Lecture 1: Stochastic Schrodinger Equation

Math Notes **Key Concepts** **Advanced Topics and Extra Details**

Contents

We have previously described the origin of a stochastic equation for open quantum systems starting from a Lindblad equation. In this lecture, we will start from the Schrödinger equation and demonstrate how to derive a stochastic differential equation that for an open quantum system provides an exact solution to the dynamics. The derivation of this is lengthy and a single lecture is insufficient to fully account for the many details involved: my solution to this challenge has been to provide a lecture that will give us an overview of the mathematical approaches used and the key physical insights arising in this derivation. I have combined the broad lecture approach with a set of lecture notes that are, to the best of my ability, a complete (possibly even painfully complete) description of the details.

You could, at this point, ask the question: is it worth this much trouble to talk about stochastic approaches to open quantum systems? I think there are two major reasons why we should answer in the affirmative. First, as I will try to show you in this lecture, stochastic methods can offer physical insights that can enrich our understanding of quantum processes. In addition, as I will discuss in my second lecture, stochastic methods provide a number of numerical advantages for modern research in open quantum systems, particularly as we continue developing towards simulating more complicated processes in extended materials.

So for this lecture, I will focus on developing a formal framework for an exact stochastic equation to solve the time evolution of the system component of a Hamiltonian in the form

$$\hat{H}_{\mathrm{tot}} = \hat{H}_{\mathrm{sys}} + \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}} \left(\hat{L} \otimes \hat{a}_i^\dagger + \hat{L}^\dagger \otimes \hat{a}_i \right) + \sum_i \hbar\omega_i \hat{a}_i^\dagger \hat{a}_i \tag{1}$$

where $\hat{H}_{\mathrm{sys}}$ is the system Hamiltonian, $\hat{a}(\hat{a}^\dagger)$ are the lowering (raising) operators for the harmonic oscillator bath, and $\hat{L}$ is the system-component of the system-bath coupling operator which describes how the environmental modes couple to the system degrees of freedom. By the end of the lecture we will have derived the non-Markovian quantum state diffusion (NMQSD) equation, found the Markovian limit, and demonstrated in what sense the system wave function localizes in the presence of a Markovian system-bath coupling. The core derivation we are tracking in this lecture was presented by *Diosi & Strunz Physics Letters A 235, 569–573 (1997).*

2 Introducing stochasticity: Decomposing the total wave function

Why is an equation of motion ever stochastic? The Schrödinger equation is a deterministic equation that fully describes the state of the particle (or any collection of particles). Even classically, Newtonian mechanics is a deterministic set of equations, so why is Brownian motion stochastic?

The key insight is to recognize that an equation is stochastic because there is a degree of freedom (or collection of degrees of freedom) that the equation is not explicitly solving. For classical Brownian motion, that is the motion of the solvent particles that are bombarding the particle of interest and causing it to move randomly. For our NMQSD equation, the stochasticity will arise because, like in the classical Brownian oscillator example, we are going to neglect the environment. Note, that when I say neglect the environment, I do not mean that we are not going to take it into account; rather, I mean we will write down an equation that accounts for the environment implicitly but does not require us to actually time evolve the environmental degrees of freedom.

2.1 Bargmann coherent states

The derivation that follows is going to require us to expand our bath states in terms of the **Bargmann coherent states**. The choice of basis is going to matter a great deal, so let's spend a moment reminding ourselves about the properties of this basis.

Coherent States
The coherent state basis is composed of states $\{|z\rangle\}$ defined as the right eigenstates of the lowering operator $\hat{a}$:

$$\hat{a}|z\rangle = z|z\rangle \tag{2}$$

with eigenvalue z. We can verify the coherent state $|z\rangle$ in the **number basis** is given by

$$|z\rangle = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}|n\rangle \tag{3}$$

by demonstrating that

$$\hat{a}|z\rangle = \hat{a}\sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}|n\rangle = \sum_{n=1}^{\infty} \frac{z^n}{\sqrt{n!}}\sqrt{n}|n-1\rangle = \sum_{n=1}^{\infty} \frac{z^n}{\sqrt{(n-1)!}}|n-1\rangle \tag{4}$$

Re-indexing with $m = n - 1$:

$$= \sum_{m=0}^{\infty} \frac{z^{m+1}}{\sqrt{m!}}|m\rangle = z\sum_{m=0}^{\infty} \frac{z^m}{\sqrt{m!}}|m\rangle = z|z\rangle \tag{5}$$

where we have made use of the action of the lowering operator in the number basis $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$. Recall that, for the harmonic oscillator, the coherent states are the most classical-like states because they move in a circle through phase space without changing their shape.

While the coherent states I have defined here form a basis, they are neither normalized nor orthogonal, so it may not be immediately obvious why it is such a convenient choice. Below, I outline the 3 additional properties of the coherent state basis that we are going to use in the derivation that follows:

<u>Property 1: Creation operator is a derivative</u>
One of special property of the coherent states is how simply they interact with the ladder operators for the harmonic oscillators the define the environment.

$$\hat{a}^\dagger|z\rangle = \frac{\partial}{\partial z}|z\rangle \tag{6}$$

Let's see why. Using $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$:

$$\hat{a}^\dagger|z\rangle = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}\sqrt{n+1}|n+1\rangle = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{(n+1)!}}\cdot(n+1)|n+1\rangle \tag{7}$$

Re-indexing with $m = n + 1$:

$$= \sum_{m=1}^{\infty} \frac{z^{m-1}}{\sqrt{m!}} \cdot m|m\rangle = \sum_{m=1}^{\infty} \frac{m\, z^{m-1}}{\sqrt{m!}}|m\rangle \tag{8}$$

Meanwhile, if we take the derivative of $|z\rangle$ directly:

$$\frac{\partial}{\partial z}|z\rangle = \frac{\partial}{\partial z}\sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}|n\rangle = \sum_{n=1}^{\infty} \frac{n\, z^{n-1}}{\sqrt{n!}}|n\rangle \tag{9}$$

These expressions are identical, confirming $\hat{a}^\dagger|z\rangle = \frac{\partial}{\partial z}|z\rangle$.

Non-normalized is simpler
Note that this property, as written, **only holds for the non-normalized coherent states (i.e. the Bargmann states)** because for normalized coherent states $|z\rangle_{\text{norm}} = e^{-|z|^2/2}|z\rangle$, the normalization factor depends on z. When $\hat{a}^\dagger$ acts, the derivative of the normalization factor contributes an extra $z^*/2$ term. Specifically, for normalized states: $\hat{a}^\dagger \to \frac{z^*}{2} + \frac{\partial}{\partial z}$ (Klauder & Sudarshan, Eq. 7-93). Only Bargmann states give pure differentiation.

Property 2: Inner product
The overlap between two Bargmann states is:

$$\langle w|z\rangle = e^{w^* z} \tag{10}$$

We can derive this using the series expansion and $\langle m|n\rangle = \delta_{mn}$:

$$\langle w|z\rangle = \sum_{m,n=0}^{\infty} \frac{(w^*)^m}{\sqrt{m!}} \frac{z^n}{\sqrt{n!}}\langle m|n\rangle = \sum_{n=0}^{\infty} \frac{(w^* z)^n}{n!} = e^{w^* z} \tag{11}$$

Setting $w = z$, we find:

$$\langle z|z\rangle = e^{|z|^2} \neq 1 \tag{12}$$

This is why they are called "non-normalized"—the norm grows exponentially with $|z|^2$.

Property 3: Completeness Relation
Despite being non-orthogonal and non-normalized, Bargmann states form an overcomplete basis:

$$\frac{1}{\pi}\int d^2 z\, e^{-|z|^2}|z\rangle\langle z| = \hat{1} \tag{13}$$

where $d^2 z = d(\operatorname{Re} z)\, d(\operatorname{Im} z)$ is the bare complex measure.

Derivation of coherent state completeness relationship
To derive the completeness relationship, we insert the Fock state expansions:

$$\frac{1}{\pi}\int d^2 z\, e^{-|z|^2} \sum_{m,n} \frac{z^n (z^*)^m}{\sqrt{n!\, m!}}|n\rangle\langle m| \tag{14}$$

The integral $\frac{1}{\pi}\int d^2z\, e^{-|z|^2} z^n (z^*)^m$ vanishes unless $n = m$ (by rotational symmetry in the complex plane: $z \to e^{i\theta} z$ gives a phase $e^{i(n-m)\theta}$ that integrates to zero). For $n = m$, the integral evaluates to $n!$, giving:

$$\sum_n \frac{n!}{n!} |n\rangle\langle n| = \sum_n |n\rangle\langle n| = \hat{1}. \tag{15}$$

2.2 Conditional system state wave function

Recall, that the total Hamiltonian is given by

$$\hat{H}_{\rm tot} = H_{\rm sys} + \sum_i^N \frac{\chi_i}{\sqrt{2m_i\omega_i}} \left(L \otimes \hat{a}_i^\dagger + L^\dagger \otimes \hat{a}_i \right) + \sum_{i=1}^N \hbar\omega_i \hat{a}_i^\dagger \hat{a}_i \tag{16}$$

where we have many harmonic oscillators composing the environment. To account for this, when we work with the environment states we will work with a product of Bargmann states - one for each harmonic oscillator. To simplify our notation, we introduce

$$|\mathbf{z}\rangle = |z_1, ..., z_i, ..., z_N\rangle \tag{17}$$

and the corresponding measure

$$d^2\mathbf{z} = \Pi_{i=1}^N \, d^2 z_i. \tag{18}$$

The corresponding resolution of identity in this notation becomes

$$\int \frac{d^2\mathbf{z}}{\pi^N} \, e^{-|\mathbf{z}|^2} |\mathbf{z}\rangle\langle\mathbf{z}|. \tag{19}$$

With these properties, we can expand the total wave function $|\Psi\rangle$ in the coherent state basis using the completeness relationship

$$|\Psi_{\rm tot}(t)\rangle = \int \frac{d^2\mathbf{z}}{\pi^N} \, e^{-|\mathbf{z}|^2} |\mathbf{z}\rangle\langle\mathbf{z}|\Psi\rangle = \int \frac{d^2\mathbf{z}}{\pi^N} \, e^{-|\mathbf{z}|^2} |\psi_{\mathbf{z}^*}(t)\rangle \otimes |\mathbf{z}\rangle. \tag{20}$$

We can physically interpret the system wave function

$$|\psi_{\mathbf{z}^*}(t)\rangle = \langle\mathbf{z}|\Psi\rangle \tag{21}$$

as the wave function the system would be in if you measured the bath to be in state $|\mathbf{z}\rangle$ (said slightly more formally, this is the system wave function conditioned on the state of the bath). [1] It is worth noting at this point, though we are not yet ready to take advantage of this property, that the system wave function $|\psi_{\mathbf{z}^*}(t)\rangle$ depends analytically on $\mathbf{z}^*$ but not on $\mathbf{z}$. This is why system states in the derivation are written as $|\psi_{\mathbf{z}^*}(t)\rangle$—the subscript reminds us that the state depends on the conjugate variable.

[1] The question of interpretation for stochastic methods in quantum mechanics is often subtle. In this case, the rather casual argument I have made can be put on rigorous footing as demonstrated in Gambetta and Wiseman Phys. Rev. A **66**, 012108 (2002).

2.3 System reduced density operator

We started this piece of our discussion by claiming we were going to find the origin of the stochasticity in our equation of motion, and - in fact - we have just done so. Allow me to explain. First, we need to recognize that the reduced density matrix for the system degrees of freedom can now be written as

$$\hat{\rho}_{\text{sys}}(t) = \int \frac{d^2\mathbf{z}}{\pi^N} e^{-|\mathbf{z}|^2} |\psi_{\mathbf{z}^*}(t)\rangle\langle\psi_{\mathbf{z}^*}(t)| \tag{22}$$

This is, by itself, a beautiful result. The reduced density operator is an integral over pure state projectors $|\psi_{\mathbf{z}^*}(t)\rangle\langle\psi_{\mathbf{z}^*}(t)|$, weighted by the Gaussian measure $e^{-|\mathbf{z}|^2} d^2\mathbf{z}$.

Bargmann reproducing kernel property
For any analytic function $g(w^*)$, the following integral

$$\frac{1}{\pi} \int d^2w \, e^{-|w|^2 + zw^*} g(w^*) = g(z^*) \tag{23}$$

is the coherent state analog of the delta function identity $\int \delta(x-y) f(y) dy = f(x)$.

Deriving the reduced density matrix
Let's compute the partial trace $\hat{\rho}_{\text{sys}} = \text{Tr}_{\text{env}}(|\Psi_{\text{tot}}\rangle\langle\Psi_{\text{tot}}|)$ step by step.

We begin by forming the total density operator:

$$|\Psi_{\text{tot}}\rangle\langle\Psi_{\text{tot}}| = \frac{1}{\pi^{2N}} \int d^2\mathbf{z} \int d^2\mathbf{w} \, e^{-|\mathbf{z}|^2 - |\mathbf{w}|^2} \left(|\psi_{\mathbf{z}^*}\rangle\langle\psi_{\mathbf{w}^*}|\right) \otimes \left(|\mathbf{z}\rangle\langle\mathbf{w}|\right) \tag{24}$$

Next, we insert the completeness relation and take the trace. For Bargmann coherent states, the completeness relation is:

$$\frac{1}{\pi^N} \int d^2\mathbf{c} \, e^{-|\mathbf{c}|^2} |\mathbf{c}\rangle\langle\mathbf{c}| = \hat{1} \tag{25}$$

so the partial trace becomes:

$$\hat{\rho}_{\text{sys}} = \frac{1}{\pi^N} \int d^2\mathbf{c} \, e^{-|\mathbf{c}|^2} \langle\mathbf{c}|\hat{\rho}_{\text{tot}}|\mathbf{c}\rangle \tag{26}$$

Substituting the total density operator and using the Bargmann inner product $\langle\mathbf{c}|\mathbf{z}\rangle = e^{\mathbf{c}^* \cdot \mathbf{z}}$:

$$\hat{\rho}_{\text{sys}} = \frac{1}{\pi^{3N}} \int d^2\mathbf{z} \int d^2\mathbf{w} \int d^2\mathbf{c} \, e^{-|\mathbf{z}|^2 - |\mathbf{w}|^2 - |\mathbf{c}|^2} e^{\mathbf{c}^* \cdot \mathbf{z} + \mathbf{w}^* \cdot \mathbf{c}} |\psi_{\mathbf{z}^*}\rangle\langle\psi_{\mathbf{w}^*}| \tag{27}$$

Now we evaluate the Gaussian integrals. The c-integral is a complex Gaussian:

$$\int d^2\mathbf{c} \, e^{-|\mathbf{c}|^2 + \mathbf{c}^* \cdot \mathbf{z} + \mathbf{w}^* \cdot \mathbf{c}} = \pi^N e^{\mathbf{w}^* \cdot \mathbf{z}} \tag{28}$$

which gives:

$$\hat{\rho}_{\text{sys}} = \frac{1}{\pi^{2N}} \int d^2\mathbf{z} \int d^2\mathbf{w} \, e^{-|\mathbf{z}|^2 - |\mathbf{w}|^2 + \mathbf{w}^* \cdot \mathbf{z}} |\psi_{\mathbf{z}^*}\rangle\langle\psi_{\mathbf{w}^*}|. \tag{29}$$

This analyticity means the only coupling between $\mathbf{z}$ and $\mathbf{w}$ in our integrand comes through the factor $e^{\mathbf{w}^* \cdot \mathbf{z}}$. Since $\langle \psi_{\mathbf{w}^*}|$ depends analytically on $\mathbf{w}^*$ we can use the **reproducing kernel property** to give our final result:

$$\hat{\rho}_{\text{sys}}(t) = \frac{1}{\pi^N} \int d^2\mathbf{z}\, e^{-|\mathbf{z}|^2} |\psi_{\mathbf{z}^*}(t)\rangle\langle\psi_{\mathbf{z}^*}(t)|. \tag{30}$$

We can write this more compactly by introducing the Gaussian ensemble average notation. Define

$$M_{\mathbf{z}}[f(\mathbf{z}, \mathbf{z}^*)] = \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2} f(\mathbf{z}, \mathbf{z}^*) \tag{31}$$

where the measure $\frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}$ defines a Gaussian probability distribution over complex configurations.

The Complex Gaussian Ensemble Average

For the coherent state labels $a = (a_1, a_2, \ldots)$ that we'll encounter in the derivation, each a_i is a complex variable. The ensemble average is defined as:

$$M_z[f(z)] = \int \frac{d^2z}{\pi}\, e^{-|z|^2} f(z) \tag{32}$$

where $d^2z = d(\text{Re}\, z)\, d(\text{Im}\, z)$ is the bare complex measure (integration over both real and imaginary parts). The factor $e^{-|z|^2}$ is a Gaussian weight centered at the origin in the complex plane. Since $|z|^2 = (\text{Re}\, z)^2 + (\text{Im}\, z)^2$, this is a two-dimensional Gaussian that decays rapidly as $|z|$ increases—most of the contribution to the integral comes from the region where $|z| \lesssim 1$.

Normalization note: With the bare measure, $\int d^2z\, e^{-|z|^2} = \pi$. In some contexts, this π factor is absorbed into the definition of $M_z[\cdot]$ to make it a normalized probability distribution. In our derivation, this normalization is explicit.

Reduced Density Operator as Ensemble Average

The reduced system density operator takes the form

$$\hat{\rho}_{\text{sys}}(t) = M_{\mathbf{z}}\left[|\psi_{\mathbf{z}^*}(t)\rangle\langle\psi_{\mathbf{z}^*}(t)|\right] \tag{33}$$

The result is that we can describe the reduced density matrix of the system in terms of a monte carlo average over different environmental configurations. This will be the first sense of stochasticity in the equation.

3 Deriving the coherent state Schrödinger equation

We have now defined a stochastic average over z for the definition of the total wave function and the system reduced density matrix. What we have not done is shown that we can time-evolve the system component of the wave function independently from the bath. The first step towards this is re-writing the full Schrödinger equation using the properties of the coherent states.

3.1 Interaction picture for OQS

To simplify the equation of motion, we will make use of the fact that harmonic oscillators have a very simple equation of motion which allows us to move into the interaction picture - where we use the Heisenberg representation for the bath operators and the Schrodinger representation for the system operators.

Heisenberg Equation of Motion
The time evolution of operators in the Heisenberg picture satisfies:

$$\frac{d\hat{A}_H}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}_H] \tag{34}$$

We can derive this by differentiating $\hat{A}_H(t) = e^{i\hat{H}t/\hbar}\hat{A}\, e^{-i\hat{H}t/\hbar}$ directly:

$$\frac{d\hat{A}_H}{dt} = \frac{i\hat{H}}{\hbar}e^{i\hat{H}t/\hbar}\hat{A}\, e^{-i\hat{H}t/\hbar} + e^{i\hat{H}t/\hbar}\hat{A}\, e^{-i\hat{H}t/\hbar}\left(-\frac{i\hat{H}}{\hbar}\right) = \frac{i}{\hbar}[\hat{H}, \hat{A}_H] \tag{35}$$

The interaction picture offers a useful compromise: we put the "easy" free evolution on operators and leave the "hard" interaction in the states. We split the Hamiltonian as $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ is solvable (like free oscillators) and $\hat{V}$ is the interaction.

Operators in the interaction picture evolve as:

$$\hat{A}_I(t) = e^{i\hat{H}_0 t/\hbar}\hat{A}\, e^{-i\hat{H}_0 t/\hbar} \tag{36}$$

while states transform according to:

$$|\psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar}|\psi_S(t)\rangle \tag{37}$$

where $|\psi_S(t)\rangle$ is the Schrödinger picture state. In a typical **interaction picture**, you will find $\hat{H}_0 = \hat{H}_{\text{sys}} + \hat{H}_{\text{bath}}$, but here we do not necessarily know the time evolution arising from the system Hamiltonian. As a result, we limit ourselves to $\hat{H}_0 = \hat{H}_{\text{bath}}$.

Bath operators in the Heisenberg representation
For our problem, we take $\hat{H}_0 = \hat{H}_{\text{env}} = \sum_i \hbar\omega_i \hat{a}_i^\dagger \hat{a}_i$ as the free bath Hamiltonian. Let's work out how the annihilation operator evolves.

We need to compute $\hat{a}_i(t) = e^{i\hat{H}_{\text{env}}t/\hbar}\hat{a}_i\, e^{-i\hat{H}_{\text{env}}t/\hbar}$. Using the Heisenberg equation with $\hat{H}_{\text{env}}$:

$$\frac{d\hat{a}_i}{dt} = \frac{i}{\hbar}[\hat{H}_{\text{env}}, \hat{a}_i] = \frac{i}{\hbar}\sum_j \hbar\omega_j[\hat{a}_j^\dagger \hat{a}_j, \hat{a}_i] \tag{38}$$

We need the commutator $[\hat{a}_j^\dagger \hat{a}_j, \hat{a}_i]$. Using the identity $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$:

$$[\hat{a}_j^\dagger \hat{a}_j, \hat{a}_i] = \hat{a}_j^\dagger[\hat{a}_j, \hat{a}_i] + [\hat{a}_j^\dagger, \hat{a}_i]\hat{a}_j \tag{39}$$

Since $[\hat{a}_j, \hat{a}_i] = 0$ and $[\hat{a}_j^\dagger, \hat{a}_i] = -\delta_{ij}$, we get:

$$[\hat{a}_j^\dagger \hat{a}_j, \hat{a}_i] = -\delta_{ij}\hat{a}_i \tag{40}$$

Therefore:

$$\frac{d\hat{a}_i}{dt} = i\sum_j \omega_j(-\delta_{ij})\hat{a}_i = -i\omega_i\hat{a}_i \tag{41}$$

This resulting equation of motion for the ladder operators of the bath degree of freedom is given by

Time Evolution of Bath Operators

$$\hat{a}_i(t) = \hat{a}_i\, e^{-i\omega_i t} \tag{42}$$

Similarly, taking the adjoint:

$$\hat{a}_i^\dagger(t) = \hat{a}_i^\dagger\, e^{+i\omega_i t}. \tag{43}$$

In this frame of reference, which moves with the harmonic oscillator states and does not affect the system operators, the effective Hamiltonian that describes the time-evolution of the wave function is given by

$$\hat{H}_{\text{eff}} = \hat{H}_{\text{sys}} + \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\left(\hat{L}\otimes\hat{a}_i^\dagger(t) + \hat{L}^\dagger\otimes\hat{a}_i(t)\right) \tag{44}$$

where the harmonic oscillator Hamiltonian terms are no longer included because their influence is accounted for in the time-evolution of the bath operators. Notice that there is no change to the behavior of the system operators since they all commute with the bath Hamiltonian. The corresponding Schrödinger equation goes from

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\text{tot}}(t)\rangle = \hat{H}_{\text{tot}}|\Psi_{\text{tot}}(t)\rangle \tag{45}$$

to

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\text{tot}}^{(I)}(t)\rangle = \hat{H}_{\text{eff}}|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{46}$$

in the interaction picture.

3.2 Deriving the coherent state Schrödinger equation

Our goal now is to derive an equation of motion for the system state conditioned on a particular coherent state configuration of the bath. To understand the behavior of the equation when we expand in the Bargmann coherent state basis, we start from the interaction picture equation and then introduce the resolution of identity in the coherent state basis on the left hand side giving:

$$\left(\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\right) i\hbar\frac{\partial}{\partial t}|\Psi_{\text{tot}}^{(I)}(t)\rangle = \left(\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\right) \hat{H}_{\text{eff}}|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{47}$$

$$= \left(\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\right) \hat{H}_{\text{sys}}|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{48}$$

$$+ \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}} \left(\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\right) \hat{L}\otimes\hat{a}_i^\dagger(t)|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{49}$$

$$+ \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}} \left(\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\right) \hat{L}^\dagger\otimes\hat{a}_i(t)|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{50}$$

Since we know the resolution of identity does not depend on time, we can move it through the time-derivative on the right hand side and notice that the only time dependence will appear in $|\psi_{\mathbf{z}^*}(t)\rangle$, leading us to

$$i\hbar\frac{\partial}{\partial t}\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\psi_{\mathbf{z}^*}(t)\rangle\otimes|\mathbf{z}\rangle = i\hbar\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\dot{\psi}_{\mathbf{z}^*}(t)\rangle\otimes|\mathbf{z}\rangle \tag{51}$$

where we use the dot notation $|\dot{\psi}_{\mathbf{z}^*}\rangle \equiv \frac{\partial}{\partial t}|\psi_{\mathbf{z}^*}\rangle$.

The first term on the right hand side, involving the system Hamiltonian, is straightforward: since $\hat{H}_{\text{sys}}$ acts only on the system Hilbert space, it commutes with the bath coherent state $|z\rangle$:

$$\left(\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\right) \hat{H}_{\text{sys}}|\Psi_{\text{tot}}^{(I)}(t)\rangle = \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}\left(\hat{H}_{\text{sys}}|\psi_{\mathbf{z}^*}(t)\rangle\right)\otimes|\mathbf{z}\rangle. \tag{52}$$

The two interaction terms requires more care, the first one (involving the raising operator) can be simplified by acting the raising operator to the left

$$\left(\hat{L}\sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\right)\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\hat{a}_i^\dagger(t)|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{53}$$

$$= \left(\hat{L}\sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\right)\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|\hat{a}_i^\dagger e^{i\omega_i t}|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{54}$$

$$= \left(\hat{L}\sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\right)\int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\mathbf{z}\rangle\langle\mathbf{z}|z_i^* e^{i\omega_i t}|\Psi_{\text{tot}}^{(I)}(t)\rangle \tag{55}$$

$$= \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}\left(\hat{L}\sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}} z_i^* e^{i\omega_i t}\right)|\psi_{\mathbf{z}^*}(t)\rangle\otimes|\mathbf{z}\rangle \tag{56}$$

making use of the fact that the raising operator acting the left behaves like the lowering operator acting to the right yielding an eigenvalue expression with the coherent state basis.

The second term is slightly more subtle and makes use of the derivative form of the raising operator to describe the action of the lowering operator acting to the left

$$\left(\hat{L}^\dagger \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\right) \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2} |\mathbf{z}\rangle\langle\mathbf{z}|\hat{a}_i(t)|\Psi^{(I)}_{\text{tot}}(t)\rangle \tag{57}$$

$$= \left(\hat{L}^\dagger \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\right) \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2} |\mathbf{z}\rangle\langle\mathbf{z}|\hat{a}_i e^{-i\omega_i t}|\Psi^{(I)}_{\text{tot}}(t)\rangle \tag{58}$$

$$= \left(\hat{L}^\dagger \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\right) \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2} |\mathbf{z}\rangle \frac{\partial}{\partial z_i^*} e^{-i\omega_i t}\langle\mathbf{z}|\Psi^{(I)}_{\text{tot}}(t)\rangle \tag{59}$$

$$= \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2} \left(\hat{L}^\dagger \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}} e^{-i\omega_i t}\right) \frac{\partial}{\partial z_i^*}|\psi_{\mathbf{z}^*}(t)\rangle \otimes |\mathbf{z}\rangle. \tag{60}$$

If we combine all of this, we find that we now have an equation that describes the time-evolution of the system wave function conditioned on observing a specific state of the bath in the coherent basis

$$\hbar\frac{d}{dt}|\psi_{\mathbf{z}^*}(t)\rangle = -i\left(\hat{H}_{\text{sys}} + \sum_i \frac{\chi_i}{\sqrt{2m_i\omega_i}}\left(\hat{L}\, z_i^* e^{i\omega_i t} + \hat{L}^\dagger\, e^{-i\omega_i t}\frac{\partial}{\partial z_i^*}\right)\right)|\psi_{\mathbf{z}^*}(t)\rangle. \tag{61}$$

Physical interpretation: This equation describes how the system wavefunction $|\psi_{z^*}(t)\rangle$ evolves for a given "configuration" z^* of the bath coherent state. The full system state is recovered by integrating over all configurations with the Gaussian weight $e^{-|z|^2}$.

At this point, we will specialize our derivation to the T=0 limit, where our initial condition will be

$$|\psi_{\mathbf{z}^*}(0)\rangle = |\psi_0\rangle. \tag{62}$$

The extension to finite temperatures is achieved through a thermofield extension, which (if I'm lucky) I have included as an appendix to these lecture notes. At the moment, it is not obvious why we need to make this approximation, but this will provide a useful boundary condition on our equation of motion.

4 Revealing the stochastic equation

At this point we have a time-evolution equation for the system wave function conditioned on a specific bath state, but the equation depends on both the system and bath degrees of freedom (as a result of the partial derivative), so we need to recognize that the bath dependence can be recast as a stochastic variable. We have actually already done this in our interpretation of the system reduced density operator

$$\hat{\rho}_{\text{sys}}(t) = M_{\mathbf{z}}\left[|\psi_{\mathbf{z}^*}(t)\rangle\langle\psi_{\mathbf{z}^*}(t)|\right] = \int \frac{d^2\mathbf{z}}{\pi^N}\, e^{-|\mathbf{z}|^2}|\psi_{\mathbf{z}^*}(t)\rangle\langle\psi_{\mathbf{z}^*}(t)| \tag{63}$$

as a complex gaussian ensemble average. This integral can be evaluated by a Monte Carlo sampling over the bath configurations $\mathbf{z}$. Extending that insight to this time-evolution equation, we can recognize that

$$Z_{\mathbf{z}^*}(t) = \sum_i (-i)\frac{\chi_i}{\sqrt{2m_i\omega_i}} z_i^* e^{i\omega_i t} \tag{64}$$

defines a stochastic process when the coherent state labels (z_i) represent a random realization of the bath state sampled from the Gaussian distribution on the camplex plane $P(z_i) = e^{-|z_i|^2}/\pi$.

4.1 Gaussian statistics

Complex Gaussian Moments
For independent complex Gaussian variables z_i with the ensemble average defined above, we have:
First moments (mean):

$$M_{\mathbf{z}}[z_i] = 0, \qquad M_{\mathbf{z}}[z_i^*] = 0 \tag{65}$$

These vanish by symmetry of the Gaussian weight under $z_i \to -z_i$.
Second moments:

$$\boxed{M_{\mathbf{z}}[z_i^* z_j] = \delta_{ij}} \tag{66}$$

$$M_{\mathbf{z}}[z_i z_j] = 0, \qquad M_{\mathbf{z}}[z_i^* z_j^*] = 0 \tag{67}$$

Notice the critical distinction here: the non-zero correlation is $M_{\mathbf{z}}[z_i^* z_j]$, **not** $M_{\mathbf{z}}[z_i z_j]$.

Now we can compute the statistics of our stochastic process. Let's start with the mean:

$$M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)] = M_{\mathbf{z}}\left[\sum_i (-i)\frac{\chi_i}{\sqrt{2m_i\omega_i}} z_i^* e^{i\omega_i t}\right] \tag{68}$$

Since the ensemble average is linear, we can pull the sum and deterministic factors outside:

$$= \sum_i (-i)\frac{\chi_i}{\sqrt{2m_i\omega_i}} e^{i\omega_i t}\, M_{\mathbf{z}}[z_i^*] \tag{69}$$

Applying the first moment identity $M_{\mathbf{z}}[z_i^*] = 0$, each term vanishes, giving us

$$\boxed{M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)] = 0} \tag{70}$$

What about correlations? Let's first compute $M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)Z_{\mathbf{z}^*}(s)]$—the correlation without complex conjugation:

$$M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)Z_{\mathbf{z}^*}(s)] = M_{\mathbf{z}}\left[\left(\sum_i (-i)\frac{\chi_i}{\sqrt{2m_i\omega_i}} z_i^* e^{i\omega_i t}\right)\left(\sum_j (-i)\frac{\chi_j}{\sqrt{2m_j\omega_j}} z_j^* e^{i\omega_j s}\right)\right] \tag{71}$$

Expanding the product:

$$= \sum_{i,j} \frac{-\chi_i\chi_j}{\sqrt{2m_i\omega_i}\sqrt{2m_j\omega_j}} e^{i\omega_i t} e^{i\omega_j s}\, M_{\mathbf{z}}[z_i^* z_j^*] \tag{72}$$

But we know $M_{\mathbf{z}}[z_i^* z_j^*] = 0$, so

$$\boxed{M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)Z_{\mathbf{z}^*}(s)] = 0} \tag{73}$$

This vanishing is a hallmark of complex Gaussian processes. It reflects the circular symmetry in the complex plane—rotating all z_i by a common phase leaves the distribution invariant but changes $z_i z_j$. Only quantities invariant under this symmetry can have non-zero averages.

Now for the crucial calculation: $M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)Z_{\mathbf{z}}^*(s)]$. First, we need the complex conjugate of our process:

$$Z_{\mathbf{z}}^*(s) = \left(\sum_j (-i)\frac{\chi_j}{\sqrt{2m_j\omega_j}} z_j^* e^{i\omega_j s}\right)^* = \sum_j (i)\frac{\chi_j}{\sqrt{2m_j\omega_j}} z_j e^{-i\omega_j s} \tag{74}$$

where we've used that χ_j, m_j, and ω_j are all real.

Now we compute:

$$M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)Z^*_{\mathbf{z}^*}(s)] = M_{\mathbf{z}}\left[\left(\sum_i (-i)\frac{\chi_i}{\sqrt{2m_i\omega_i}} z_i^* e^{i\omega_i t}\right)\left(\sum_j (i)\frac{\chi_j}{\sqrt{2m_j\omega_j}} z_j e^{-i\omega_j s}\right)\right] \tag{75}$$

$$= \sum_{i,j} \frac{\chi_i\chi_j}{\sqrt{2m_i\omega_i}\sqrt{2m_j\omega_j}} e^{i\omega_i t} e^{-i\omega_j s}\, M_{\mathbf{z}}[z_i^* z_j] \tag{76}$$

Applying the fundamental identity $M_{\mathbf{z}}[z_i^* z_j] = \delta_{ij}$:

$$= \sum_{i,j} \frac{\chi_i\chi_j}{\sqrt{2m_i\omega_i}\sqrt{2m_j\omega_j}} e^{i\omega_i t} e^{-i\omega_j s}\, \delta_{ij} \tag{77}$$

$$= \sum_i \frac{\chi_i^2}{2m_i\omega_i} e^{i\omega_i t} e^{-i\omega_i s} = \sum_i \frac{\chi_i^2}{2m_i\omega_i} e^{i\omega_i (t-s)}. \tag{78}$$

If we recall that at T=0, the bath correlation function is given by

$$\alpha(t,s) = \alpha(t-s) = \sum_i \frac{\chi_i^2}{2m_i\omega_i} e^{-i\omega_i (t-s)} \tag{79}$$

then we can see that

$$M_z[Z_{\mathbf{z}^*}(t)Z^*_{\mathbf{z}^*}(s)] = \alpha^*(t-s)\,\delta_{i,j}. \tag{80}$$

Statistics of the Stochastic Process $Z_{\mathbf{z}^*}(t)$

The stochastic process defined in terms of coherent state labels has statistics that exactly reproduce the bath correlation function:

$$M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)] = 0, \quad M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)Z_{\mathbf{z}^*}(s)] = 0, \quad M_{\mathbf{z}}[Z_{\mathbf{z}^*}(t)Z^*_{\mathbf{z}^*}(s)] = \alpha^*(t,s) \tag{81}$$

4.2 Non-Markovian Quantum State Diffusion Equation

Chain rule for functional derivatives

Let $F[Z_{\mathbf{z}^*}]$ be a function that depends on a stochastic process $Z_{\mathbf{z}^*}(t)$, where

$$Z_{\mathbf{z}^*}(t) = \sum_i c_i(t) z_i^* \tag{82}$$

then we write the chain rule as

$$\frac{\partial}{\partial z_\lambda^*} F[Z_{\mathbf{z}^*}] = \int_{-\infty}^{\infty} ds\, \frac{\partial Z_{\mathbf{z}^*}(s)}{\partial z_\lambda^*} \frac{\delta F}{\delta Z_{\mathbf{z}^*}(s)}. \tag{83}$$

This is the infinite-dimensional generalization of the familiar chain rule $\frac{\partial}{\partial x} = \sum_i \frac{\partial y_i}{\partial x}\frac{\partial}{\partial y_i}$, where the sum over discrete indices becomes an integral over the continuous variable s.

Example

Suppose we have a process $Z(s)$ defined as a linear combination:

$$Z(s) = \sum_i c_i(s)\, a_i^* \tag{84}$$

where the a_i^* are the fundamental variables. We want to compute $\frac{\partial}{\partial a_i^*}$ acting on a functional $F[Z]$. Applying the chain rule:

$$\frac{\partial}{\partial a_i^*} F[Z] = \int ds\, \frac{\partial Z(s)}{\partial a_i^*} \frac{\delta F}{\delta Z(s)} \tag{85}$$

Since $Z(s) = \sum_j c_j(s) a_j^*$, we have:

$$\frac{\partial Z(s)}{\partial a_i^*} = c_i(s) \tag{86}$$

Therefore:

$$\frac{\partial}{\partial a_i^*} = \int ds\, c_i(s) \frac{\delta}{\delta Z(s)} \tag{87}$$

Having recognized the presence of a stochastic process in equation of motion, we are left with the final task of rewriting the partial derivative in terms of the coherent state index into this stochastic form which will remove the last remnants of tracking the explicit bath state from our equation of motion which is hiding in the third term with the partial derivative of the coherent state index. Noting that

$$\frac{\partial Z_{\mathbf{z}^*}(s)}{\partial z_\lambda^*} = (-i) \frac{\chi_\lambda}{\sqrt{2 m_\lambda \omega_\lambda}} e^{i\omega_\lambda s} \tag{88}$$

and using the chain rule we can rewrite

$$\begin{aligned}
\sum_\lambda (-i) \frac{\chi_\lambda}{\sqrt{2 m_\lambda \omega_\lambda}} e^{-i\omega_\lambda t} \frac{\partial}{\partial z_\lambda^*} &= \sum_\lambda (-i) \frac{\chi_\lambda}{\sqrt{2 m_\lambda \omega_\lambda}} e^{-i\omega_\lambda t} \int_{-\infty}^{\infty} ds\, \frac{\partial Z_z(s)}{\partial z_\lambda^*} \frac{\delta}{\delta Z_z(s)} &(89)\\
&= \sum_\lambda (-i) \frac{\chi_\lambda}{\sqrt{2 m_\lambda \omega_\lambda}} e^{-i\omega_\lambda t} \int_{-\infty}^{\infty} ds\, (-i) \frac{\chi_\lambda}{\sqrt{2 m_\lambda \omega_\lambda}} e^{i\omega_\lambda s} \frac{\delta}{\delta Z_z(s)} &(90)\\
&= -\int_{-\infty}^{\infty} ds \left[\frac{\chi_\lambda^2}{2 m_\lambda \omega_\lambda} e^{-i\omega_\lambda (t-s)} \right] \frac{\delta}{\delta Z_z(s)} &(91)
\end{aligned}$$

where we exchange the sum and integral (valid for absolutely convergent sums). The expression in brackets is precisely the zero-temperature bath correlation function:

$$\alpha(t, s) = \alpha(t - s) = \sum_\lambda \frac{\chi_\lambda^2}{2 m_\lambda \omega_\lambda} e^{-i\omega_\lambda (t-s)} \tag{92}$$

which depends only on the time difference $\tau = t - s$ due to the time-translation invariance of the free bath Hamiltonian.

We can now rewrite the total expression for the time-evolution of our conditional system wave function as

$$\hbar \frac{d}{dt} |\psi_{\mathbf{z}^*}(t)\rangle = -i\hat{H}_{\text{sys}} |\psi_{\mathbf{z}^*}(t)\rangle + Z_{\mathbf{z}^*}(t) \hat{L} |\psi_{\mathbf{z}^*}(t)\rangle - \hat{L}^\dagger \int_{-\infty}^{\infty} \alpha(t-s) \frac{\delta}{\delta Z_{\mathbf{z}^*}(s)} |\psi_{\mathbf{z}^*}(t)\rangle ds. \tag{93}$$

We can simplify the limits of integration by recognizing that since our thermal environment is in the vacuum state at t=0, there cannot be any dependence of the wave function on the stochastic trajectory before time t=0. This, as a reminder, was why we needed to assume everything is at zero temperature, in the absence of that the limits of integration do not have a simple lower bound. Similarly, causality restricts us so that the wave function cannot depend on the future values of the stochastic trajectory, leaving us with the

Non-Markovian quantum state diffusion (NMQSD) equation

$$\hbar\frac{d}{dt}|\psi_{\mathbf{z}^*}(t)\rangle = -i\hat{H}_{\text{sys}}|\psi_{\mathbf{z}^*}(t)\rangle + Z_{\mathbf{z}^*}(t)\hat{L}|\psi_{\mathbf{z}^*}(t)\rangle - \hat{L}^\dagger\int_0^t \alpha(t-s)\frac{\delta}{\delta Z_{\mathbf{z}^*}(s)}|\psi_{\mathbf{z}^*}(t)\rangle ds. \tag{94}$$

5 Example: Markovian limit

What happens when the environment has no memory? This is the Markov limit, where the bath correlation time $\tau_c \to 0$, meaning the environment forgets its interaction with the system essentially instantaneously. Let's see how the full NMQSD machinery simplifies in this case.

The Markov limit is characterized by a delta-correlated bath:

$$\alpha(t-s) = \gamma\delta(t-s) \tag{95}$$

where the parameter γ sets the decay rate. This singular correlation function captures the physical situation where bath correlations exist only at equal times—a memoryless environment.

In the Markov limit, the NMQSD equation reduces to the quantum state diffusion (QSD) equation (derived in Appendix A)

$$\hbar\frac{d}{dt}|\psi_{\mathbf{z}^*}(t)\rangle = -i\hat{H}_{\text{sys}}|\psi_{\mathbf{z}^*}(t)\rangle + \hat{L}Z_t^*|\psi_{\mathbf{z}^*}(t)\rangle - \frac{\gamma}{2}\hat{L}^\dagger\hat{L}|\psi_{\mathbf{z}^*}(t)\rangle. \tag{96}$$

This limiting equation is much simpler because we have removed the functional derivative that sits inside of the NMQSD equation. We have done this at the price of assuming that environment relaxes infinitely quickly, which restricts our ability to simulate many physical processes. Nevertheless, this is a useful model for us to consider as we think about the dynamics of these conditional system wave functions.

Wide open quantum system

A **wide open system** is one where we can write the Hamiltonian in a block-diagonal form with (at least one) different $\hat{L}_n$ operators associated with each block that do not drive transition between blocks.

Exercise 1: Wide open systems

We can define the **delocalization entropy** of a system wave function in terms of the coefficients of that wave function

$$S(\psi) = -\sum_k |c_k|^2 \ln(|c_k|^2). \tag{97}$$

Note that this sense of entropy is not defined on the ensemble but on a single wave function.

(a) Demonstrate that the entropy is 0 when the exciton is fully localized on 1 site.

(b) Calculate the entropy for the fully delocalized state

$$|\psi\rangle = \frac{1}{\sqrt{4}}(|1\rangle + |2\rangle + |3\rangle + |4\rangle). \tag{98}$$

Is the entropy higher in the localized or delocalized state?

(c) The dispersion entropy theorem for quantum state diffusion states that for a wide open system

$$\frac{d}{dt}\left(\mathcal{M}_z[S(|\psi_z(t)\rangle)]\right) = -\sum_k \frac{1-|c_k|^2}{|c_k|^2} \langle\psi_z|\hat{L}_k|\psi_z\rangle \leq 0. \tag{99}$$

What does this mean for the average delocalization of the wave function as a function of time? Imagine you start the system in a fully delocalized state, what should happen? On the other hand, if the wave function starts in the totally localized state, what should happen?

(d) Returning to our original formulation of the problem, recognizing that $|\Psi\rangle$ is the total wave function for the system and bath. Explain what your result for part (c) means in terms of this total wave function. What does the dispersion entropy theorem say in terms of the total wave function?

Exercise 2: Limitations of the method

Looking back over this method, what are the major limitations of the method presented? We spoke at the very beginning about the long timescale of method development, so there have been a lot of developments since this method was first developed - what are the key developments you would want to go look for in the literature if you were interested in this method?

6 Appendix A: Deriving the Markovian limit

Our starting point is the linear NMQSD equation with its memory integral:

$$\partial_t \psi_t = -iH\psi_t + LZ_t\psi_t - L^\dagger \int_0^t \alpha(t-s)\frac{\delta\psi_t}{\delta Z_s^*}\,ds \tag{100}$$

To proceed, we need to understand what happens to the functional derivative $\frac{\delta\psi_t}{\delta Z_s^*}$ when evaluated at the boundary point $s = t$.

6.1 The Boundary Functional Derivative

A key result that requires careful derivation is:

$$\frac{\delta\psi_t}{\delta Z_t^*} = \frac{1}{2}L\psi_t \quad (t > 0) \tag{101}$$

The factor of 1/2 might seem surprising. It arises because when we differentiate at the boundary point $s = t$, the delta function contribution sits at the edge of the integration domain $[0, t]$, contributing only half its weight. This differs from the O-operator initial condition $O(s, s, Z^*) = L$ by exactly this factor of 1/2.

To establish this result, we work with the Dyson series solution for ψ_t:

$$\psi_t(Z^*) = \sum_{n=0}^{\infty}(-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, H_{\text{tot}}(t_1)\cdots H_{\text{tot}}(t_n)\psi_0 \tag{102}$$

where the effective Hamiltonian can be written as

$$H_{\text{tot}}(t) = -iH_{\text{sys}} + \hat{L}Z_t^* - \hat{L}^\dagger \int_{-\infty}^{\infty} ds\,\alpha(t-s)\frac{\delta}{\delta Z_s^*} \tag{103}$$

Now let's compute the functional derivative order by order. Using the fundamental identity

$$\frac{\delta Z_t^*}{\delta Z_s^*} = \delta(t-s) \tag{104}$$

we can work out what happens at each order of the Dyson expansion.

At first order, the functional derivative acts on the noise term $\hat{L}Z_{t_1}^*$:

$$\frac{\delta}{\delta Z_t^*}\int_0^t dt_1\,(-i)H_{\text{tot}}(t_1)\psi_0 = \int_0^t dt_1\,\delta(t-t_1)L\psi_0 = \frac{1}{2}L\psi_0 \tag{105}$$

Notice that the integral $\int_0^t \delta(t-t_1)dt_1 = \frac{1}{2}$ because the delta function peak sits exactly at the upper boundary of the integration domain.

What about second order? The derivative can act on either $H_{\text{tot}}(t_1)$ or $H_{\text{tot}}(t_2)$. When it acts on the outer integral (giving $\delta(t-t_1)$), setting $t_1 = t$ leaves the inner integral intact:

$$\frac{\delta}{\delta Z_t^*}\int_0^t dt_1 \int_0^{t_1} dt_2\,(-i)^2 H_{\text{tot}}(t_1)H_{\text{tot}}(t_2)\psi_0 = \frac{1}{2}L\int_0^t dt_2\,(-i)H_{\text{tot}}(t_2)\psi_0 \tag{106}$$

When the derivative acts on the inner integral (giving $\delta(t-t_2)$), this requires $t_2 = t$. But the time-ordering constraint $t_2 \leq t_1 \leq t$ means this only has support when $t_1 = t$ exactly, which contributes nothing to the outer integral.

This pattern persists to all orders:

$$\frac{\delta}{\delta Z_t^*}\left[n\text{-th order term of } \psi_t\right] = \frac{1}{2}L\left[(n-1)\text{-th order term of } \psi_t\right] \tag{107}$$

Summing the entire series (and re-indexing) leads to:

$$\frac{\delta \psi_t}{\delta Z_t^*} = \frac{1}{2}L\sum_{n=0}^{\infty}(-i)^n\int_0^t dt_1\cdots\int_0^{t_{n-1}} dt_n\, H_{\text{tot}}(t_1)\cdots H_{\text{tot}}(t_n)\psi_0 = \frac{1}{2}L\psi_t \tag{108}$$

which confirms our key result.

6.2 Eliminating the Memory Integral

With the boundary functional derivative in hand, we can now apply the delta-function correlation to collapse the memory integral. The memory-weighted functional derivative operator becomes:

$$\mathcal{D}_t = \int ds\, \alpha(t-s)\frac{\delta}{\delta Z_s^*} = \int ds\, \gamma\delta(t-s)\frac{\delta}{\delta Z_s^*} = \gamma\frac{\delta}{\delta Z_t^*} \tag{109}$$

The delta function has selected only the contribution at $s = t$—the non-local memory integral has collapsed to a local operator. Combining this with our boundary result:

$$\mathcal{D}_t\psi_t = \gamma\frac{\delta\psi_t}{\delta Z_t^*} = \gamma\cdot\frac{1}{2}L\psi_t = \frac{\gamma}{2}L\psi_t \tag{110}$$

Substituting back into the NMQSD equation, the memory term $-L^\dagger\int_0^t \alpha(t-s)\frac{\delta\psi_t}{\delta Z_s^*}ds$ becomes simply $-L^\dagger\cdot\frac{\gamma}{2}L\psi_t = -\frac{\gamma}{2}L^\dagger L\psi_t$. We arrive at the Markovian stochastic Schrödinger equation:

$$\partial_t\psi_t(Z^*) = -iH\psi_t(Z^*) + LZ_t^*\psi_t(Z^*) - \frac{\gamma}{2}L^\dagger L\psi_t(Z^*) \tag{111}$$

driven by complex white noise Z_t with statistics:

$$\mathbb{E}[Z_t] = 0, \quad \mathbb{E}[Z_tZ_s] = 0, \quad \mathbb{E}[Z_tZ_s^*] = \gamma\delta(t-s) \tag{112}$$

6.3 Standard Stochastic Differential Form

Converting to standard notation with $Z_t^* = \sqrt{\gamma}\dot{\xi}_t^*$ where ξ_t is a standard complex Brownian motion:

$$d\psi_t = \left(-iH\psi_t - \frac{\gamma}{2}L^\dagger L\psi_t\right)dt + \sqrt{\gamma}L\psi_t\, d\xi_t^* \tag{113}$$

with $\mathbb{E}[d\xi_t\, d\xi_s^*] = \delta_{ts}dt$.

Itô vs. Stratonovich Interpretation
Since the original NMQSD is treated in Euler calculus (for finite environments), its Markovian limit inherits Stratonovich interpretation. However, for complex noise satisfying $\mathbb{E}[\xi_t\xi_s] = 0$, the correction term between Itô and Stratonovich forms vanishes.

The Markovian Diffusive SSE

In the Markov limit $\alpha(t-s) = \gamma\delta(t-s)$, the NMQSD reduces to:

$$d\psi_t = \left(-iH - \frac{\gamma}{2}L^\dagger L\right)\psi_t\,dt + \sqrt{\gamma}L\psi_t\,d\xi_t^* \tag{114}$$

with complex white noise increments $d\xi_t^*$ satisfying $\mathbb{E}[d\xi_t\,d\xi_s^*] = \delta_{ts}dt$.

This is the well-known linear diffusive stochastic Schrödinger equation from quantum optics and continuous measurement theory. The deterministic part $-\frac{\gamma}{2}L^\dagger L$ provides non-unitary decay, while the stochastic term $\sqrt{\gamma}L\,d\xi_t^*$ provides diffusive noise.

Physical Interpretation of the Factor of $1/2$

The appearance of $1/2$ in $\frac{\delta\psi_t}{\delta Z_t^*} = \frac{1}{2}L\psi_t$ is a boundary effect from integrating a delta function at the edge of its domain. This is *not* the same as the O-operator initial condition $O(s,s) = L$, which is derived without encountering this boundary issue. The distinction matters when connecting the functional derivative formalism to the O-operator formalism.

Why Memory Disappears

The delta-correlated bath $\alpha(t-s) = \gamma\delta(t-s)$ contains no information about correlations at different times. The integral over past history collapses to a single point, eliminating all memory effects. The parameter γ sets the relaxation timescale: it corresponds to decay rates in spontaneous emission problems and relates to the spectral density via $\gamma = 2\pi J(\omega_0)$ evaluated at the system frequency.

Connection to Measurement Theory

The Markovian SSE admits interpretation as describing pure states conditioned on continuous heterodyne detection outcomes. This measurement interpretation generally becomes more complicated for non-Markovian dynamics, which is one reason the Markov case is so much better understood.