad (3.2.9)$$

This 'jump' situation occurs with total probability δp .

It is easy to show that this method is equivalent to the master equation as written in equation (3.0.2). First we define the density operator in the usual manner,

$$\sigma(t) = |\phi(t)\rangle \langle \phi(t)|. \quad (3.2.10)$$

Then using equations (3.2.7) and (3.2.9) the statistical average of the density operator is

$$\overline{\sigma(t + \delta t)} = (1 - \delta p) \frac{|\phi^{(1)}(t + \delta t)\rangle \langle \phi^{(1)}(t + \delta t)|}{\sqrt{1 - \delta p}} + \delta p \sum_m \Pi_m \frac{c_m |\phi(t)\rangle \langle \phi(t)| c_m^\dagger}{\sqrt{\frac{\delta p_m}{\delta t}}}, \quad (3.2.11)$$

where we have used the notation convention outlined in Sub-section (3.1). Using the definitions in equations (3.2.10), (3.2.1) and (3.2.8) we obtain

$$\overline{\sigma(t + \delta t)} = \sigma(t) - i\delta t(H_{\text{eff}}\sigma(t) - \sigma(t)H_{\text{eff}}^\dagger) + \delta t \sum_m c_m \sigma(t) c_m^\dagger, \quad (3.2.12)$$

which holds regardless of whether $\sigma(t)$ comprises of pure or mixed states. Rearranging slightly leads to

$$\dot{\sigma}(t) = \lim_{\delta t \rightarrow 0} \left(\frac{\overline{\sigma(t + \delta t)} - \sigma(t)}{\delta t} \right) \quad (3.2.13)$$

$$= -i(H_{\text{eff}}\sigma(t) - \sigma(t)H_{\text{eff}}^\dagger) + \sum_m c_m \sigma(t) c_m^\dagger, \quad (3.2.14)$$

which is identical to equation (3.0.2) demonstrating that taking a stochastic average over trajectories is equivalent to the master equation.

3.3. Statistical errors

3.4. Physical interpretation

3.5. Higher-order methods

3.6. Illustrative Examples

We now look to apply the quantum trajectory technique to the two illustrative examples discussed at the end of Section (2), namely the optical Bloch equations and spin-boson model.

3.6.1 Optical Bloch Equations

Using the optical master in the rotating frame, as stated in equation (2.4.24), and the general form of the Lindbladian master equation, as in equation (3.0.1), we can read off the form of the effective Hamiltonian using equation (3.0.3)

$$H_{\text{eff}} = \frac{\nu'}{2}\sigma_z + \frac{\Omega}{2}\sigma_x - i\Gamma(\epsilon)N(\epsilon)\sigma_-\sigma_+ - i\Gamma(\epsilon)(1+N(\epsilon))\sigma_+\sigma_-.$$
 (3.6.1)

Using this equation and the algorithm outline in Sub-section (3.2) we propagate an initial state forward in time. Two sample trajectories are shown in Figure (2) for the specific case with detuning $\nu' = 0$, Rabi frequency $\Omega = 1$, rate $\Gamma = \frac{\Omega}{6}$, $\epsilon = 1\text{eV}$, a typical optical transition frequency, and temperature $T = 25^\circ$, i.e room temperature. The trajectories undergo Rabi oscillations which are intermittently broken by quantum jumps at random points. A jump to the ground state corresponds to stimulated or spontaneous emission, whereas a jump to the excited state corresponds to absorption.

Jumps?

green Kelvin

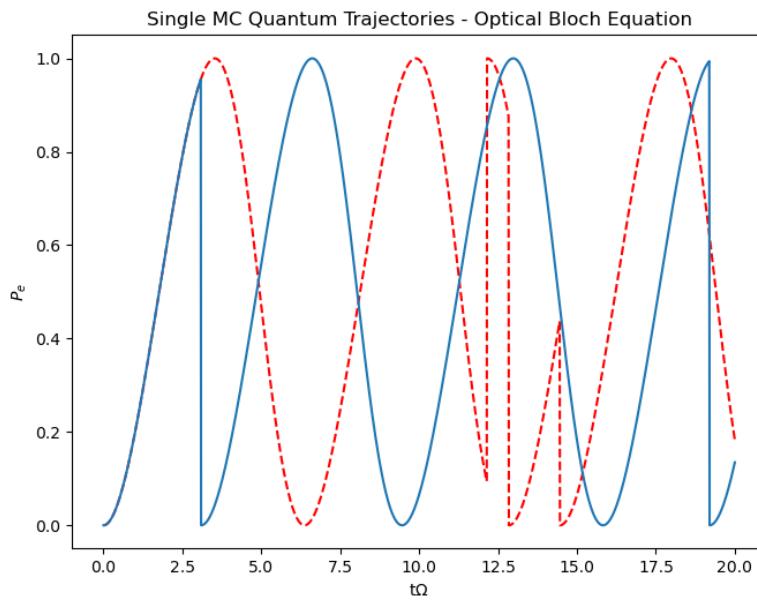


Figure 2: Illustrative example of quantum trajectories for the optical Bloch equations. The plot shows the population of the excited state, i.e the probability to find the atom in the excited state, for two random sample trajectories propagating in time as a function of $t\Omega$. Here we choose detuning $\nu' = 0$, Rabi frequency $\Omega = 1$, rate $\Gamma = \frac{\Omega}{6}$, optical transition frequency $\epsilon = 1\text{eV}$ and temperature $T = 25^\circ$.

We can now repeat this for multiple sample trajectories and take the stochastic average to determine the ensemble behaviour. This is shown in Figure (3). In the long time limit, the average population of the excited states tends to slightly less than 0.5, which physically we interpret as the decay being approximately equal to the pumping.

Due to elevated
temperature

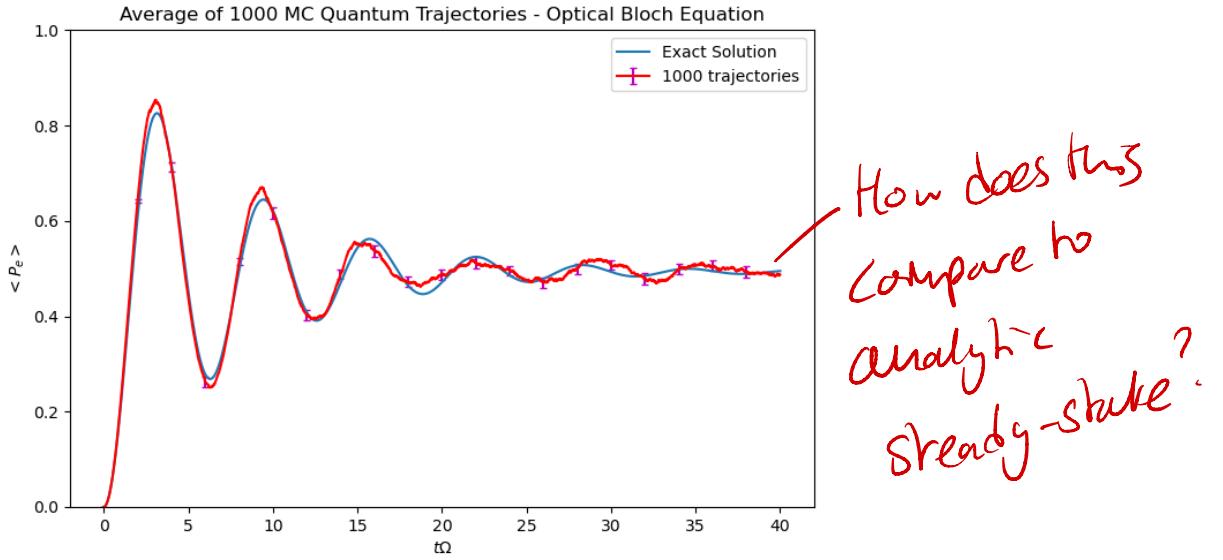


Figure 3: Illustrative example of quantum trajectories for the optical Bloch equations. The plot shows the population of the excited state averaged over 1000 trajectories (red line), compared with the exact solution found from direct integration of the master equation (blue line). Here we choose detuning $\nu' = 0$, Rabi frequency $\Omega = 1$, rate $\Gamma = \frac{\Omega}{6}$ and temperature $T = 25^\circ$. The results agree within the statistical errors, shown as error bars which have been calculated as described in Sub-section (3.3)

3.6.2 Spin-boson model

In an analogous fashion to the analysis of the optical Bloch equations we use the specific form of the master equation in Lindblad form for the spin-boson model, as written in equation (2.4.30), to read off the effective Hamiltonian

$$\begin{aligned} H_{\text{eff}} = H_S - i \frac{\Gamma_0}{2} P_0^2 \\ - i \frac{\Gamma(\eta)}{2} (1 + N(\eta)) P_\eta^\dagger P_\eta \\ - i \frac{\Gamma(\eta)}{2} N(\eta) P_\eta P_\eta^\dagger. \end{aligned} \quad (3.6.2)$$

The H_{LS} term has been ignored as it is usually negligible but could always be absorbed into the original Hamiltonian, just list assumption (2) in the derivation of the Markovian master equation. We require a specific form for Γ_0 and Γ_η , which from equations (2.4.33) and (2.4.34) requires specifying a form for $J(\omega)$. The simplest choice is an Ohmic form, i.e $J(\omega) = \alpha\omega$, where α is the coupling strength. We now re-write the expressions for the rates explicitly as

$$\begin{aligned} \Gamma_0 &= 2\pi \lim_{\omega \rightarrow 0} \alpha\omega(1 + 2N(\omega)) \\ &\approx 2\pi \lim_{\omega \rightarrow 0} \alpha\omega(1 + \frac{2k_B T}{\omega}) \\ &= 4\pi\alpha k_B T, \end{aligned} \quad (3.6.3)$$

Physically justified for an
electromagnetic environment

where we have used the fact that

$$N(\omega) = \frac{1}{e^{\frac{\omega}{k_B T}} - 1} \approx \frac{k_B T}{\omega}. \quad \text{for small } \omega \quad (3.6.4)$$

Similarly,

$$\Gamma(\eta) = 2\pi J(\omega) = 2\pi\alpha\eta. \quad (3.6.5)$$

Choosing similar parameters to our analysis of the optical Bloch equations, we set the bias $\epsilon = 0$, then η becomes equivalent to the tunnelling coefficient Δ which is set to 1. The optical transition frequency is again $\omega = 1\text{eV}$ and $\Gamma = \frac{\Delta}{6}$, so equation (3.6.5) implies that $\alpha = \frac{1}{12\pi}$.

Since we chose to work in the energy eigenbasis rather than the z-basis, we no longer get oscillations like those of Figure (2). Instead our initial state is not affected by propagation under the effective Hamiltonian, it remains as is until a quantum jump occurs, at which time it moves to the other eigenstate. Two random sample trajectories, plotting the excited population with time, are shown in Figure (4), one starting in the ground state (solid blue line) and the other starting in the excited state (dashed red line). Again, repeating averaging over 1000 trajectories we obtain

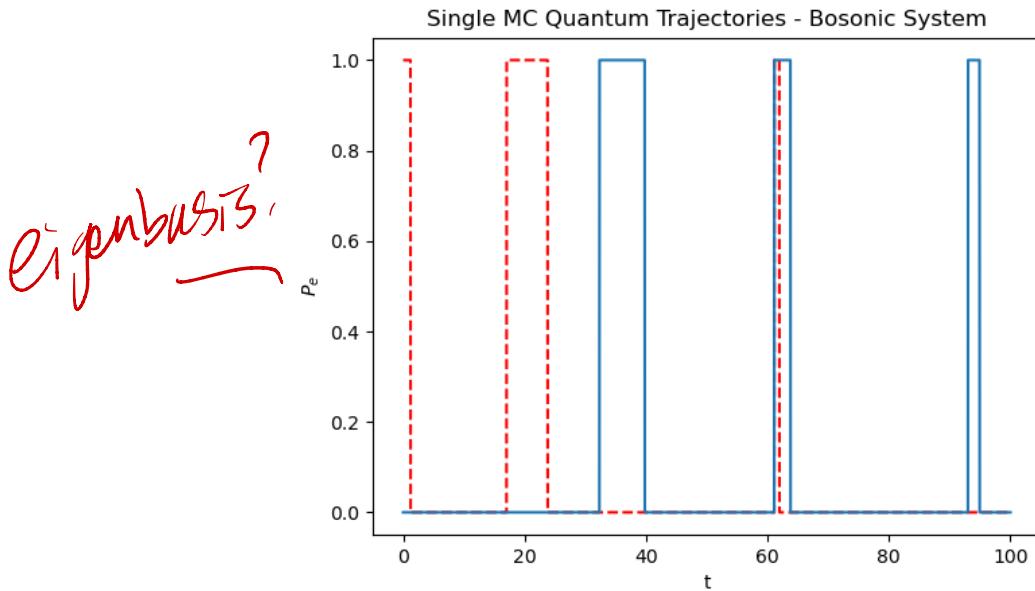


Figure 4: Illustrative example of quantum trajectories for the spin-boson model working in the energy eigenbasis.

The plot shows the population of the excited state for two random sample trajectories propagating in time, one starting in the ground state and one in the excited state. Here we choose detuning $\epsilon = 0$, tunnelling $\Delta = 1$, optical transition frequency $\omega = 1\text{eV}$, coupling strength $\alpha = \frac{1}{12\pi}$ and temperature $T = 5000\text{K}$.

the ensemble behaviour. We see in the long time limit, our bosonic bath thermalises the system.

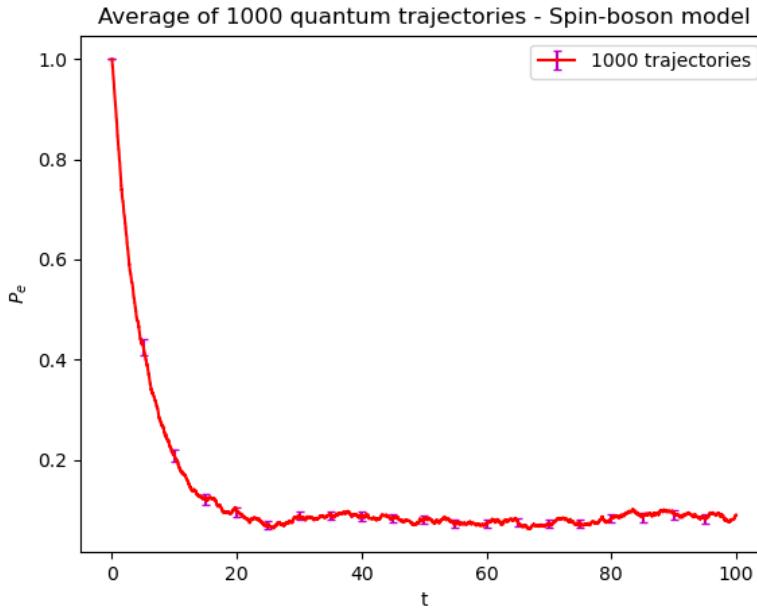


Figure 5: Illustrative example of quantum trajectories for the spin-boson model working in the energy eigenbasis. The plot shows the population of the excited state averaged over 1000 trajectories. Here we choose detuning $\epsilon = 0$, tunnelling $\Delta = 1$, coupling strength $\alpha = \frac{1}{12\pi}$ and temperature $T = 5000K$.

3.7. Entropy

4. Conclusion

5. Length and date

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