
Stochastic Processes: From Classical to Quantum

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October 30, 2019

ABSTRACT

The goal of this review¹ paper is to give an introduction to the mathematics of quantum noise and some of its applications in non-equilibrium statistical mechanics. We start with some reminders from the theory of classical stochastic processes. We then provide a brief overview of quantum mechanics and quantum field theory, from the viewpoint of quantum probability and adopting the language of Hudson and Parthasarathy [123]. We introduce quantum stochastic processes on a boson Fock space and their calculus. Whenever possible, we make connections with the relevant concepts in classical probability theory. As an application of the theory, we introduce the theory of open quantum systems, with emphasis on the physics and modeling aspects of these systems.

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¹This is a work in progress and the contents will be updated from time to time. Any comments and suggestions from the readers are welcomed. Last updated: June 2019.

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1 Theory of Classical Stochastic Processes

To understand quantum mechanics, it is important to first have a firm grasp of the classical world and its laws, in particular how randomness comes into play in classical systems. This section gives an overview (and a bit more) of open classical systems and their stochastic modeling, keeping in mind that the ideas for these classical systems can often be extended to study the quantum ones.

1.1 Motivation from Non-Equilibrium Statistical Mechanics

A central topic in non-equilibrium statistical mechanics is the study of open classical systems. An open system is a component of a larger closed system and interacts with other components of the larger system. We first briefly review the mechanics of a closed classical system, in the Hamiltonian formulation. The *states* of the system are specified by points in a *phase space* (or state space), which can be a finite or infinite dimensional manifold. Let us assume for now that its phase space is finite dimensional and is taken to be the $2n$ -dimensional manifold, $P = O \times \mathbb{R}^n$, where n is an integer and $O \subset \mathbb{R}^n$ is an open set. In this case, points in the phase space can be represented as (\mathbf{x}, \mathbf{p}) , where the point $\mathbf{x} \subset O$ describes the configuration of the various objects in the system and the point $\mathbf{p} \subset \mathbb{R}^n$ describes the momenta of the various objects in the system.

The time evolution of the system is specified by a *trajectory*, a function $\mathbf{z}(t) := (\mathbf{x}(t), \mathbf{p}(t))$ from an interval in \mathbb{R} to P . The fundamental dynamical principle says that the allowed trajectories are determined, uniquely in terms of the initial condition $\mathbf{z}(0)$, by the solutions of the well-known *Hamilton's equations*. The Hamilton's equations is a system of $2n$ ordinary differential equations of the form

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i}, \quad (1)$$

for $i = 1, \dots, n$, where $H = H(\mathbf{x}, \mathbf{p})$ is a function on the phase space called the *Hamiltonian*, whose choice depending on the system one wishes to describe. The Hamiltonian can be interpreted as the total energy on the phase space and the trajectory defines a *flow* $\mathbf{z}(t) = \Phi(t)\mathbf{z}(0)$ on the phase space that leaves invariant the total energy $H(\mathbf{z}(t))$ of the system, conveying conservation of energy of the system.

Often times, one would like to have a dynamical description for $F(\mathbf{z})$, an arbitrary smooth function on the phase space, called a *classical observable*. If $\mathbf{z}(t)$ satisfies the Hamilton's equations, then $F(t) := F(\mathbf{z}(t))$ evolves according to:

$$\frac{dF}{dt} = \{F, H\}, \quad (2)$$

where the right hand side above denotes the Poisson bracket of F and H , the function evaluated at $(\mathbf{x}(t), \mathbf{p}(t))$ as follows:

$$\{F, H\} := \sum_{i=1}^n \frac{\partial F}{\partial x_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial x_i}. \quad (3)$$

In particular, we have $\{x_i, x_j\} = \{p_i, p_j\} = 0$ and $\{x_i, p_j\} = \delta_{ij}$, where δ_{ij} denotes the Kronecker delta. For properties of the Poisson bracket and details on structures and symmetries in Hamiltonian dynamics, see [107].

Generally, a system has, possibly infinitely, many states and one usually does not have a priori knowledge about all the initial values of these states². Treating the system in a statistical manner allows us to bring the problem into a tractable one. An important notion in statistical mechanics is that of *thermal equilibrium*, which, roughly speaking, is a condition that the states of the system be statistically distributed according to a probability distribution on the phase space that is invariant for the Hamiltonian flow $\Phi(t)$. In particular, the distribution of the state variable \mathbf{z} at time zero remains the same for all times. The introduction of such invariant probability measure randomizes the phase space, allowing one to simplify the description of the system at the cost of introducing uncertainty.

It is well known that in a finite dimensional phase space, any absolutely continuous $\Phi(t)$ -invariant probability measure admits a Boltzmann-Gibbs type density, $\rho(\mathbf{z}) = e^{-\beta H(\mathbf{z})}/Z$, where Z is the normalization constant (partition function)

²Typically one deals with systems containing Avogadro's number $N_A = 6 \times 10^{23}$ of particles. Interestingly, this number was computed by Perrin experimentally in his attempt to test Einstein's explanation of Brownian motion in terms of atoms and thereby confirming Dalton's atomic theory of matter. Perrin received a Nobel prize in 1926 for this.

and $\beta = 1/(k_B T) > 0$, k_B is the Boltzmann's constant and $T > 0$ is the temperature. As probabilistic framework takes its place in the thermal equilibrium setting, a natural question is whether a sufficiently smooth function on the phase space can be regarded as a stochastic process. It turns out that this is only true when the underlying phase space is infinite dimensional and, moreover, the Hamiltonian must have continuous spectrum [129]. In this case, the process is stationary and Gaussian (if the system is linear). We will keep in mind the above result when building a stochastic model for an open system later. The above question is related to the problem of stochastic aggregation of [128, 127], where it was found that any stationary Gaussian process with a rational spectral density can be represented as the output of a linear infinite dimensional Hamiltonian system in a thermal equilibrium.

1.2 A Hamiltonian Model for Open Classical Systems

We consider a toy model describing a Brownian particle in contact with a heat bath, which is initially in a thermal equilibrium. The particle is modeled as a Hamiltonian system and it moves in a potential U . The heat bath is modeled as a system of non-interacting harmonic oscillators whose initial energy is distributed according to the Gibbs distribution at temperature T . The Brownian particle is coupled to each harmonic oscillator in the bath. This model is used widely to study many systems in statistical physics [49, 114]. Our goal is to derive, at a formal level, a stochastic integro-differential equation (SIDE) for the position and momentum variable of the particle from a specified Hamiltonian. This derivation serves to motivate the class of SIDEs that we are studying in this subsection. We emphasize that our derivation here is certainly not original and follows closely that in [64] (see also an abstract approach in [156]). In fact, the derivation follows along the line of the program of Gibbs [49].

One approach to derive the equations is to assume first that there are finitely many harmonic oscillators in the bath (Kac-Zwanzig model [157, 9]). We then takes the thermodynamic limit by sending the number of oscillators to infinity in the resulting equations (replacing finite sum over oscillator frequencies by an integral), arguing that the set of frequencies must be dense to allow dissipation of energy from the system to the bath and to eliminate Poincaré recurrence. Another approach, which is more technically involved, is to replace the finite system of oscillator equations by an infinite system modeled by a wave equation [133, 126] (see Remark 1). See also [94, 31] and the references therein for an approach based on the Mori-Zwanzig projection formalism. We will derive the SIDEs by adopting the former approach in the multi-dimensional case.

We consider the situation where the coupling is nonlinear in the particle's position and linear in the bath variables. Let $\hat{\mathbf{x}} = (\mathbf{x}, \mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{d+d_1+\dots+d_N}$ and $\hat{\mathbf{p}} = (\mathbf{p}, \mathbf{p}_1, \dots, \mathbf{p}_N) \in \mathbb{R}^{d+d_1+\dots+d_N}$. Hereafter, the subscript $*$ denotes transposition and $|\mathbf{b}|^2 := \mathbf{b}^* \mathbf{b} = \sum_{k=1}^n b_k^2$ denotes the norm of vector $\mathbf{b} := (b_1, \dots, b_n) \in \mathbb{R}^n$.

The Hamiltonian of the system plus bath is:

$$H(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \frac{|\mathbf{p}|^2}{2m} + U(\mathbf{x}) + \sum_{k=1}^N \left(\frac{|\mathbf{p}_k|^2}{2} + \frac{1}{2} \omega_k^2 \left| \mathbf{x}_k - \frac{\mathbf{c}_k^*}{\omega_k^2} \mathbf{f}(\mathbf{x}) \right|^2 \right), \quad (4)$$

where m is the particle's mass, $\mathbf{x} \in \mathbb{R}^d$ and $\mathbf{p} \in \mathbb{R}^d$ are respectively the particle's position and momentum, $\mathbf{x}_k \in \mathbb{R}^{d_k}$, $\mathbf{p}_k \in \mathbb{R}^{d_k}$ and $\omega_k \in \mathbb{R}^+$ ($k = 1, \dots, N$) are respectively the position, momentum and frequency of the k th bath oscillator, $\mathbf{f}(\mathbf{x}) := (f_1(\mathbf{x}), \dots, f_r(\mathbf{x})) \in \mathbb{R}^r$ is a vector function of $\mathbf{x} := (x^{(1)}, \dots, x^{(d)})$ and the $\mathbf{c}_k \in \mathbb{R}^{r \times d_k}$ (so $\mathbf{c}_k^* \in \mathbb{R}^{d_k \times r}$) are coupling matrices that specify the coupling strength between the system and the k th bath oscillator. We assume each f_j ($j = 1, \dots, r$) is continuously differentiable in $x^{(k)}$, for every $k = 1, \dots, d$.

To derive an equation for the particle's position and momentum, we start by plugging the expression for $H(\hat{\mathbf{x}}, \hat{\mathbf{p}})$ into the Hamilton's equations to obtain:

$$\dot{\mathbf{x}} = \frac{\mathbf{p}}{m}, \quad (5)$$

$$\dot{\mathbf{p}} = -\nabla_{\mathbf{x}} U(\mathbf{x}) + \mathbf{g}(\mathbf{x}) \sum_k \mathbf{c}_k \left(\mathbf{x}_k - \frac{\mathbf{c}_k^*}{\omega_k^2} \mathbf{f}(\mathbf{x}) \right), \quad (6)$$

$$\mathbf{x}_k = \mathbf{p}_k, \quad k = 1, \dots, N, \quad (7)$$

$$\mathbf{p}_k = -\omega_k^2 \mathbf{x}_k + \mathbf{c}_k^* \mathbf{f}(\mathbf{x}), \quad k = 1, \dots, N, \quad (8)$$

where $\mathbf{g}(\mathbf{x}) \in \mathbb{R}^{d \times r}$ denotes the Jacobian matrix $\left(\frac{\partial f_i}{\partial x^{(j)}} \right)_{ij}$.

Next, we eliminate the bath variables $\mathbf{x}_k, \mathbf{p}_k$, $k = 1, \dots, N$, from the system's dynamics. Solving for $\mathbf{x}_k(t)$ in terms of $\mathbf{x}(t)$:

$$\mathbf{x}_k(t) = \mathbf{x}_k(0) \cos(\omega_k t) + \frac{\mathbf{p}_k(0)}{\omega_k} \sin(\omega_k t) + \frac{\mathbf{c}_k^*}{\omega_k} \int_0^t \sin(\omega_k(t-s)) \mathbf{f}(\mathbf{x}(s)) ds. \quad (9)$$

Plugging this into (6), we obtain:

$$\begin{aligned} \dot{\mathbf{p}}(t) = & -\nabla_{\mathbf{x}} U(\mathbf{x}(t)) + \mathbf{g}(\mathbf{x}(t)) \sum_k \frac{\mathbf{c}_k \mathbf{c}_k^*}{\omega_k^2} \left(\int_0^t \omega_k \sin(\omega_k(t-s)) \mathbf{f}(\mathbf{x}(s)) ds - \mathbf{f}(\mathbf{x}(t)) \right) \\ & + \mathbf{g}(\mathbf{x}(t)) \mathbf{F}(t), \end{aligned} \quad (10)$$

where

$$\mathbf{F}(t) = \sum_k \mathbf{c}_k \left(\mathbf{x}_k(0) \cos(\omega_k t) + \frac{\mathbf{p}_k(0)}{\omega_k} \sin(\omega_k t) \right). \quad (11)$$

In the integral term above, we integrate by parts to obtain:

$$\int_0^t \omega_k \sin(\omega_k(t-s)) \mathbf{f}(\mathbf{x}(s)) ds = \mathbf{f}(\mathbf{x}(t)) - \cos(\omega_k t) \mathbf{f}(\mathbf{x}(0)) - \int_0^t \cos(\omega_k(t-s)) \mathbf{g}^*(\mathbf{x}(s)) \dot{\mathbf{x}}(s) ds. \quad (12)$$

Using this, the equation for $\mathbf{p}(t)$ becomes the *generalized Langevin equation (GLE)*:

$$\dot{\mathbf{p}}(t) = -\nabla_{\mathbf{x}} U(\mathbf{x}(t)) - \mathbf{g}(\mathbf{x}(t)) \int_0^t \boldsymbol{\kappa}(t-s) \mathbf{g}^*(\mathbf{x}(s)) \dot{\mathbf{x}}(s) ds + \mathbf{g}(\mathbf{x}(t)) \boldsymbol{\xi}(t), \quad (13)$$

where

$$\boldsymbol{\kappa}(t) = \sum_k \frac{\mathbf{c}_k \mathbf{c}_k^*}{\omega_k^2} \cos(\omega_k t) \in \mathbb{R}^{r \times r} \quad (14)$$

and

$$\boldsymbol{\xi}(t) = \mathbf{F}(t) - \boldsymbol{\kappa}(t) \mathbf{f}(\mathbf{x}(0)) = \sum_k \mathbf{c}_k \left(\left(\mathbf{x}_k(0) - \frac{\mathbf{c}_k^*}{\omega_k^2} \mathbf{f}(\mathbf{x}(0)) \right) \cos(\omega_k t) + \frac{\mathbf{p}_k(0)}{\omega_k} \sin(\omega_k t) \right). \quad (15)$$

Note that $\boldsymbol{\xi}(t) \in \mathbb{R}^r$ is expressed in terms of the initial values of the variables $\mathbf{x}'_k(0) := \mathbf{x}_k(0) - \frac{\mathbf{c}_k^*}{\omega_k^2} \mathbf{f}(\mathbf{x}(0)) \in \mathbb{R}^p$ and $\mathbf{p}_k(0) \in \mathbb{R}^p$. If all these initial values are known, then $\boldsymbol{\xi}(t)$ is a deterministic force. However, one rarely has a complete information about these initial values and this is where the introduction of randomness can help to simplify the model. In view of this, we assume that the variables $\mathbf{x}'_k(0)$ and $\mathbf{p}_k(0)$ are random and are distributed according to a Gibbs measure, with the density:

$$\rho((\mathbf{x}_k, \mathbf{p}_k) \mid \mathbf{x}(0) = \mathbf{x}) = Z^{-1} \exp \left(-\beta \left(\sum_{k=1}^N \frac{|\mathbf{p}_k|^2}{2} + \frac{1}{2} \omega_k^2 \left| \mathbf{x}_k - \frac{\mathbf{c}_k^*}{\omega_k^2} \mathbf{f}(\mathbf{x}) \right|^2 \right) \right), \quad (16)$$

where $\beta = 1/(k_B T)$ and Z is the partition function. Taking the averages of the bath variables with respect to the above density:

$$E_\rho[\mathbf{x}'_k(0) \mid \mathbf{x}(0) = \mathbf{x}] = 0, \quad E_\rho[\mathbf{p}_k(0) \mid \mathbf{x}(0) = \mathbf{x}] = 0, \quad (17)$$

$$E_\rho[\mathbf{x}'_k(0)(\mathbf{x}'_k(0))^* \mid \mathbf{x}(0) = \mathbf{x}] = \frac{k_B T}{\omega_k^2} \mathbf{I}, \quad E_\rho[(\mathbf{p}_k(0)(\mathbf{p}_k(0))^* \mid \mathbf{x}(0) = \mathbf{x}] = k_B T \mathbf{I}, \quad (18)$$

where E_ρ denotes mathematical expectation with respect to ρ and $\mathbf{I} \in \mathbb{R}^{p \times p}$ is identity matrix.

Note that $\boldsymbol{\xi}(t)$ is a stationary, Gaussian process, if it is conditionally averaged with respect to ρ [157]. It follows from this distribution of the bath variables that we have the *fluctuation-dissipation relation*:

$$E_\rho[\boldsymbol{\xi}(t)] = 0, \quad E_\rho[\boldsymbol{\xi}(t) \boldsymbol{\xi}(s)^*] = k_B T \boldsymbol{\kappa}(t-s), \quad (19)$$

where $\boldsymbol{\kappa}(t-s)$ is the memory kernel whose formula is given in (14). Later, we will generalize the resulting covariance of the process $\boldsymbol{\xi}(t)$ to an integral expression. We remark that the memory function $\boldsymbol{\kappa}(t)$ and the ‘‘color’’ of the noise $\boldsymbol{\xi}(t)$ are determined by the bath spectrum and the system-bath coupling.

Now we pass to the continuum limit by replacing the sum over k in $\boldsymbol{\kappa}(t)$ by an integral $\int_{\mathbb{R}^+} d\omega n(\omega)$, where $n(\omega)$ is a density of states. Then, if the \mathbf{c}_k are replaced by $\mathbf{c}(\omega) \in \mathbb{R}^{r \times p}$, the memory function $\boldsymbol{\kappa}(t)$ becomes the function:

$$\boldsymbol{\kappa}(t) = \int_{\mathbb{R}^+} d\omega n(\omega) \frac{\mathbf{c}(\omega) \mathbf{c}(\omega)^*}{\omega^2} \cos(\omega t), \quad (20)$$

where $\hat{\kappa}_c(\omega) := n(\omega)c(\omega)c(\omega)^*/\omega^2 \in L^1(\mathbb{R}^+)$. Repeating the same procedure for the noise process and also replacing the $x'_k(0)$ and $p_k(0)$ by $x'(\omega)$ and $p(\omega)$ respectively, $\xi(t)$ becomes:

$$\xi(t) = \int_{\mathbb{R}^+} d\omega n(\omega)c(\omega) \left(x'(\omega) \cos(\omega t) + \frac{p(\omega)}{\omega} \sin(\omega t) \right). \quad (21)$$

The choice of the $n(\omega)$ and $c(\omega)$ specifies the memory function and therefore (by the fluctuation-dissipation relation) the statistical properties of the noise process. We write $\kappa(t)$ as an inverse Fourier transform of a measure:

$$\kappa(t) = \frac{1}{2\pi} \int_{\mathbb{R}} S(\omega) e^{i\omega t} d\omega, \quad (22)$$

where the measure is absolutely continuous with respect to the Lebesgue measure, with the density $S(\omega) = \pi \hat{\kappa}_c(\omega) \geq 0$. The density $S(\omega)$ is known as the *spectral density* of the bath.

Remark 1. As the heat bath has infinitely many degrees of freedom, it is physically more correct to derive the *SIDEs* starting from a an infinite dimensional Hamiltonian with continuous spectrum (as discussed in the introduction). We briefly mention how this can be done at the cost of higher level of difficulties. We restrict to one dimension for simplicity. This discussion will be useful when we consider a quantum version of open system. For details, we refer to Chapter 2 in [11]. The model for the heat bath, in accordance to the classical field theory, is modeled by the wave equation in \mathbb{R} :

$$\frac{\partial^2}{\partial t^2} \varphi_t(\omega) = \Delta_\omega \varphi_t(\omega), \quad (23)$$

where $\omega \in \Omega = \mathbb{R}$, $t \in \mathbb{R}$ and Δ_ω denotes the Laplacian. The wave equation is a second-order equation which can be written as the following system of first-order equations:

$$d\varphi_t(\omega) = \pi_t(\omega) dt, \quad (24)$$

$$d\pi_t(\omega) = \Delta_\omega \varphi_t(\omega) dt, \quad (25)$$

with initial conditions $\varphi_0(\omega) = \varphi(\omega)$ and $\pi_0(\omega) = \pi(\omega)$ to be specified. These are the Hamiltonian equations of motion whose dynamics are specified by the Hamiltonian function:

$$H_B(\varphi, \pi) = \frac{1}{2} \int_{\Omega} (|\nabla_\omega \varphi(\omega)|^2 + |\pi(\omega)|^2) d\omega. \quad (26)$$

Note that in the above, we have taken the frequency representation for modeling the environment, in contrast to the dual representation (via Fourier transformation) in spatial domain as adopted in Chapter 2 of [11]. The total system of the particle plus its environment is described by the Hamiltonian:

$$H = H_S + H_B + H_I, \quad (27)$$

where H_I describes the interaction between the particle and its environment and is assumed to be of the following dipole form:

$$H_I = -f(\mathbf{x}) \int_{\Omega} \nabla_\omega \varphi(\omega) c(\omega) d\omega, \quad (28)$$

where $c(\omega)$ is a coupling function and $f(\mathbf{x})$ is a (generally nonlinear) function of the particle's position $\mathbf{x} \in \mathbb{R}^d$.

So far we have not specified the initial conditions for the above model for the total system. Our goal is to model a situation where the particle not only dissipates energy into the environment but also “fluctuates” and eventually its dynamics relax to a “stationary state”. To allow this, we assume that the model is initially in thermal equilibrium at positive temperature $T > 0$, i.e. the initial conditions, $\{(\varphi(\omega), \pi(\omega)) : \omega \in \Omega\}$, of the wave equations are distributed according to a Gibbs measure at this temperature. In this case, the environment has infinite energy (or heat capacity) and therefore provides sufficient energy to achieve our goal. In fact, one expects “return to equilibrium” for the system, i.e. an initial distribution of the system will converge to a stationary state which is given by the Gibbs distribution, $Z^{-1} e^{-\beta H_S(\mathbf{x}, \mathbf{p})} d\mathbf{x} d\mathbf{p}$, where Z is the partition function and $\beta = 1/k_B T$. This introduces randomness³ into the otherwise deterministic Hamiltonian dynamics.

Now, technical difficulties arise when one tries to extend the Gibbs distribution to the infinite-dimensional setting as the following expression for the Gaussian measure, $\mu_\beta(d\pi d\varphi) = Z^{-1} e^{-\beta H_B(\varphi, \pi)} \prod_{\omega \in \mathbb{R}} d\pi d\varphi$, does not define a Gaussian density with respect to the Lebesgue measure (which does not exist in infinite dimensions!). One has to deal with this using the theory of Gaussian measures in Hilbert spaces (see [20, 78]). Once these are dealt with carefully, one can then show that the dynamics specified by the Hamiltonian above are equivalent to those by a *SIDE* of the form (13).

³Our notation of Ω resembles that for a sample space of elementary events in probability theory but this is actually not a deliberate choice of ours here!

Remark 2. An alternative approach, natural from the approximation theory and as outlined before Remark 1, is to justify rigorously the passage from (14) and (15) to (20) and (21) respectively. In our context, such limiting procedure constructs stationary Gaussian processes from deterministic ODEs with random initial conditions. Such construction can indeed be done and justified rigorously by adapting techniques from [149, 90, 88, 9], in which one of the key techniques is the Skorokhod embedding theorem [53]. Other approximation methods such as Monte Carlo approximation of (20) can also be considered [74]. See also [89, 111] for related results concerning derivation of stochastic models from deterministic ones and [146, 63] for numerical experiments. Note that, in this approach (15) is viewed as a random trigonometric series⁴, with the randomness coming from the initial variables $\mathbf{x}'_k(0)$ and $\mathbf{p}_k(0)$.

1.3 SDE Representation and Quasi-Markov Stationary Gaussian Processes

In this section, we define a class of stationary Gaussian processes [41, 155, 42] known as the quasi-Markov processes and characterize these processes in terms of Markovian representations in the form of Itô type stochastic differential equations (SDEs) on Euclidean space \mathbb{R}^n (n is a positive integer) driven by Wiener processes⁵. We assume familiarity⁶ with basic concepts in the theory of probability and stochastic processes in the following.

Fix a probability space (Ω, \mathcal{F}, P) and denotes expectation with respect to P by \mathbb{E} .

Definition 1. We say that a stochastic process, $\{\mathbf{y}_t \in \mathbb{R}^m; t \in [0, T]\}$, admits a SDE representation if it can be represented as $\mathbf{y}_t = \mathbf{c}(\mathbf{x}_t)$, where $\mathbf{x}_t \in \mathbb{R}^n$ is the solution of the following Itô SDE:

$$d\mathbf{x}_t = \mathbf{a}(t, \mathbf{x}_t)dt + \mathbf{b}(t, \mathbf{x}_t)d\mathbf{W}_t, \quad (29)$$

with initial condition $\mathbf{x}_0 = \mathbf{x}$. In the above, $\mathbf{a} : [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}^n$, $\mathbf{b} : [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}^{n \times r}$, $\mathbf{c} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ are measurable functions, and $\{\mathbf{W}_t \in \mathbb{R}^r : t \geq 0\}$ is a Wiener process, i.e. a family of random variables which is Gaussian with mean $\mathbb{E}\mathbf{W}_t = 0$ and has covariance $\mathbb{E}\mathbf{W}_t\mathbf{W}_s^* = \min(t, s)\mathbf{I}$, where $\mathbf{I} \in \mathbb{R}^{r \times r}$ is identity matrix. The initial condition \mathbf{x} can be either deterministic or a random variable that is independent of the Wiener process.

The formal derivative of the Wiener process, $\zeta_t := \frac{d\mathbf{W}_t}{dt}$, is a white noise process, i.e. a (generalized⁷) mean-zero Gaussian vector-valued stochastic process with correlation function $\mathbb{E}\zeta_t\zeta_s^* = \delta(t-s)\mathbf{I}$. It serves as an idealized model for a random disturbance imparted to the otherwise deterministic ordinary differential equation, $d\mathbf{x}_t = \mathbf{a}(t, \mathbf{x}_t)dt$. We call \mathbf{a} the *drift coefficient* and the amplitude of the noise, \mathbf{b} , the *noise coefficient* or *diffusion coefficient* of the SDE. In the context of stochastic modeling, it is useful to distinguish two different natures of the driving noise in the SDE. If \mathbf{b} is a constant, we will say that the noise is additive. If \mathbf{b} depends on the state \mathbf{x}_t of the system, we will say that the noise is multiplicative.

The correct interpretation for the SDE (29) is as the stochastic integral equation:

$$\mathbf{x}_t = \mathbf{x} + \int_0^t \mathbf{a}(s, \mathbf{x}_s)ds + \int_0^t \mathbf{b}(s, \mathbf{x}_s)d\mathbf{W}_s, \quad (30)$$

almost surely (a.s.), where the last integral term above is an Itô integral, as carefully⁸ defined in the Itô theory of stochastic integration. A precise notion of solution to the SDE (1) involves the above integral interpretation, specification of appropriate classes of functions which \mathbf{a} and \mathbf{b} belong to, as well as desired properties of the solution \mathbf{x}_t . There are different notions of solution for SDE of type (1).

In the Definition 1, the functions \mathbf{a} and \mathbf{b} are assumed to be belong to appropriate classes of functions such that the SDE (29) has a pathwise unique solution up to the time T . A general sufficient condition for existence and uniqueness of solution, up to its explosion time⁹, of the SDE is, roughly speaking¹⁰, when \mathbf{a} and \mathbf{b} are locally Lipschitz (see Theorem

⁴This viewpoint is an old one, dated as early as the days of Paley, Wiener and Zygmund. We refer to [80, 48, 81] for review, history and connection to other areas of mathematics.

⁵One could consider, for instance, SDEs on manifolds driven by continuous semimartingales. We will not treat classes of SDEs that are more general than the one defined here in this thesis.

⁶We refer to [10, 44, 121] for mathematically rigorous introductions and [50, 140] for applications.

⁷See [77, 52, 68] for alternative approaches to study white noise. Note that the SDE is written in a differential form due to the generalized nature of the white noise.

⁸Recall that the Wiener paths $t \mapsto W_t(\omega)$ ($\omega \in \Omega$) are continuous but nowhere differentiable a.s.. Moreover, it is not of bounded variation, so the integral cannot be defined as a Riemann-Stieltjes integral in a unique way. Different Riemann-Stieltjes approximations lead to different stochastic integrals (the Itô integrals and Stratonovich integrals are two important ones), which, in turn, lead to SDEs with different properties. This is an important lesson from the point of view of stochastic modeling.

⁹i.e. the maximum stopping time up to which a solution of the SDE can be defined.

¹⁰These conditions depend on the notion of “solution” to the SDE that one introduces.

1.1.8 in [69] for precise formulation; see also [75, 100]). The global existence and uniqueness result (i.e. for all time $t \geq 0$) can be obtained by imposing additional assumptions on \mathbf{a} and \mathbf{b} . Typically, one additionally imposes a linear growth type condition (see [106]) or assumption on a Lyapunov function associated to the SDE (see Theorem 5.9 in [17] or the text [83]).

We now elaborate more on the above discussions through a simple mathematical formulation¹¹. We emphasize that in the following we are not including various extensions of the formulation to keep the technicalities involved to a bare minimum. Let us start by defining Itô stochastic integrals. For simplicity, we restrict to scalar processes. Generalization to vector-valued processes is straightforward. Let $b(t)$ be a random process on $[0, T]$ which is adapted to the filtration $\mathcal{F}_t = \sigma(\{W_s : s \leq t\})$ generated by the Wiener process $\{W_s : s \leq t\}$, i.e. it is an \mathcal{F}_t -measurable function for all $t \in [0, T]$. Assume that $b(\cdot)$ is square-integrable, i.e. $\mathbb{E} \int_0^T |b(s)|^2 ds < \infty$. We define the stochastic integral:

$$B(t) = \int_0^t b(s) dW_s, \quad (31)$$

as the $L_2(\Omega)$ limit of the Riemann sum approximation:

$$B_a(t) = \lim_{N \rightarrow \infty} \sum_{n=0}^{N-1} b(\tau_n)(W(t_{n+1}) - W(t_n)), \quad (32)$$

where we have introduced a partition of the interval $[0, t]$ by letting $t_n = n\Delta t$, $n = 0, 1, \dots, N-1$ and $N\Delta t = t$, and for $a \in [0, 1]$, $\tau_n := (1-a)t_n + at_{n+1}$ for $n = 0, 1, \dots, N-1$. The *Itô stochastic integral* is defined as the integral $B_0(t)$, corresponding to the choice of $a = 0$ in the formula for $B_a(t)$ above. It is a diffusion process (i.e. it is a Markov¹² process with a continuous sample path), satisfies the Itô isometry:

$$\mathbb{E} \left(\int_0^T b(s) dW_s \right)^2 = \int_0^T \mathbb{E} |b(s)|^2 ds, \quad (33)$$

and has the quadratic variation:

$$\langle B \rangle_t := \lim_{|P| \rightarrow 0} \sum_{n=0}^{N-1} |B_{t_{n+1}} - B_{t_n}|^2 = \int_0^t b(s)^2 ds, \quad (34)$$

where P ranges over the partition $\{t_0, \dots, t_{N-1}\}$ of $[0, t]$ and $|P|$ is the mesh of the partition P .

We now define a notion of solution to SDE (1) and provide a result on the existence and uniqueness of its solution.

Definition 2. Strong solution of SDE. A process \mathbf{x}_t with continuous paths defined on the probability space (Ω, \mathcal{F}, P) is called a *strong solution*¹³ to the SDE (1) if:

- (i) \mathbf{x}_t is almost surely continuous and adapted to the filtration \mathcal{F}_t generated by the Wiener process $\{\mathbf{W}_s, s \leq t\}$ and \mathbf{x} (independent of the Wiener process)¹⁴;
- (ii) $\mathbf{b}(\cdot, \mathbf{x}_\cdot) \in L^1([0, T]; \mathbb{R}^n)$ and $\boldsymbol{\sigma}(\cdot, \mathbf{x}_\cdot) \in L^2([0, T]; \mathbb{R}^{n \times r})$ almost surely;
- (iii) For every $t \geq 0$, the stochastic integral equation (30), with $\mathbf{x}_0 = \mathbf{x}$, holds almost surely.

A simple approach to obtain result on existence and uniqueness of solution for SDEs is to impose the Lipschitz continuity assumption and a linear growth condition (which prevents the solution from exploding in finite time), familiar from the existence and uniqueness theory of ordinary differential equations.

Theorem 1. Global existence and uniqueness of solution to SDE. Assume that $\mathbf{a}(\cdot, \cdot)$ and $\mathbf{b}(\cdot, \cdot)$ satisfy the following (global) Lipschitz continuity assumption and linear growth condition, i.e. there exists a positive constant C such that for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and $t \in [0, T]$,

$$|\mathbf{a}(t, \mathbf{x}) - \mathbf{a}(t, \mathbf{y})| + |\mathbf{b}(t, \mathbf{x}) - \mathbf{b}(t, \mathbf{y})|_F \leq C|\mathbf{x} - \mathbf{y}|, \quad (35)$$

¹¹ At the introductory level of, for instance, [44].

¹² Recall that an adapted process x_t (with respect to $\{\mathcal{F}_t : t \geq 0\}$) is *Markov* if for any $s, t \geq 0$ and any bounded continuous real-valued function f , $\mathbb{E}[f(x_{s+t})|\mathcal{F}_s] = \mathbb{E}[f(x_{s+t})|x_s]$ a.s..

¹³ There is also a notion of weak solution. Throughout this paper, a solution to a SDE is meant in the strong sense.

¹⁴ Condition (i) implies that \mathbf{x}_t is progressively measurable with respect to \mathcal{F}_t , so our definition here is a bit less general than the one in page 81-82 of [44].

and

$$|\mathbf{a}(t, \mathbf{x})| + |\mathbf{b}(t, \mathbf{x})|_F \leq C(1 + |\mathbf{x}|), \quad (36)$$

where $|\cdot|_F$ denotes Frobenius norm. Moreover, assume that $\mathbf{x}_0 = \mathbf{x}$ is a random variable independent of the Wiener process \mathbf{W}_t with finite second moment, $\mathbb{E}|\mathbf{x}|^2 < \infty$.

Then the SDE (1) has a unique (strong) solution \mathbf{x}_t with $\mathbb{E} \int_0^t |\mathbf{x}_s|^2 ds < \infty$ for every $t > 0$.

Proof. See page 90-94 in [44]. □

The uniqueness of the solution is in the sense that if there exists two solutions \mathbf{x}_t and \mathbf{y}_t satisfying the SDE, then $\mathbf{x}_t = \mathbf{y}_t$ for all t almost surely. Note that when the above globally Lipschitz condition on the drift and noise coefficient holds, the linear growth condition above is equivalent to the condition that both $|\mathbf{a}(t, \mathbf{0})|$ and $|\mathbf{b}(t, \mathbf{0})|$ be bounded for every $t \geq 0$. It can also be shown that the solution \mathbf{x}_t of the SDE is a semimartingale and a diffusion process.

Usually one is interested in the case when the SDE is autonomous, i.e. $\mathbf{a} = \mathbf{a}(\mathbf{x}_t)$ and $\mathbf{b} = \mathbf{b}(\mathbf{x}_t)$ do not show explicit dependence on the time t . In this case, recall that \mathbf{x}_t is a diffusion process and there is an associated second-order differential operator, the infinitesimal generator of the process:

$$\mathcal{L} = \sum_{i=1}^n a_i(\mathbf{x}) \frac{\partial}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^n \Sigma_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} =: \mathbf{a}(\mathbf{x}) \cdot \nabla + \frac{1}{2} \Sigma(\mathbf{x}) : D^2, \quad (37)$$

where the $\Sigma_{i,j}$ denote the matrix elements of the matrix $\Sigma(\mathbf{x}) = \mathbf{b}(\mathbf{x})\mathbf{b}(\mathbf{x})^T$, ∇ denotes the gradient operator, D^2 denotes the Hessian matrix and $:$ denotes inner product between two matrices defined by $\mathbf{A} : \mathbf{B} = \text{Tr}(\mathbf{A}^T \mathbf{B}) = \sum_{i,j} A_{i,j} B_{i,j}$ (the superscript T denotes transposition).

Of interest is a formula that allows us to compute the rate of change in time of a sufficiently nice function $F : [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}$ evaluated at the solution $\mathbf{x}_t \in \mathbb{R}^n$ of the SDE. This is an important result at the heart¹⁵ of stochastic calculus.

Theorem 2. Itô's formula^a. Assume that the assumptions in Theorem 1 hold and let \mathbf{x}_t be the solution of the autonomous SDE (1). Assume that $F \in C^{1,2}([0, T] \times \mathbb{R}^n)$. Then the process $F(\mathbf{x}_t)$ satisfies:

$$F(t, \mathbf{x}_t) = F(\mathbf{x}_0) + \int_0^t \frac{\partial F}{\partial s}(s, \mathbf{x}_s) ds + \int_0^t \mathcal{L}F(s, \mathbf{x}_s) ds + \int_0^t (\nabla F(s, \mathbf{x}_s)) \cdot \mathbf{b}(\mathbf{x}_s) d\mathbf{W}_s, \quad (38)$$

where \mathcal{L} is the infinitesimal generator for the process \mathbf{x}_t , or, in the differential form:

$$dF(t, \mathbf{x}_t) = \frac{\partial F}{\partial t} dt + \sum_{i=1}^n \frac{\partial F}{\partial x_i} dx_i + \frac{1}{2} \sum_{i,j=1}^n \frac{\partial^2 F}{\partial x_i \partial x_j} dx_i dx_j, \quad (39)$$

where the convention $dW_i(t)dW_j(t) = \delta_{i,j}dt$, $dW_i(t)dt = 0$ for $i, j = 1, \dots, n$ is used.

^aItô's formula also holds for stopping times.

Proof. See page 78-79 in [44]. □

Using the Itô's formula, one can obtain a partial differential equation (PDE) describing the expectation of a functional, $u(\mathbf{x}, t) := \mathbb{E}[\phi(\mathbf{x}_t) | \mathbf{x}_0 = \mathbf{x}]$, $\phi \in C^2(\mathbb{R}^n)$, of the solution \mathbf{x}_t to the SDE. Indeed, applying the Itô's formula to u , using the martingale property of stochastic integrals and differentiating with respect to time gives the *backward Kolmogorov equation*:

$$\frac{\partial u}{\partial t} = \mathcal{L}u, \quad u(\mathbf{x}, 0) = \phi(\mathbf{x}), \quad (40)$$

and its solution can be expressed via the semigroup generated by \mathcal{L} , i.e. $u(\mathbf{x}, t) = (e^{t\mathcal{L}}\phi)(\mathbf{x})$. The adjoint equation of the backward Kolmogorov equation is the *forward Kolmogorov equation* (Fokker-Planck equation) for the probability

¹⁵There are many important applications of Itô's formula. Perhaps an intriguing example is the computation of the stochastic integral $\int_0^t W_s dW_s \in \mathbb{R}$. More generally, one compute $\int_0^t h_n(W_s, s) dW_s = h_{n+1}(W_t, t)$, where $h_n(x, s)$ ($n = 0, 1, \dots$) is the n th Hermite polynomial. This result can also be derived using the exponential martingale (generating function of the Hermite polynomial), which has connections to the quantum stochastic calculus (see Example 5).

density $\rho(\mathbf{x}, t) \in C^{2,1}(\mathbb{R}^n \times (0, \infty))$ of the process \mathbf{x}_t (with initial density $\rho_0(\mathbf{x})$):

$$\frac{\partial \rho}{\partial t} = \mathcal{L}^* \rho, \quad \rho = \rho_0 \text{ for } \mathbf{x} \in \mathbb{R}^n \times \{0\}, \quad (41)$$

where $\mathcal{L}^* = \nabla \cdot (-\mathbf{a}(\mathbf{x}) \cdot + \frac{1}{2} \nabla \cdot (\Sigma(\mathbf{x}) \cdot))$ is the L_2 -adjoint of the generator \mathcal{L} .

In the context of stochastic modeling of the noise process $\xi(t)$ in (13), we are interested in real-valued processes that are mean-square continuous, mean-zero Gaussian and stationary ($\mathbb{E}\mathbf{y}_t = \mathbf{0}$ and $\mathbb{E}\mathbf{y}_t^2 < \infty$) [34]. The Gaussianness and stationarity of \mathbf{y}_t should be inherited by the Markov process \mathbf{x}_t . Therefore, we are led to consider linear time-invariant SDE representation of the type

$$d\mathbf{x}_t = \mathbf{A}\mathbf{x}_t dt + \mathbf{B}d\mathbf{W}_t, \quad (42)$$

$$\mathbf{y}_t = \mathbf{C}\mathbf{x}_t, \quad (43)$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times r}$, $\mathbf{C} \in \mathbb{R}^{m \times n}$ are constant matrices. Therefore,

$$\mathbf{y}_t = \mathbf{C}e^{\mathbf{A}t}\mathbf{x} + \int_0^t \mathbf{C}e^{\mathbf{A}(t-s)}\mathbf{B}d\mathbf{W}_s, \quad (44)$$

where the initial time is taken to be $t = 0$, and we see that the SDE representation is a particular time representation of the process \mathbf{y}_t .

We assume that \mathbf{A} is *Hurwitz stable* (or $-\mathbf{A}$ is *positive stable*), i.e. the real parts of all eigenvalues of \mathbf{A} are negative, and the initial condition \mathbf{x} is a mean-zero Gaussian random variable with covariance matrix \mathbf{M} satisfying the *Lyapunov equation*¹⁶:

$$\mathbf{A}\mathbf{M} + \mathbf{M}\mathbf{A}^T = -\mathbf{B}\mathbf{B}^T. \quad (45)$$

Then one computes that the covariance function of \mathbf{y}_t equals:

$$\mathbf{R}(t-s) := \mathbb{E}\mathbf{y}_t\mathbf{y}_s^T = \mathbf{C}e^{\mathbf{A}(t-s)}\mathbf{M}\mathbf{C}^T, \quad (46)$$

where $t > s \geq 0$. Note that since \mathbf{y}_t is stationary, the covariance function depends only on the time difference $\tau = t - s$.

Denote by \mathcal{G} the class of the real-valued, mean-square continuous, mean-zero stationary Gaussian processes. A subclass of \mathcal{G} known as the quasi-Markov processes is of particular interest to us.

Definition 3. Let $\{\mathbf{y}_t \in \mathbb{R}^m : t \in [0, T]\}$ be a stochastic process in \mathcal{G} . We say that \mathbf{y}_t is a quasi-Markov process in \mathcal{G} if it has a SDE representation of the form (42)-(43), specified by the triple $(\mathbf{A}, \mathbf{B}, \mathbf{C})$ of matrices of appropriate dimensions. Here \mathbf{A} is Hurwitz stable and the initial condition \mathbf{x} is a mean-zero Gaussian random variable with covariance matrix \mathbf{M} such that the Lyapunov equation $\mathbf{A}\mathbf{M} + \mathbf{M}\mathbf{A}^T = -\mathbf{B}\mathbf{B}^T$ is satisfied.

We now look at an equivalent representation in the frequency domain. It is useful to view the Gaussian process, $t \rightarrow \mathbf{y}_t = (y_t^1, \dots, y_t^m)$ ($t \in [0, T]$), as a curve in the real Hilbert space of $L^2(\Omega, \mathcal{F}, P)$. In particular, all the probability information about \mathbf{y}_t is encoded in the subspace $\mathcal{H}(\mathbf{y}) \subset L^2(\Omega, \mathcal{F}, P)$, where $\mathcal{H}(\mathbf{y})$ is the closed subspace spanned by the process \mathbf{y}_t , i.e. $\mathcal{H}(\mathbf{y}) = \text{span}\{y_t^k : t \in [0, T], k = 1, \dots, m\}$. Recall that for a (mean-square continuous) stationary stochastic process, $t \mapsto \mathbf{y}_t$, there exists a (strongly continuous) one-parameter group $\{\mathbf{U}_t : t \in \mathbb{R}\}$ of unitary operators on $\mathcal{H}(\mathbf{y})$ such that for any time $t > 0$, one has $\mathbf{y}_t = \mathbf{U}_t\mathbf{y}$. Note that the group preserves expectation.

By the Stone-von Neumann theorem [131], \mathbf{y}_t can be written uniquely as

$$\mathbf{U}_t\mathbf{y} = \int_{\mathbb{R}} e^{i\omega t} d\mathbf{E}(\omega)\mathbf{y}, \quad (47)$$

where $\mathbf{E}(\cdot)$ is the spectral measure mapping Borel subsets of real line into orthogonal projection operators on $\mathcal{H}(\mathbf{y})$ and $d\mathbf{E}(\omega)\mathbf{y}$ can be viewed as a stochastic measure. In this way, one obtains a spectral representation for the stationary Gaussian process \mathbf{y}_t . More generally:

Theorem 3. Every stationary process $\{\mathbf{y}_t : t \in \mathbb{R}\}$, continuous in mean-square, admits a representation

$$\mathbf{y}_t = \int_{\mathbb{R}} e^{i\omega t} d\hat{\mathbf{y}}(\omega), \quad t \in \mathbb{R}, \quad (48)$$

where $d\hat{\mathbf{y}}$ is a finite vector-valued orthogonal stochastic measure uniquely determined by the process, and satisfies

$$\mathbb{E}d\hat{\mathbf{y}}(\omega) = \mathbf{0}, \quad \mathbb{E}|d\hat{\mathbf{y}}(\omega)|^2 = d\mathbf{F}(\omega), \quad (49)$$

¹⁶By our assumption on \mathbf{A} , there exists a unique solution to the Lyapunov equation. Furthermore, the solution is given by $\mathbf{M} = \int_0^\infty e^{\mathbf{A}y}\mathbf{B}\mathbf{B}^T e^{\mathbf{A}^T y} dy$ (also known as the controllability gramian) [18].

where \mathbf{F} is the spectral distribution function of (\mathbf{y}_t) . The orthogonal stochastic measure $\hat{\mathbf{y}}(\omega)$ is called the Fourier transform of the stationary process \mathbf{y}_t .

Proof. See Theorem 3.3.2 in [99]. □

In particular, consider the one-dimensional stationary linear process of form

$$\xi_t = \int_{\mathbb{R}} w(t-s)\eta(ds), \quad (50)$$

$t \in \mathbb{R}$, where $\eta(dt)$ is the standard stochastic measure with orthogonal values on $t \in \mathbb{R}$ such that $\mathbb{E}\eta(dt) = 0$, $\mathbb{E}|\eta(dt)|^2 = dt$, with the weight function $w(t)$ satisfying $\int_{\mathbb{R}} |w(t)|^2 dt < \infty$ (for instance, ξ_t is a stochastic integral). Then ξ_t has a spectral representation:

$$\xi_t = \int_{\mathbb{R}} e^{i\omega t} \phi(\omega) d\hat{W}(\omega), \quad (51)$$

where $d\hat{W}(\omega)$ is a stochastic measure with orthogonal values on \mathbb{R} such that $\mathbb{E}\hat{W}(\omega) = 0$ and $\mathbb{E}|d\hat{W}(\omega)|^2 = d\omega/(2\pi)$, i.e. \hat{W} is the Fourier transform of the Wiener process (W_t) , and $\phi(\omega)$ is a non-random function expressible as the Fourier transform of the weight function $w(t)$:

$$\phi(\omega) = \int_{\mathbb{R}} e^{-i\omega t} w(t) dt. \quad (52)$$

Equation (51) represents the harmonic oscillations $\phi(\omega)e^{i\omega t}$ of frequency ω and the spectral density $S(\omega) = |\phi(\omega)|^2$ characterizes the weight of the different harmonic components of the process depending on the frequency ω [135].

One natural task is to characterize all processes that admit a (finite-dimensional) SDE representation in terms of their statistical properties (i.e. their covariance function and spectral distribution function).

Theorem 4. *The following statements are equivalent.*

- (i) *There exists finite-dimensional SDE representations of $\mathbf{y}_t \in \mathcal{G}$;*
- (ii) *The spectral distribution function, \mathbf{F} , of the process is absolutely continuous with a rational spectral density \mathbf{S} , i.e. $\mathbf{S}(\omega) = \frac{d}{d\omega} \mathbf{F}(\omega)$;*
- (iii) *The covariance function, $\mathbf{R}(t) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathbf{S}(\omega) e^{i\omega t} d\omega$, of the process is a Bohl function, i.e. its matrix elements are finite linear combination of products of an exponential, a polynomial, a sine or cosine function.*

Proof. To show (i) is equivalent to (ii), see Corollary 10.3.4 in [99]. To show (ii) is equivalent to (iii), apply Theorem 2.20 in [148] to $\mathbf{R}(t)$. □

In experimental situations, one typically only has spectral information about a noise process; for instance its spectral density [54]. It is then important to be able to model the noise process based on this information. The construction of a SDE representation (i.e. identification of the triple $(\mathbf{A}, \mathbf{B}, \mathbf{C})$) for a quasi-Markov process in \mathcal{G} given its spectral density or covariance function is the problem of stochastic realization, which has interesting connections to the Lax-Phillips scattering theory and can be formulated in a coordinate-free approach (see the monograph [99]), that are worth mentioning. The following result solves the problem in our case (see [99, 129] for details).

Algorithm 1. *A SDE representation of a quasi-Markov process \mathbf{y}_t , given its spectral density \mathbf{S} , can be computed via the following procedures:*

- (1) *Find a spectral factorization of $\mathbf{S}(\omega)$, i.e. find a rational $m \times r$ matrix function Φ such that $\mathbf{S}(\omega) = \Phi(i\omega)\Phi(i\omega)^*$, where Φ is an analytic spectral factor (i.e. all its poles lie in the left half plane) and $*$ denotes conjugate transpose. For simplicity, restrict to left-invertible factors, with the rank of \mathbf{S} equals to r .*
- (2) *For each such spectral factor Φ , define the Gaussian process \mathbf{W}_t by specifying its Fourier transform $\hat{\mathbf{W}}(\omega)$ as:*

$$d\hat{\mathbf{W}}(\omega) = \Phi^{-L}(i\omega) d\hat{\mathbf{y}}(\omega), \quad (53)$$

where $-L$ denotes left inverse. Then it is easy to see that \mathbf{W}_t is a \mathbb{R}^d -valued Wiener process and \mathbf{y}_t admits the spectral representation:

$$\mathbf{y}_t = \int_{\mathbb{R}} e^{i\omega t} \Phi(i\omega) d\hat{\mathbf{W}}(\omega). \quad (54)$$

(3) Compute a minimal realization of the spectral factor $\Phi(i\omega)$ of the form

$$\Phi(i\omega) = \mathbf{C}(i\omega \mathbf{I} - \mathbf{A})^{-1} \mathbf{B}, \quad (55)$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$ is a Hurwitz stable matrix, $\mathbf{B} \in \mathbb{R}^{n \times r}$ and $\mathbf{C} \in \mathbb{R}^{m \times n}$ are constant matrices such that $\mathbf{A}\mathbf{M} + \mathbf{M}\mathbf{A}^T = -\mathbf{B}\mathbf{B}^T$, with n as small as possible.

Therefore, corresponding to every spectral factor Φ , \mathbf{y}_t admits a SDE representation of the form as defined in Definition 3. The representation obtained is unique up to a change of basis on the state space and an orthogonal transformation on the Wiener process \mathbf{W}_t .

Now we return to our earlier discussions of open systems. Observe that after taking the thermodynamic limit the noise process $\xi(t)$ in (21) can be seen to be already in a form of spectral representation, with the initial “field variables” $(\mathbf{x}'(\omega), \mathbf{p}(\omega))$ (conditionally) distributed according to a Gibbs measure. This justifies our stochastic modeling of the noise process.

We now apply the above algorithm by factorizing $\mathbf{S}(\omega) = \Phi(i\omega)\Phi^*(i\omega)$, where $\Phi(i\omega) = \sqrt{\pi n(\omega)/\omega^2} \mathbf{c}(i\omega)$ is a spectral factor of the spectral density. The following examples give realization of a few noise processes. We take $n(\omega) = 2\omega^2/\pi$ (Debye-type spectrum for phonon bath) in all these examples.

Example 1. If we choose $\mathbf{c}(\omega) \in \mathbb{R}^{d \times d}$ to be a scalar multiple of the identity matrix \mathbf{I} , then $\kappa(t)$ is proportional to $\delta(t)\mathbf{I}$. This leads to a Langevin equation driven by white noise, in which the damping term is instantaneous. In this case, we have the SDE system for $(\mathbf{x}_t, \mathbf{v}_t) \in \mathbb{R}^{d \times d}$:

$$d\mathbf{x}_t = \mathbf{v}_t dt, \quad (56)$$

$$m d\mathbf{v}_t = -\nabla_{\mathbf{x}} U(\mathbf{x}_t) dt - \mathbf{g}^2(\mathbf{x}_t) \mathbf{v}_t dt + \mathbf{g}(\mathbf{x}_t) d\mathbf{W}_t, \quad (57)$$

where \mathbf{W}_t is the Wiener process.

The above SDE system can also be obtained as a Markovian limit of the GLE [126].

In the special case where $\mathbf{g}(\mathbf{x}_t) = \mathbf{g}$ is a constant matrix and $U(\mathbf{x}) = \frac{1}{2} k \mathbf{x}^2$ (harmonic potential) or $U(\mathbf{x}) = \mathbf{0}$ (free particle case), both the GLE and the SDE system (56)-(57) are exactly solvable. Interestingly, in this special case and in one dimension ($d = 1$), the SDE system (56)-(57) can be derived from the Lamb’s model [91] and constructed using a dilation procedure (see [104, 96] for details and other Hamiltonian models for open systems).

Example 2. If we choose $\mathbf{c}(\omega) \in \mathbb{R}^{d \times d}$ to be the diagonal matrix with the k th entry

$$\frac{\alpha_k}{\sqrt{\alpha_k^2 + \omega^2}}, \quad (58)$$

where the $\alpha_k > 0$, then we have:

$$\kappa(t) = \mathbf{A} e^{-\mathbf{A}t}, \quad (59)$$

where \mathbf{A} is the constant diagonal matrix with the k th entry equal α_k . On the other hand, choosing $\mathbf{c}(\omega)$ to be the diagonal matrix with the k th entry

$$\left(\frac{\omega_{kk}}{\tau_{kk}} \right)^2 \frac{1}{\sqrt{\omega^2 (\omega_{kk}^2 / \tau_{kk})^2 + (\omega^2 - (\omega_{kk} / \tau_{kk})^2)^2}} \quad (60)$$

allows us to obtain the covariance function of a harmonic noise process, where the ω_{kk} and τ_{kk} are the diagonal entries of the matrix Ω and τ respectively. In the general case where $\kappa(t)$ is written as $\mathbf{C}_1 e^{-\Gamma_1 t} \mathbf{M}_1 \mathbf{C}_1^*$, one may take $\mathbf{M}_1 = \mathbf{I}$, Γ_1 to be positive definite, in which case the Lyapunov equation gives $\Gamma_1 = \Sigma_1 \Sigma_1^* / 2$, and choose

$$\mathbf{c}(\omega) = \frac{1}{\sqrt{2}} \mathbf{C}_1 (\Gamma_1^2 + \omega^2 \mathbf{I})^{-1/2} \Sigma_1. \quad (61)$$

To summarize, stochastic integro-differential equations (SIDEs) of the following form appear naturally from the studies of open classical systems:

$$m \ddot{\mathbf{x}}(t) = \mathbf{F}(\mathbf{x}(t)) - \mathbf{g}(\mathbf{x}(t)) \int_0^t \kappa(t-s) \mathbf{h}(\mathbf{x}(s)) \dot{\mathbf{x}}(s) ds + \sigma(\mathbf{x}(t)) \xi(t), \quad (62)$$

where $m > 0$ is the mass of the particle, \mathbf{F} represents the external force, $\kappa(t)$ is a memory function, $\xi(t)$ is a stationary Gaussian process, and \mathbf{g} , \mathbf{h} and σ are state-dependent coefficients.

Let us consider the special case where the memory function and the covariance function of the driving noise are Bohl. An immediate consequence of Theorem 4 allows us to embed the resulting process $\mathbf{x}(t)$, satisfying (62), as a component of a higher dimensional process which admits a SDE representation. This approach makes available various tools and techniques from the Markov theory of stochastic processes and can be exploited to study homogenization of GLEs.

To end this section, we give a brief literature review on works related to the GLEs. A basic form of the GLEs (62) was first introduced by Mori in [114] and subsequently used to model many systems in statistical physics [87, 147, 59]. As remarked by van Kampen in [150], “Non-Markov is the rule, Markov is the exception”. Therefore, it is not surprising that non-Markovian equations (including those of form (62)) find numerous applications and thus have been studied widely in the mathematical, physical and engineering literature (see [101, 138] for surveys of non-Markovian processes). In particular, GLEs have been widely used as models to study many systems and have attracted increasing interest in recent years. We refer to, for instance, [144, 110, 102, 5, 141, 67, 33, 93] for various applications of GLEs and [122, 109, 1, 94, 117] for asymptotic analysis of GLEs.

2 Mathematical Concepts and Formulations of Quantum Mechanics

We now switch our attention to the quantum theory formulated in the language of quantum probability. Quantum probability is a version of noncommutative probability theory that not only extends Kolmogorov’s classical probability theory, but also provides a natural framework to study quantum mechanical systems. In fact, its development was aided by statistical ideas and concepts from quantum theory. It is the foundation for construction of quantum stochastic calculus (QSC) and quantum stochastic differential equations (QSDEs), which extend classical stochastic calculus and SDEs. The basic rigorous construction of QSC and QSDEs was first laid out in the seminal¹⁷ work of Hudson and Parthasarathy (H-P) [72]. Modeling quantum mechanics as a noncommutative probability theory is a fruitful mathematical approach. In the last few decades, the quantum probability formalism has been widely applied to study open quantum systems. On the other hand, the classical stochastic calculus of Itô has deep connection with objects such as the Fock space and the Heisenberg uncertainty principle [19].

In this section, we give a quick overview of quantum probability. We follow closely the notations and expositions in [123]. For comprehensive accounts of quantum probability, we refer to the monographs [123] and [113]. For recent developments, perspectives and applications of the calculus to the study of open quantum systems, we refer to [70, 45, 11, 23, 119, 43, 15, 61, 58, 143].

Notation. $[A, B] := AB - BA$ and $\{A, B\} := AB + BA$ denote, respectively, the commutator and anti-commutator of the operators A and B . The symbol I denotes identity operator on an understood space. We denote by $\mathcal{B}(\mathcal{H})$ the algebra of all bounded operators on the Hilbert space \mathcal{H} , with the inner product $\langle \cdot | \cdot \rangle$, which is linear in the second argument and antilinear in the first. We are using Dirac’s bra-ket notation, so we will write, for instance, the vector $u \in \mathcal{H}$ as the ket $|u\rangle$. For $X \in \mathcal{B}(\mathcal{H})$, $u, v \in \mathcal{H}$, we write $\langle u | X | v \rangle = \langle u | Xv \rangle = \langle X^*u | v \rangle$. We recall that unbounded operators are defined only on a linear manifold in \mathcal{H} (the domain of the operators). Two unbounded operators X and Y are equal if their domains coincide and both of them agree on the common domain. The adjoint operator of the unbounded operator X is denoted as X^\dagger (whenever it exists). Any projections considered hereafter are orthogonal projections.

2.1 Postulates of Quantum Mechanics

The essence of quantum probability is best illustrated in line with the mathematical formulation of non-relativistic quantum mechanics, which is based on a set of commonly accepted postulates [116]. We will do so in this subsection and make connection to relevant concepts in classical probability along the way. For simplicity, we focus on description of a single, isolated particle in the following.

Roughly speaking, classical mechanics describes the dynamical state variables of a particle as functions of position and momentum on a phase space. Quantum mechanics describes the state of a particle by an abstract “wave function”

¹⁷For an account of the developments that preceded the publication of this seminal paper, see [7].

obeying wave mechanics¹⁸. More precisely, following closely the Dirac-von Neumann axioms¹⁹, quantum mechanics is formulated based on the following principles.

- (A1) **Spaces.** For every quantum system, there is an associated complex separable Hilbert space \mathcal{H} (with an inner product $\langle \cdot | \cdot \rangle$) on which an algebra of linear operators, \mathcal{A} , is defined.
- (A2) **States.** Given an algebra of operators \mathcal{A} on \mathcal{H} for a quantum system, the space of *quantum states*, $\mathcal{S}(\mathcal{A})$ of the system consists of all positive trace class operators $\rho \in \mathcal{A}$ with unit trace, i.e. $\text{Tr}(\rho) = 1$. The pure states are projection operators (rays) onto one-dimensional subspaces of \mathcal{H} , with $\text{Tr}(\rho^2) = 1$. All other states, with $\text{Tr}(\rho^2) < 1$, are called mixed states. For instance, if $|u\rangle$ is a unit vector in \mathcal{H} , then the density operator defined by $|u\rangle\langle u|$ is a pure state. For our convenience, we will also refer to $|u\rangle$ as the state. In finite-dimensional spaces, the general density operator representing a mixed state is a statistical mixture of pure states of the form $\rho = \sum_j p_j |u_j\rangle\langle u_j|$, where $\sum_j p_j = 1$.
- (A3) **Observables.** An *observable* of the quantum system is represented by a self-adjoint linear (not necessarily bounded) operator, X , on \mathcal{H} . By von Neumann's spectral theorem [132], it admits a spectral representation,

$$X = \int_{\mathbb{R}} x P^X(dx), \quad (63)$$

where P^X is a spectral measure on the Borel σ -algebra of \mathbb{R} . For instance, for a self-adjoint operator $X \in \mathcal{B}(\mathcal{H})$ with \mathcal{H} finite-dimensional, the spectral representation becomes $X = \sum_{\lambda \in \text{Spec}(X)} \lambda E_\lambda$, where the λ are the eigenvalues of X with E_λ the orthogonal projection on the corresponding eigenspace such that $E_\lambda E_{\lambda'} = 0$ for $\lambda \neq \lambda'$ and $\sum_{\lambda \in \text{Spec}(X)} E_\lambda = I$.

- (4) **Measurements and Statistics.** Let X represent an observable, $|u\rangle$ be a state²⁰ and $E \subset \mathbb{R}$ be a Borel subset. Then the spectral projection $P^X(E)$ is the *event* that the value of the observable X lies in E and the probability that the event $P^X(E)$ occurs in the state $|u\rangle$ is given by $\langle u | P^X(E) | u \rangle$. From this, one sees that the *probability measure* μ_X is given by

$$\mu_X(E) = \langle u | P^X(E) | u \rangle, \quad (64)$$

on the Borel σ -algebra of \mathbb{R} . A process of *measurement*²¹ on a quantum system is the correspondence between the observable-state pair $(X, \rho = |u\rangle\langle u|)$ and the probability measure μ_X . In other words, for any Borel subset $E \in \mathcal{B}(\mathbb{R})$, the quantity $\mu_X(E) \in [0, 1]$ is the probability that the result of the measurement of the observable X belongs to E when a quantum system is in the state ρ . We say that μ_X is the *distribution* of the observable X in the state $|u\rangle$ and define the *expectation* of the observable X in this state by

$$\langle X \rangle = \text{Tr}(X\rho) = \int_{\mathbb{R}} x \mu_X(dx) = \langle u | X | u \rangle, \quad (65)$$

whenever it is finite. If f is a Borel function (real or complex-valued), then $f(X)$ is an observable with expectation $\langle f(X) \rangle = \int_{\mathbb{R}} f(x) \mu_X(dx) = \langle u | f(X) | u \rangle$, if it is finite. An important example is the *characteristic function* of X in the state $|u\rangle$, defined as:

$$\langle e^{itX} \rangle = \int_{\mathbb{R}} e^{itx} \mu_X(dx) = \langle u | e^{itX} | u \rangle. \quad (66)$$

From the above discussion, one can therefore view a quantum state as quantum analogue of probability distribution in classical probability and a quantum observable as quantum analogue of random variable (classical observable). There are important distinctions between these notions in the classical versus quantum case. In particular, the set of quantum observables generally forms a noncommutative algebra while the set of classical observables forms a commutative one. The noncommutativity of quantum observables leads to notable departure of quantum mechanics from its classical counterpart, in particular:

- Non-commuting operators do not, in general, admit a “joint distribution”²² in a particular state [26].

¹⁸The wave nature of the particle in the theory is consistent with the observation in the double-slit experiment – see Chapter 1 in [62, 137] for a brief description.

¹⁹Here we are following the orthodox version of quantum mechanics. Interpretations of quantum mechanics belong to the foundations of quantum mechanics and we will not discuss them (however, see [2] for a fun digression).

²⁰Any (mixed) state can be purified, i.e. it can be written as a partial trace of a pure state on an enlarged Hilbert space. Purification is a central idea in the theory of quantum information [118].

²¹For the theory of quantum measurement from a physicist's perspective, see [152].

²²Non-commuting observables cannot be simultaneously realized classically. Generally, there is no sensible notion of joint quantum probability distribution for them.

- Noncommutativity of operators also gives rise to interesting inequalities for statistical quantities of observables. We mention one such inequality in the following.

Define the *covariance* between $X, Y \in \mathcal{B}(\mathcal{H})$ in the state ρ as:

$$\text{cov}_\rho(X, Y) = \text{Tr}(\rho X^* Y) - \text{Tr}(\rho X^*) \text{Tr}(\rho Y),$$

which might be a complex number if the two observables are non-commuting (interference) [123].

Proposition 1. (*Uncertainty Principle*) Let $\text{var}_\rho(X) = \text{cov}_\rho(X, X)$, then for any pure state $|u\rangle$ and observables X, Y , we have the following inequality:

$$\text{var}_u(X) \text{var}_u(Y) \geq \frac{1}{4} |\langle u | i[X, Y] | u \rangle|^2.$$

Proof. See Proposition 5.1 in [123]. □

This is an abstract version of the Heisenberg uncertainty principle in quantum mechanics. It conveys the impossibility of measuring both X and Y with total precision in the pure state $|u\rangle$ (see also Appendix A in [92]).

A comparison between notions arising in classical probability and the notions in the above postulates for quantum mechanics is summarized in Table 1.

We demonstrate the notions introduced so far and the above consequences of noncommutativity in an example. These consequences should be kept in mind when we study open quantum systems in the next section.

Example 3. The following describes a quantum particle moving in a three dimensional space. The wave function, i.e. the complex-valued function of the particle's position, $|\psi(x)\rangle \in \mathcal{H} = L^2(\mathbb{R}^3) := \{|\psi(x)\rangle : \mathbb{R}^3 \rightarrow \mathbb{C} : \int_{\mathbb{R}^3} |\psi(x)|^2 dx < \infty\}$ (with the inner product, $\langle \phi | \psi \rangle = \int_{\mathbb{R}^3} \overline{\phi(x)} \psi(x) dx$), determines the pure state, $|\psi(x)\rangle \langle \psi(x)|$.

Two important observables are the position q and momentum p , defined as

$$q\psi(x) = x\psi(x), \quad p\psi(x) = -i\hbar \nabla_x \psi(x), \quad (67)$$

where $\psi(x)$ belongs to a dense domain²³ of \mathcal{H} and $\hbar \approx 1.05 \times 10^{-34}$ joule-second is the (reduced) Planck constant. They are unbounded self-adjoint operators and are noncommuting, since $[q, p]\psi(x) = i\hbar\psi(x)$, which is the canonical commutation relation (CCR) between q and p . By Nelson's theorem, which states that two observables have a joint probability distribution (in the sense as described in Section 2 of [26]) if and only if they commute, it follows that q and p do not admit a joint distribution in the same state. Applying the uncertainty principle, we see that formally $\text{var}_u(q)\text{var}_u(p) \geq \hbar^2/4$ when the particle is in the normalized state u .

Later we will describe a system of infinitely many identical quantum particles. In that case, we will see that the CCRs among their observables specify the quantum statistics and the properties of the representation of these CCRs will be exploited to build a theory of quantum stochastic integration.

Table 1: Notions in Classical and Quantum Probability

Notions	Classical Probability	Quantum Probability
State Space	Set of all possible outcomes, Ω	Complex separable Hilbert space, \mathcal{H}
Events	\mathcal{F} , set of all indicator functions in Ω	$\mathcal{P}(\mathcal{H})$, set of all projections in \mathcal{H}
Observables	Measurable functions	Self-adjoint operators in \mathcal{H}
States	Probability measure, μ	Positive operators of unit trace, ρ
Prob. Space	Measure space $(\Omega, \mathcal{F}, \mu)$	The triple $(\mathcal{H}, \mathcal{P}(\mathcal{H}), \rho)$

Remark 3. Interplay between classical and quantum probability. Quantum probability, in its algebraic formulation, can be seen as a generalization of classical probability as follows. The algebra $\mathcal{B}(\mathcal{H})$ contains many σ -algebras of mutually commuting projectors. Consider for instance, $\mathcal{H} = L^2(\Omega, \mathcal{F}, P)$, then $L^\infty(\Omega, \mathcal{F}, P)$ is a commutative (von Neumann) algebra acting on $\mathcal{H} = L^2(\Omega, \mathcal{F}, P)$ by multiplication. The projectors (events) in $L^\infty(\Omega, \mathcal{F}, P)$ are the operators of multiplication by indicator functions of elements of \mathcal{F} . The spectral theorem below provides the crucial link between classical and quantum probability.

²³It is useful to consider wave functions $\psi(x)$ that live in a suitable test function space, i.e. a linear subspace $\mathcal{D} \subset \mathcal{H}$. For example, \mathcal{D} can be the set of all smooth functions with support in some compact subset $K \subset \mathbb{R}$. Physically, this choice of \mathcal{D} says that the particle is confined to the region K in space.

Theorem 5. *There exists a probability space (Ω, \mathcal{F}, P) and an $*$ -isomorphic map ϕ from a commutative $*$ -algebra of operators on \mathcal{H} onto the set of measurable functions on Ω (i.e. a linear bijection with $\phi(AB) = \phi(A)\phi(B)$ and $\phi(A^*) = \phi(A)^*$).*

Proof. See [21]. □

The probability measure P induces a state ρ on the commutative algebra by $\rho(f) = \int_{\Omega} f(w) dP(w)$. A classical random variable X can be described as a quantum random variable (observable) by the $*$ -homomorphism $J : L^{\infty}(E, \mathcal{E}, P) \rightarrow L^{\infty}(\Omega, \mathcal{F}, P)$, $J(f) = f \circ X$, where (E, \mathcal{E}) is a measurable space. However, two non-commuting self-adjoint operators cannot be represented as multiplication operators on the same Hilbert space $L^2(\Omega, \mathcal{F}, P)$.

(A5) **Dynamics.** The (reversible) time evolution of a pure state (wave function) in \mathcal{H} is determined by a unitary operator $U : \mathcal{H} \rightarrow \mathcal{H}$. By Stone's theorem, if $t \mapsto U_t$ is a strongly continuous, one-parameter unitary group, then there exists a unique linear self-adjoint operator H , the *Hamiltonian*, such that $U(t) = e^{-itH}$. In this case, the pure state $|u\rangle$ evolves according to $|u(t)\rangle = U(t)|u\rangle$, $U_0 = I$, $\langle u|u\rangle = 1$, and satisfies the celebrated *Schrodinger equation*:

$$i\hbar \frac{d}{dt} |u(t)\rangle = H |u(t)\rangle, \quad |u(0)\rangle = |u\rangle, \quad t \geq 0. \quad (68)$$

Physically, the Schrodinger equation is sensible, as the linearity of the dynamics ensures the superposition principle for states is satisfied and the fact that the Schrodinger equation is first order in time guarantees causality of the states. The self-adjointness (in particular, the symmetry) of H is important to conserve the probability at all times, i.e. $\|u(t)\| = 1$ for all $t \geq 0$.

For general states which are represented by density operators, they evolve via the map $\rho \mapsto \rho(t) = U_t \rho U_t^*$. This is the so-called *Schrodinger picture*, where the states evolve in time while the observables are fixed. The dual picture, where the states are fixed while the observables evolve in time, is called the *Heisenberg picture*. In this picture, an observable evolves according to the map ($*$ -automorphism) $X \mapsto X(t) = \tau_t(X) = U_t^* X U_t$ and satisfies the *Heisenberg equation of motion*:

$$\frac{d}{dt} X(t) = \frac{i}{\hbar} [H, X(t)], \quad X(0) = X. \quad (69)$$

The two pictures are related via $\text{Tr}(\rho X(t)) = \text{Tr}(\rho(t) X)$ (by the cyclic property of trace). Taking the expectation of X with respect to the state $|u\rangle$, one obtain the *Ehrenfest equation*, a quantum analogue of the classical Hamilton's equation:

$$\frac{d}{dt} \langle X(t) \rangle = \frac{i}{\hbar} \langle [H, X(t)] \rangle, \quad \langle X(0) \rangle = \langle X \rangle \in \mathbb{R}. \quad (70)$$

Example 4. Suppose that the single particle in the previous example is a quantum harmonic oscillator and so is described by the Hamiltonian:

$$H_{ho} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2, \quad (71)$$

where m and ω denote the mass and frequency of the particle respectively. Then the Heisenberg equation of motions for its position and momentum give

$$\dot{q}(t) = p(t)/m, \quad \dot{p}(t) = -m\omega^2 q(t), \quad (72)$$

which can be seen to be quantum analogue of the Newton's second law, $\ddot{q}(t) = -\omega^2 q(t)$.

2.2 Composite Systems

We need to be able to describe a family of independent systems (recall that so far we have focused on a system – that of a single particle). Let \times and \otimes denote the Cartesian and tensor product²⁴ respectively in the following.

In classical probability, if $(\Omega_1, \mathcal{F}_1, P_1), \dots, (\Omega_n, \mathcal{F}_n, P_n)$ are probability spaces describing n independent statistical systems, then the product probability space $(\Omega, \mathcal{F}, P) := (\Omega_1 \times \dots \times \Omega_n, \mathcal{F}_1 \times \dots \times \mathcal{F}_n, P_1 \times \dots \times P_n)$ describes a single system consisting of the n systems, and

$$P(F_1 \times \dots \times F_n) = P_1(F_1) \dots P_n(F_n),$$

²⁴For definitions of tensor product, see [123] (for a coordinate-free approach based on positive definite kernels) and [?] (for the usual approach).

for any event $F_i \in \mathcal{F}_i$. In quantum mechanics, the Hilbert space of a composite system consisting of independent component systems is the Hilbert space tensor product of the state spaces associated with the component systems. More precisely, if $(\mathcal{H}_1, \rho_1), \dots, (\mathcal{H}_n, \rho_n)$ describe n independent quantum systems, then $(\mathcal{H}, \rho) := (\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n, \rho_1 \otimes \dots \otimes \rho_n)$ describes a single quantum system consisting of the n systems, where $\rho_1 \otimes \dots \otimes \rho_n$ is a state on $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n$.

For $i = 1, \dots, n$, let X_i be an observable on \mathcal{H}_i and the spectral projection $P^{X_i}(E_i)$ be the event that the value of the observable X_i lies in the Borel subset $E_i \in \mathbb{R}$. Then $X = X_1 \otimes \dots \otimes X_n$ is an observable on \mathcal{H} and the probability that the value of the observable X lies in $E = E_1 \times \dots \times E_n$ is given by

$$\begin{aligned} \mu_{X_1, \dots, X_n}(E_1 \times \dots \times E_n) &= \text{Tr}((\rho_1 \otimes \dots \otimes \rho_n)(P^{X_1}(E_1) \otimes \dots \otimes P^{X_n}(E_n))) \\ &= \text{Tr}(\rho_1 P^{X_1}(E_1)) \dots \text{Tr}(\rho_n P^{X_n}(E_n)) = \mu_{X_1}(E_1) \dots \mu_{X_n}(E_n). \end{aligned} \quad (73)$$

Other notions introduced in the Postulate (A4)-(A5) can be extended analogously to composite systems. The above descriptions can be generalized to infinitely many independent systems and in the case when the systems are also identical it is convenient to achieve this task on a Hilbert space endowed with a certain structure: the Fock space, to be introduced next.

3 Elements of Quantum Stochastic Analysis

We provide a minimal review of the basic ideas and results from Hudson-Parthasarathy (H-P) quantum stochastic calculus, which is a bosonic²⁵ Fock space stochastic calculus based on the creation, conservation and annihilation operators of quantum field theory. The goal of our review is to convince, at least at a formal level, the readers that a quantum version of stochastic calculus can be developed in parallel with the classical calculus. For details of the calculus, we refer to the monographs [113] and [123]. Again, we follow [123] closely in the following.

Recall that a classical stochastic process is a family of random variables (classical observables) on a probability space (Ω, \mathcal{F}, P) indexed by $t \in \mathbb{R}^+ := [0, \infty)$. To see how one could formulate the concept of quantum stochastic process, let us first consider a family of commuting observables, $\{X(t), t \in T\}$ where $T \subset \mathbb{R}^+$ is a time interval. Since this family can be simultaneously diagonalized, we are allowed to consider observables of the form $\sum_{j=1}^n \xi_j X(t_j)$ for any finite set $\{t_1, \dots, t_n\} \subset T$ and real constants ξ_j ($j = 1, \dots, n$) and define the *joint characteristic function* of $\mathbf{X} := (X(t_1), \dots, X(t_n))$, i.e. Fourier transform of the joint probability distribution $\mu_{X(t_1), \dots, X(t_n)}$ in \mathbb{R}^n :

$$\langle e^{i\boldsymbol{\xi} \cdot \mathbf{X}} \rangle := \langle u | e^{i \sum_{j=1}^n \xi_j X(t_j)} | u \rangle, \quad (74)$$

where $|u\rangle$ is a state and $\boldsymbol{\xi} = (\xi_1, \dots, \xi_n) \in \mathbb{R}^n$. Then the family $\{\mu_{X(t_1), \dots, X(t_n)} : \{t_1, \dots, t_n\} \subset T, n = 1, 2, \dots\}$ of all finite-dimensional distributions is consistent. Therefore, it follows from Kolmogorov's theorem that the family $\{X(t), t \in T\}$ defines a stochastic process. Note that the correspondence $\boldsymbol{\xi} \rightarrow e^{i\boldsymbol{\xi} \cdot \mathbf{X}}$ is a unitary representation of \mathbb{R}^n .

An important example of classical stochastic process that can be constructed via the above procedure is the Wiener process, with respect to which a stochastic integral can be defined [82]. Adapting the above view point to a family of commuting (operator-valued and not necessarily bounded) quantum observables with respect to a class of states in a Hilbert space, one can construct quantum stochastic processes [3]. A particular quantum analogue of the above unitary representation (the Weyl representation) will be important in the case when the observables are unbounded. We will focus on the construction of quantum analogue of Wiener process within the setting of a bosonic Fock space.

3.1 Bosonic Fock Space

A Fock space describes states of a quantum field consisting of an indefinite number of identical particles. It is a crucial object in the formalism of second quantization used to study quantum many-body systems. The main idea of second quantization is to specify quantum states by the number of particles occupying the states, rather than labeling each particle with its state, thereby eliminating redundant information concerning identical particles and allowing an efficient description of quantum many-body states. From the perspective of quantum stochastic modeling, it is a natural space²⁶ to support the quantum noise, describing the effective action of the environment on a system of interest.

²⁵A stochastic calculus can also be constructed in the setting of a fermionic Fock space and in fact such calculus is related to the one based on the Fock space [71].

²⁶The theory of Fock space provides a convenient framework to study not only quantum fields, but also other objects, such as the Carleman linearization techniques in nonlinear dynamical systems [85, 84] and classical stochastic mechanics [13].

A system of identical particles is described by either a totally symmetric wave function (invariant under exchange of any two coordinates) or a totally asymmetric wave function. This gives rise to two distinct types of particles: bosons in the former case and fermions in the latter case. We are only interested in description for bosonic systems.

Definition 4. The bosonic Fock space, over the one-particle space \mathcal{H} , is defined as the countable direct sum:

$$\Gamma(\mathcal{H}) = \mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}^{\otimes 2} \oplus \cdots \oplus \mathcal{H}^{\otimes n} \oplus \cdots, \quad (75)$$

where \mathbb{C} , denoting the one-dimensional space of complex scalars, is called the vacuum subspace and $\mathcal{H}^{\otimes n}$, denoting the symmetric tensor product of n copies of \mathcal{H} , is called the n -particle subspace. Any element in an n -th particle subspace is called an n -particle vector. For any n elements $|u_1\rangle, |u_2\rangle, \dots, |u_n\rangle$ in \mathcal{H} , the vector $\otimes_{j=1}^n |u_j\rangle$ is known as the finite particle vector (or Fock vector). The dense linear manifold $\mathcal{F}(\mathcal{H})$ of all finite particle vectors is called the finite particle domain.

Since the particles constituting the noise space (and in each of the n -particle space) are bosons, in order to describe the n -particle state (i.e. to belong to the n -particle space, $\mathcal{H}^{\otimes n}$), a Fock vector has to be symmetrized:

$$|u_1\rangle \circ |u_2\rangle \circ \cdots \circ |u_n\rangle = \frac{1}{n!} \sum_{\sigma \in \mathcal{P}_n} |u_{\sigma(1)}\rangle \otimes |u_{\sigma(2)}\rangle \otimes \cdots \otimes |u_{\sigma(n)}\rangle, \quad (76)$$

where \mathcal{P}_n is the set of all permutations, σ , of the set $\{1, 2, \dots, n\}$. The n -particle space is invariant under the action of the permutation group \mathcal{P}_n .

Important elements of the bosonic Fock space, $\Gamma(\mathcal{H})$, are the *exponential vectors*:

$$|e(u)\rangle = 1 \oplus |u\rangle \oplus \frac{|u\rangle^{\otimes 2}}{\sqrt{2!}} \oplus \cdots \oplus \frac{|u\rangle^{\otimes n}}{\sqrt{n!}} \oplus \cdots, \quad (77)$$

where $|u\rangle \in \mathcal{H}$ and $|u\rangle^{\otimes n}$ denotes the tensor product of n copies of $|u\rangle$. We call $|\Omega\rangle := |e(0)\rangle$ the *Fock vacuum vector*, which corresponds to the state with no particles. Note that $|\psi(u)\rangle = e^{-\langle u|u\rangle/2} |e(u)\rangle$ is a unit vector. The pure state with the density operator $|\psi(u)\rangle\langle\psi(u)|$ is called the *coherent state* associated with $|u\rangle$. In the special case when $\mathcal{H} = \mathbb{C}$, the coherent states on $\Gamma(\mathcal{H}) = \mathbb{C} \oplus \mathbb{C} \oplus \cdots$ are sequences of the form:

$$|\psi(\alpha)\rangle = e^{-|\alpha|^2/2} \left(1, \alpha, \frac{\alpha^2}{\sqrt{2!}}, \dots, \frac{\alpha^n}{\sqrt{n!}}, \dots \right). \quad (78)$$

We collect some basic properties of exponential vectors in the following.

Proposition 2. Basic properties of exponential vectors.

For all $|u\rangle, |v\rangle \in \mathcal{H}$, the exponential vectors satisfy the following scalar product formula:

$$\langle e(u)|e(v)\rangle = e^{\langle u|v\rangle}, \quad (79)$$

with the same notation for scalar products in appropriate spaces.

- (ii) The map $|u\rangle \mapsto |e(u)\rangle$ from \mathcal{H} into $\Gamma(\mathcal{H})$ is continuous.
- (iii) The set $\{|e(u)\rangle : |u\rangle \in \mathcal{H}\}$ of all exponential vectors is linearly independent and total in $\Gamma(\mathcal{H})$, i.e. the smallest closed subspace containing the set is the whole space $\Gamma(\mathcal{H})$.
- (iv) Let S be a dense set in \mathcal{H} . Then the linear manifold $\mathcal{E}(S)$ generated by $M := \{|e(u)\rangle : |u\rangle \in S\}$ is dense in $\Gamma(\mathcal{H})$. For every map $T : M \rightarrow \Gamma(\mathcal{H})$, there exists a unique linear operator T' on $\Gamma(\mathcal{H})$ with domain $\mathcal{E}(S)$ such that $T'|e(u)\rangle = T|e(u)\rangle$ for all $|u\rangle \in S$.
- (v) Let \mathcal{H}_i be Hilbert spaces, $|u_i\rangle \in \mathcal{H}_i$ ($i = 1, \dots, n$) and $\mathcal{H} = \oplus_{i=1}^n \mathcal{H}_i$. Then there exists a unique unitary isomorphism $U : \Gamma(\mathcal{H}) \rightarrow \Gamma(\mathcal{H}_1) \otimes \cdots \otimes \Gamma(\mathcal{H}_n)$ satisfying the relation:

$$U|e(u_1 \oplus \cdots \oplus u_n)\rangle = |e(u_1)\rangle \otimes \cdots \otimes |e(u_n)\rangle, \quad (80)$$

for every $|u_i\rangle \in \mathcal{H}_i$.

Proof. (i) follows from a straightforward computation. (ii) follows from the proof in Corollary 19.5 in [123]. (iii)-(v) follow from Proposition 19.4, Corollary 19.5 and Proposition 19.6 in [123] respectively. One key ingredient in showing (iv)-(v) is Proposition 7.2 in [123]. \square

When $S = \mathcal{H}$ in (iv), we call $\mathcal{E} = \mathcal{E}(\mathcal{H})$ the *exponential domain* in $\Gamma(\mathcal{H})$. By (iv), \mathcal{E} is dense in $\Gamma(\mathcal{H})$. Therefore, any linear operator on $\Gamma(\mathcal{H})$ can be determined by its action on the exponential vectors.

It turns out that bosonic Fock spaces have many interesting connections with Gaussian stochastic processes (see [78] and Example 19.8-19.12 in [123]). We only mention one such connection: that with the Wiener process in classical probability.

Example 5. (From Example 19.9 in [123]) Consider the Hilbert spaces $L^2(\mathbb{R}^+)$, $\Gamma(L^2(\mathbb{R}^+))$, where $\mathbb{R}^+ = [0, \infty)$ is equipped with Lebesgue measure, and $L^2(\mu)$, where μ is the probability measure of the standard Wiener process $\{W(t), t \geq 0\}$. For any complex-valued function $f \in L^2(\mathbb{R}^+)$, let $\int_0^\infty f dW$ denote the stochastic integral of f with respect to the path W of the Wiener process. Then there exists a unique unitary isomorphism (the Wiener-Segal duality transformation) $U : \Gamma(L^2(\mathbb{R}^+)) \rightarrow L^2(\mu)$ satisfying:

$$[U|e(f)\rangle](W) = \exp \left\{ \int_0^\infty f dW - \frac{1}{2} \int_0^\infty f(t)^2 dt \right\} =: e^W(f), \quad (81)$$

and

$$\langle e(f)|e(g)\rangle = e^{\langle f|g\rangle} = \mathbb{E}_\mu \overline{e^W(f)} e^W(g)$$

for all $f, g \in L^2(\mathbb{R}^+)$.

In particular, this implies that $|e(1_{[0,t]}f)\rangle$ can be identified with the exponential martingale $\exp\{\int_0^t f dW - \frac{1}{2} \int_0^t f^2(s) ds\}$ in classical probability for every $t > 0$. This suggests that the operators of multiplication by an indicator function (with respect to time intervals), together with (v) in Proposition 2, will be crucial when building a theory of quantum stochastic integration.

3.2 The Weyl Representation and Stochastic Processes in Bosonic Fock Spaces

An important group in the theory of quantum stochastic calculus is the translation group on the Hilbert space \mathcal{H} . Indeed, any Hilbert space, \mathcal{H} , being a vector space, is an additive group, which has a natural translation action on the set of all exponential vectors by $|u\rangle : |e(v)\rangle \mapsto |e(v+u)\rangle$, where $|u\rangle, |v\rangle \in \mathcal{H}$. By requiring this action to be scalar product preserving, we define the *Weyl operator* (displacement operator):

$$W(u)|e(v)\rangle = e^{-\frac{1}{2}\|u\|^2 - \langle u|v\rangle} |e(u+v)\rangle, \quad (82)$$

for every $|v\rangle \in \mathcal{H}$. Note that $\langle W(u)e(v_1)|W(u)e(v_2)\rangle = \langle e(v_1)|e(v_2)\rangle$ for every $|v_1\rangle, |v_2\rangle \in \mathcal{H}$. By the totality of the set of all exponential vectors, it follows that there exists a unique unitary operator $W(u)$ in $\Gamma(\mathcal{H})$ satisfying the above formula for every $|u\rangle \in \mathcal{H}$.

Theorem 6. Let \mathcal{H} be a complex separable Hilbert space. Let $W(u)$ be the Weyl operator defined in (82). The correspondence $|u\rangle \rightarrow W(u)$ from \mathcal{H} into the set of unitary operators on \mathcal{H} is strongly continuous and irreducible in $\Gamma(\mathcal{H})$, in the sense that there is no proper subspace in $\Gamma(\mathcal{H})$ that is invariant under all $W(u)$.

Moreover, for every $|u_1\rangle, |u_2\rangle \in \mathcal{H}$, we have:

$$W(u_1)W(u_2) = e^{-i\text{Im}(\langle u_1|u_2\rangle)} W(u_1 + u_2), \quad (83)$$

$$W(u_1)W(u_2) = e^{-2i\text{Im}(\langle u_1|u_2\rangle)} W(u_2)W(u_1). \quad (84)$$

It follows that for every $|u\rangle \in \mathcal{H}$, the map $t \mapsto W(tu)$, $t \in \mathbb{R}$, is a one-parameter group of unitary operators with the self-adjoint Stone generator $p(u)$, satisfying

$$W(tu) = e^{-itp(u)}, \quad (85)$$

for all $t \in \mathbb{R}$. The observables $p(u)$ obey the following commutation relation:

$$[p(u), p(v)]|e(w)\rangle = 2i\text{Im}\langle u, v\rangle |e(w)\rangle$$

for all $|u\rangle, |v\rangle, |w\rangle \in \mathcal{H}$.

Proof. This is a special case of Theorem 20.10 in [123]. □

The correspondence $|u\rangle \rightarrow W(u)$ is called a *projective unitary representation*. The formula (83) implies that it is a homomorphism modulo a phase factor of unit modulus. The formula (84) is known as the *Weyl commutation relation*.

Such representation allows one to obtain a rich class of observables, which are the building blocks of the calculus, on the Fock space $\Gamma(\mathcal{H})$. From these observables, one can then build quantum analogues of Wiener process. Illustrating this is the focus of this subsection.

Remark 4. A more general group called the Euclidean group, which contains the translation group as a subgroup, would allow one to obtain a richer class of observables, including quantum analogue of Lévy processes [123]. This shows the power of the formalism, as it allows realization of processes such as Wiener process and Poisson process on the same space. However, since we are only interested in the stochastic integration theory with respect to quantum analogue of the Wiener process in this paper, we omit further discussions on the general construction. For details, see [123].

We now introduce a family of operators in terms of which not only computations involving the $p(u)$ become simplified but can also be related to operators familiar from quantum field theory.

We define, for any $|u\rangle \in \mathcal{H}$,

$$q(u) = -p(iu) = p(-iu), \quad a(u) = \frac{1}{2}(q(u) + ip(u)), \quad a^\dagger(u) = \frac{1}{2}(q(u) - ip(u)). \quad (86)$$

The operators $a^\dagger(u)$ and $a(u)$ defined above are canonical observables on the bosonic Fock space, called the *creation operators* and *annihilation operators* associated to the vector $|u\rangle \in \mathcal{H}$, respectively. Following [123], we will refer to them as the *fundamental fields*. Note that $p(u) = i(a^\dagger(u) - a(u))$ and $q(u) = a^\dagger(u) + a(u)$.

We collect some useful properties, which will be crucial for the development of quantum stochastic calculus, of these operators in the following.

Proposition 3. The domain of product of finitely many operators from the family $\{a(u), a^\dagger(u) : |u\rangle \in \mathcal{H}\}$ contains the exponential domain \mathcal{E} . Moreover, for any $|u\rangle, |v\rangle \in \mathcal{H}$, $\psi, \psi_1, \psi_2 \in \mathcal{E}$,

(i)

$$a(u)|e(v)\rangle = \langle u|v\rangle|e(v)\rangle, \quad a^\dagger(u)|e(v)\rangle = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n!}} \sum_{r=0}^{n-1} |v\rangle^{\otimes r} \otimes |u\rangle \otimes |v\rangle^{\otimes (n-r-1)}; \quad (87)$$

(ii) the creation and annihilation operators are mutually adjoint, i.e. $\langle a^\dagger(u)\psi_1|\psi_2\rangle = \langle \psi_1|a(u)\psi_2\rangle$;

(iii) the restrictions of $a(u)$ and $a^\dagger(u)$ to \mathcal{E} are antilinear and linear in $|u\rangle$ respectively. Moreover, they satisfy the canonical commutation relations (CCRs): $[a(u), a(v)]\psi = [a^\dagger(u), a^\dagger(v)]\psi = 0$ and $[a(u), a^\dagger(v)]\psi = \langle u|v\rangle\psi$.

(iv)

$$a^\dagger(u)|e(v)\rangle = \left. \frac{d}{d\epsilon} |e(v + \epsilon u)\rangle \right|_{\epsilon=0}, \quad (88)$$

(v) the linear manifold of all finite particle vectors is contained in the domain of $a(u)$ and $a^\dagger(u)$. Moreover,

$$a(u)|\Omega\rangle = 0, \quad (89)$$

$$a(u)|v\rangle^{\otimes n} = \sqrt{n}\langle u|v\rangle|v\rangle^{\otimes (n-1)}, \quad (90)$$

$$a^\dagger(u)|v\rangle^{\otimes n} = \frac{1}{\sqrt{n+1}} \sum_{r=0}^n |v\rangle^{\otimes r} \otimes |u\rangle \otimes |v\rangle^{\otimes (n-r)}. \quad (91)$$

Proof. See Proposition 20.12-20.14 in [123]. The key idea to obtain the formula in (i), (iii)-(v) is to replace, in the definition of Weyl operator in (82), u by tu , $t \in \mathbb{R}$, and then differentiating with respect to t at $t = 0$, so that one obtains:

$$p(u)|e(v)\rangle = -i\langle u|v\rangle|e(v)\rangle + i \sum_{n=1}^{\infty} \frac{1}{\sqrt{n!}} \sum_{r=0}^{n-1} |v\rangle^{\otimes r} \otimes |u\rangle \otimes |v\rangle^{\otimes (n-r-1)}. \quad (92)$$

The formula there then lead to (ii) and the statements about the domain of the operators. \square

Note that in the special case $|u\rangle = |v\rangle$ in (i), we have $a(u)|\psi(u)\rangle = \langle u|u\rangle|\psi(u)\rangle$, which is an eigenvalue relation similar to the one that defines the coherent state as eigenvector of annihilation operator in quantum optics [55]. Since

vectors of the form $|v\rangle^{\otimes n}$ linearly span the n -particle space, (v) shows that $a(u)$ maps the n -particle subspace into the $(n-1)$ -particle subspace while $a^\dagger(u)$ maps the n -particle subspace into the $(n+1)$ -particle subspace, justifying their names as annihilation and creation operators respectively.

Remark 5. Connection to quantum field theory. By working with appropriate basis in \mathcal{H} , we can relate the above creation and annihilation operators (the fundamental fields) to those familiar from quantum field theory. For instance, choose and fix an orthonormal basis $\{|e_k\rangle, k = 1, 2, \dots\}$ and define $a_k = a(e_k)$, $a_k^\dagger = a^\dagger(e_k)$. Then on the exponential domain \mathcal{E} , these operators satisfy the commutation relations $[a_k, a_l] = [a_k^\dagger, a_l^\dagger] = 0$ and $[a_k, a_l^\dagger] = \delta_{kl}$. These are the commutation relations describing the ladder operators for a set of independent harmonic oscillators.

Now, let us move to a different basis of single particle state, say the position eigenstates $|r\rangle$, corresponding to the unitary transformation $|r\rangle = \sum_k \langle e_k | r \rangle |e_k\rangle$. Note that $\langle e_k | r \rangle = \varphi_k^*(r)$, the complex conjugate of the wavefunction $\varphi_k(r)$. The transformation gives a new set of creation operators, $\psi^\dagger(r) = \sum_k \varphi_k^*(r) a_k^\dagger$, and annihilation operators, $\psi(r) = \sum_k \varphi_k(r) a_k$. They satisfy the commutation relations $[\psi(r_1), \psi^\dagger(r_2)] = \delta(r_1 - r_2)$, $[\psi(r_1), \psi(r_2)] = [\psi^\dagger(r_1), \psi^\dagger(r_2)] = 0$ for $r_1, r_2 \in \mathbb{R}$, which are commutation relations describing operator-valued functions called the quantum fields.

Lastly, we investigate statistical features of observables arising from Weyl representation and show that these observables can be viewed as quantum analogue of stochastic processes. From definition, we have:

$$\left\langle \Omega \left| W \left(\sum_{j=1}^n t_j u_j \right) \right| \Omega \right\rangle = \exp \left(-\frac{1}{2} \sum_{i,j} t_i t_j \langle u_i | u_j \rangle \right) \quad (93)$$

for $|u_j\rangle \in \mathcal{H}$, $t_j \in \mathbb{R}$, $1 \leq j \leq n$. Let $\mathcal{H}_{\mathbb{R}}$ be a real subspace of \mathcal{H} such that $\mathcal{H} = \mathcal{H}_{\mathbb{R}} \oplus i\mathcal{H}_{\mathbb{R}}$. Then $\langle u | v \rangle \in \mathbb{R}$ for $|u\rangle, |v\rangle \in \mathcal{H}_{\mathbb{R}}$ and $\{W(u) : |u\rangle \in \mathcal{H}_{\mathbb{R}}\}$ is a commutative family of operators (due to (84)). In particular, $\{p(u) : |u\rangle \in \mathcal{H}_{\mathbb{R}}\}$ is a commutative family of observables, and so from (93), one has

$$\left\langle \Omega \left| \exp \left(-i \sum_{j=1}^n t_j p(u_j) \right) \right| \Omega \right\rangle = \exp \left(-\frac{1}{2} \sum_{i,j} t_i t_j \langle u_i | u_j \rangle \right), \quad (94)$$

which is the characteristic function of the n -dimensional Gaussian distribution with zero means and covariance matrix $(\langle u_i | u_j \rangle)_{i,j=1,\dots,n}$. Therefore, the above commutative family of observables in the Fock space realizes a zero mean classical Gaussian random field [105] in the vacuum state $|\Omega\rangle$ (more generally, in the coherent states; see Proposition 21.1 in [123]).

Example 6. (From Example 21.3 in [123]) Let $S \subset \mathcal{H}$ be a real subspace and P be a spectral measure on \mathbb{R}^+ for which S is invariant. Let $|u_t\rangle = P([0, t])|u\rangle$, $X_t = p(u_t)$ and $R(t) = \langle u | P([0, t]) | u \rangle$, where $|u\rangle \in S$ and $p(u_t)$ is the Stone generator of the map $t \mapsto W(u_t)$. Then $\{X_t : t \in \mathbb{R}\}$ is a family of commuting observables (with common domain \mathcal{E}) whose distribution in the vacuum state is a mean zero Gaussian process with independent increments and $\text{cov}(X_t, X_s) = R(\min(t, s))$. Note that when $\langle u | P([0, t]) | u \rangle = t$, $\{X_t : t \in \mathbb{R}\}$ realizes the standard Wiener process in classical probability.

3.3 Elements of Quantum Stochastic Calculus

Example 6 suggests that we can turn the fundamental fields on a bosonic Fock space into continuous time quantum stochastic processes²⁷ provided that an appropriate time parameter is introduced in the fields. Then one could develop a quantum stochastic differential description for a large class of observable-valued maps $t \mapsto X(t)$ in terms of these quantum stochastic processes, in parallel with classical integration theory. This is the basic idea in the seminal work [72] and will be elaborated in the following.

To introduce the time parameter in the fundamental fields, we take the one-particle space to be $\mathcal{H} = L^2(\mathbb{R}^+) \otimes \mathcal{Z} = L^2(\mathbb{R}^+; \mathcal{Z})$, with its Borel structure and Lebesgue measure. Symmetrically second quantizing this space leads to the bosonic Fock space $\Gamma(L^2(\mathbb{R}^+) \otimes \mathcal{Z})$. Here \mathcal{Z} is a complex separable Hilbert space, equipped with a complete orthonormal basis $(|z_k\rangle)_{k \geq 1}$. The space \mathcal{Z} is called the *multiplicity space* of the noise. The space \mathcal{H} is equipped with the scalar product:

$$\langle f | g \rangle = \int_0^\infty \langle f(t) | g(t) \rangle_{\mathcal{Z}} dt, \quad (95)$$

²⁷See also the more abstract definition in [3], which defines quantum stochastic process $J_t(X)$ as a family of continuous $*$ -homomorphisms on (\mathcal{H}, ρ) indexed by t .

and any element in it can be viewed as a norm square integrable function from \mathbb{R}^+ into \mathcal{Z} . As we will be formulating a differential (in time) description of processes on the Fock space, \mathbb{R}^+ represents the time semi-axis.

Physically, the dimension of \mathcal{Z} is the number of field channels that ones can couple to a system. When $\mathcal{Z} = \mathbb{C}$ (one-dimensional), the corresponding bosonic Fock space, $\Gamma(L^2(\mathbb{R}^+))$, describes a single field channel [119]. When $\mathcal{Z} = \mathbb{C}^d$ and the $|z_i\rangle = (0, \dots, 0, 1, 0, \dots, 0)$ with 1 in the i -th slot, $i = 1, 2, \dots, d$, is fixed as a canonical orthonormal basis in \mathbb{C}^d , the corresponding Fock space describes d field channels coupled to the system. Since the dimension of \mathcal{Z} can be infinite, it allows considering infinitely many field channels. To take advantage of this generality, we take the quantum noise space to be the bosonic Fock space $\Gamma(\mathcal{H})$ over $\mathcal{H} = L^2(\mathbb{R}^+) \otimes \mathcal{Z}$ in the following.

To introduce quantum probabilistic analogues of stochastic integrals, one needs an appropriate notion of time to formulate the notion of filtration and adapted processes. We consider the canonical spectral measure $P(\cdot)$ on \mathbb{R}^+ , defined by:

$$(P(E)f)(t) = 1_E(t)f(t), \quad (96)$$

for $f \in \mathcal{H}$, where 1_E denotes the indicator function of a Borel subset $E \subset \mathbb{R}^+$. One can interpret $P(\cdot)$ as a time observable in the Hilbert space \mathcal{H} which, as a spectral measure, is continuous, i.e. $P(\{t\}) = 0$ for all t .

Note that the $P(\cdot)$ are orthogonal projections, in terms of which a decomposition of the Hilbert space \mathcal{H} as the direct sum of a closed subspace and its orthogonal complement can be obtained. We define:

$$\mathcal{H}_t := \text{Ran}(P([0, t])), \quad \mathcal{H}_{[s, t]} := \text{Ran}(P([s, t])), \quad \mathcal{H}_{[t, \infty)} := \text{Ran}(P([t, \infty))),$$

where Ran denotes the range. Then for $0 < t_1 < t_2 < \dots < t_n < \infty$, we have the decomposition:

$$\mathcal{H} = \mathcal{H}_{t_1} \oplus \mathcal{H}_{[t_1, t_2]} \oplus \dots \oplus \mathcal{H}_{[t_{n-1}, t_n]} \oplus \mathcal{H}_{[t_n, \infty)}.$$

Now let \mathcal{H}_S be a fixed Hilbert space called the *initial Hilbert space* and consider the space $\mathcal{F} = \mathcal{H}_S \otimes \Gamma_s(\mathcal{H})$. Physically, one view \mathcal{H}_S as describing a system of interest, $\Gamma(\mathcal{H})$ as describing a noise process (modeling, for instance, a heat bath) and \mathcal{F} as the total space for the time evolution of the system in the presence of quantum noise.

Denote:

$$\mathcal{F}_0 = \mathcal{H}_S, \quad \mathcal{F}_t = \mathcal{H}_S \otimes \Gamma(\mathcal{H}_t), \quad \mathcal{F}_{[s, t]} = \Gamma(\mathcal{H}_{[s, t]}), \quad \mathcal{F}_t = \Gamma(\mathcal{H}_{[t, \infty)}).$$

Then, by (v) of Proposition 2, for $0 \leq t_1 < \dots < t_n < \infty$, we have the following continuous tensor product factorization over \mathbb{R}^+ :

$$\mathcal{F} = \mathcal{F}_{t_1} \otimes \mathcal{F}_{[t_1, t_2]} \otimes \dots \otimes \mathcal{F}_{[t_{n-1}, t_n]} \otimes \mathcal{F}_{[t_n, \infty)}.$$

The identification above is based on the factorization of the exponential vectors:

$$|\psi\rangle \otimes |e(u)\rangle = |\psi\rangle \otimes |e(u_{[0, t_1]})\rangle \otimes |e(u_{[t_1, t_2]})\rangle \otimes \dots \otimes |e(u_{[t_{n-1}, t_n]})\rangle \otimes |e(u_{[t_n, \infty)})\rangle, \quad (97)$$

where $|\psi\rangle \in \mathcal{H}_S$, $u_A(\tau) = P(A)u(\tau)$. Note that $\mathcal{F}_{t_1}, \mathcal{F}_{[t_j, t_{j+1}]}$ ($j = 1, \dots, n-1$) and $\mathcal{F}_{[t_n, \infty)}$ embed naturally into \mathcal{F} as subspaces by tensoring with the vacuum vectors in appropriate sectors of the total space.

The basic idea of H-P quantum stochastic calculus comes from this continuous tensor product factorization property of bosonic Fock space. One can obtain a quantum analogue of the filtration by generalizing the viewpoint that filtrations in classical probability can be represented as a commutative algebra.

Definition 5. A filtration $(\mathcal{B}_t)_{t \geq 0}$ in \mathcal{F} is an increasing family of (von Neumann) algebras, where

$$\mathcal{B}_t = \{X \otimes 1_t : X \in \mathcal{B}(\mathcal{F}_t), 1_t \text{ is the identity operator in } \mathcal{F}_{[t, \infty)}\}. \quad (98)$$

Roughly speaking, a process $\{X_t, t \geq 0\}$ is adapted to the filtration $(\mathcal{B}_t)_{t \geq 0}$, if X_t acts trivially on $\mathcal{F}_{[t, \infty)}$, i.e. such that $X_t = X_t \otimes 1_t$ for all t . From now on, we assume the following for simplicity. All the operators in a bosonic Fock space have domains that include the exponential domain. Let $D_0 \subset \mathcal{H}_S$ be a dense subspace, $\mathcal{M} \subset \mathcal{H}$ be linear manifold such that $P([s, t])|u\rangle \in \mathcal{M}$ whenever $|u\rangle \in \mathcal{M}$ for every $0 \leq s < t < \infty$. Also, the linear manifold generated by all vectors of the form $f e(u) := |f\rangle \otimes |e(u)\rangle$, $f := |f\rangle \in D_0$, $u := |u\rangle \in \mathcal{M}$, is contained in the domain of any operators in \mathcal{F} . More precisely:

Definition 6. (i) A family $X = \{X_t : t \geq 0\}$ of operators in \mathcal{F} is an adapted process if the map $t \rightarrow X_t f e(u)$ is measurable and there exists an operator X'_t in \mathcal{F}_t such that

$$X(t) f e(u) = (X'_t f e(u_t)) \otimes e(u_{[t, \infty)}), \quad (99)$$

for all $t \geq 0$, $f \in D_0$ and $u \in \mathcal{M}$. Such an adapted process is called regular if the map $t \rightarrow X_t f e(u)$ is continuous for every $f \in D_0$, $u \in \mathcal{M}$.

(ii) A map $m : t \rightarrow m_t$ from \mathbb{R}^+ into \mathcal{F} is a martingale if $m_t \in \mathcal{F}_t$ for every t and $P([0, s])m_t = m_s$ for all $s < t$.

Remark 6. Take $\mathcal{H}_S = \mathbb{C}$, $\mathcal{N}_1 = \mathcal{B}(\mathcal{F})$, $\mathcal{N}_2 = \mathcal{B}(\mathcal{F}_t) \otimes P_{\mathcal{F}_t}$, where $P_{\mathcal{F}_t}$ denotes the set of projections $P([t, \infty))$ into the space \mathcal{F}_t . Then for $X \in \mathcal{N}_1$, there exists a unique operator $X' \in \mathcal{N}_2$ such that for all $u, v \in \mathcal{M}$,

$$\langle e(u_t), X'e(v_t) \rangle = \langle e(u_t) \otimes e(u_t), Xe(v_t) \otimes e(v_t) \rangle$$

The map $X \mapsto X' \otimes P([t, \infty))$ can thus be viewed as a (quantum) conditional expectation $E[\cdot | \mathcal{N}_2]$. Therefore, one can view m_t , the martingale in a bosonic Fock space, as a martingale in the more familiar form in classical probabilistic sense, i.e. $E(m_t | \mathcal{F}_s) = m_s$ for all $s \leq t$.

An important class of martingales is of the form $|u_t\rangle = P([0, t])|u\rangle$ for $|u\rangle \in \mathcal{M}$ (c.f. Example 6). We now introduce two families of regular, adapted processes associated with this class of martingales (see other processes that can be studied in [123]). These are the processes in a bosonic Fock space with respect to which stochastic integrals will be defined later.

Any vector $|u\rangle \in \mathcal{H}$ may be regarded as a \mathcal{Z} -valued function. For a fixed basis of \mathcal{Z} (e.g. in the case when \mathcal{Z} is the space \mathbb{C}^d with the canonical basis $|z_k\rangle$), we set $u_k(t) = \langle z_k | u(t) \rangle_{\mathcal{Z}}$ for $k \geq 1$, where $\langle \cdot | \cdot \rangle_{\mathcal{Z}}$ denotes scalar product on \mathcal{Z} .

Definition 7. Let $\mathcal{H}_S = \mathbb{C}$ so that $\mathcal{F} = \Gamma(L^2(\mathbb{R}^+) \otimes \mathcal{Z})$. The creation and annihilation processes associated with the martingales $\{1_{[0, t]} |z_k\rangle\}_{k \geq 1}$ are linear operators with their domains equal the exponential domain \mathcal{E} and:

$$A_k^\dagger(t) = a^\dagger(1_{[0, t]} \otimes z_k), \quad A_k(t) = a(1_{[0, t]} \otimes z_k), \quad (100)$$

for $k = 1, 2, \dots$, where $1_{[0, t]}$ denotes indicator function of $[0, t]$ as an element of $L^2(\mathbb{R}^+)$.

Each A_k (respectively, A_k^\dagger) is defined on a distinct copy of the Fock space $\Gamma(L^2(\mathbb{R}^+))$ and therefore, the A_k 's (respectively, A_k^\dagger) are commuting. Physically, each of them represents a single channel of quantum noise input coupled to the system. Note that in the special case $\mathcal{Z} = \mathbb{C}$, the above construction only gives a single pair of creation and annihilation process and in the case $\mathcal{Z} = \mathbb{C}^d$, we have d pairs of creation and annihilation processes associated with d distinct noise inputs. The actions of the $A_k(t)$ on the exponential vectors are given by the eigenvalue relations:

$$A_k(t)|e(u)\rangle = \left(\int_0^t u_k(s) ds \right) |e(u)\rangle, \quad (101)$$

and the $A_k^\dagger(t)$ are the corresponding adjoint processes:

$$\langle e(v) | A_k^\dagger(t) | e(u) \rangle = \left(\int_0^t \overline{v_k(s)} ds \right) \langle e(v) | e(u) \rangle. \quad (102)$$

The above processes, which are time integrated versions of instantaneous creation and annihilation operators are two of the three kinds of *fundamental noise processes* introduced by Hudson and Parthasarathy. They satisfy an integrated version of the CCR: $[A_k(t), A_l^\dagger(s)] = \delta_{kl} \min(t, s)$, $[A_k(t), A_l(s)] = [A_k^\dagger(t), A_l^\dagger(s)] = 0$.

For each k , their ‘future pointing’ infinitesimal time increments, $dA_k^\#(t) := A_k^\#(t + dt) - A_k^\#(t)$, where $\#$ denotes either creation or annihilation processes, with respect to the time interval $[t, t + dt]$, are *independent* processes. The independence is due to the fact that time increments with respect to non-overlapping time intervals are commuting since they are *adapted* with respect to \mathcal{F} , i.e. they act non-trivially on the factor $\mathcal{F}_{[t, t+dt]}$ of the space $\mathcal{F} = \mathcal{F}_t \otimes \mathcal{F}_{[t, t+dt]} \otimes \mathcal{F}_{[t+dt, \infty)}$ and trivially, as identity operator on the remaining two factors. In other words, for a fixed k ,

$$dA_k^\#(t)|e(u)\rangle = (A_k^\#(t + dt) - A_k^\#(t))|e(u)\rangle \quad (103)$$

$$= e(u_{[0, t]}) \otimes a^\#(1_{[t, t+dt]} \otimes z_k) e(u_{[t, t+dt]}) \otimes e(u_{[t+dt, \infty)}), \quad (104)$$

where the operators $a^\#$ are defined in (100). Therefore, any Hermitian noise processes $M(t)$ that are appropriate combinations of the $A_k^\#(t)$ (for instance, the quantum Wiener processes introduced later in (110)) have independent time increments, i.e. if we define the characteristic function of M with respect to the coherent state, $|\psi(u)\rangle$, as $\varphi_M(\lambda) := \langle \psi(u) | e^{i\lambda M} | \psi(u) \rangle$, then for any two times $s \leq t$, we see that their joint characteristic function with respect to the coherent states is the product of individual characteristic functions:

$$\begin{aligned} \varphi_{M(s), M(t)-M(s)}(\lambda_s, \lambda_t) &:= \langle \psi(u) | e^{i\lambda_s M(s) + i\lambda_t (M(t)-M(s))} | \psi(u) \rangle \\ &= \varphi_{M(s)}(\lambda_s) \varphi_{M(t)-M(s)}(\lambda_t). \end{aligned} \quad (105)$$

This property is a quantum analog of the notion of processes with independent increments in classical probability.

Remark 7. In quantum field theory, the operators $A_k^\dagger(t)$ and $A_k(t)$ are called the smeared field operators and are usually written formally as:

$$A_k(t) = \int_0^t b_k(s)ds, \quad A_k^\dagger(t) = \int_0^t b_k^\dagger(s)ds, \quad (106)$$

where the $b_k(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{b}_k(\omega) e^{-i\omega t} d\omega$ and $b_k^\dagger(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{b}_k^\dagger(\omega) e^{i\omega t} d\omega$ are the idealized Bose field processes satisfying the singular CCR: $[b_k(t), b_l^\dagger(s)] = \delta_{kl} \delta(t-s)$ [51]. Physically, since $b_k^\dagger(s)$ creates a particle at time s through the k th noise channel, $A_k^\dagger(t)$ creates a particle that survives up to time t . These formal expressions for the annihilation and creation processes are simpler to work with than the more regular integrated processes defined in (101)-(102). As remarked on page 39 of [119], the more fundamental processes from the underlying physics point of view are the quantum field processes, not the rigorously defined, more regular integrated processes.

Exploiting the structure of bosonic Fock space and the properties of the fundamental noise processes outlined above, Hudson and Parthasarathy developed and studied *quantum stochastic integrals* with respect to these fundamental processes for a suitable class of adapted integrand processes, in analogy with the constructions in the classical Itô theory. These integrals are, for instance, of the form:

$$M_k(t) := \int_0^t F_k(s) dA_k(s) + G_k(s) dA_k^\dagger(s) \quad (107)$$

$$= F_k(t_1) \otimes (A_k(t_2 \wedge t) - A_k(t_1 \wedge t)) + G_k(t_1) \otimes (A_k^\dagger(t_2 \wedge t) - A_k^\dagger(t_1 \wedge t)), \quad (108)$$

defined on \mathcal{F}_{t_1} for $t > 0$, where the adapted operator-valued processes $F_k(s) := F_k(t_1)1_{[t_1, t_2)}(s)$ and $G_k(s) := G_k(t_1)1_{[t_1, t_2)}(s)$ are step functions of s , $t_1 \wedge t_2$ denotes minimum of t_1 and t_2 , and A_k, A_k^\dagger are the annihilation and creation processes on \mathcal{F} . In parallel with the construction in classical Itô calculus, the above stochastic integral can be extended to include integrands that belong to a large class of adapted operator-valued processes²⁸. We will only sketch selected important results of the calculus in the following. For rigorous statements (including existence and uniqueness results etc.), see [123].

The most important result of the calculus is the *quantum Itô formula*²⁹, which describes how the classical Leibnitz formula for the time-differential of a product of two functions gets corrected when these functions depend explicitly on the fundamental processes. In the vacuum state, the quantum Itô formula can be summarized by:

$$dA_k(t) dA_l^\dagger(t) = \delta_{kl} dt \quad (109)$$

and all other products of differentials that involve $dA_k(t), dA_k^\dagger(t)$ and dt vanish. This can be viewed as a chain rule with Wick ordering [145] and as a quantum analogue of the classical Itô formula. Also, when the $F_k(s)$ and $G_k(s)$ in (107) are bounded (so that multiplications of operators are free of domain issue), we have:

$$d(M_i M_j) = (dM_i) M_j + M_i (dM_j) + dM_i dM_j,$$

where the Itô correction term $dM_i dM_j$ is evaluated according to the rule (109).

In particular, with respect to the initial vacuum state, the field quadratures $W_k^0(t) = A_k(t) + A_k^\dagger(t)$ ($k = 1, 2, \dots$) are mean zero Hermitian Gaussian processes with variance t . Therefore, they can be viewed as quantum analogue of classical Wiener processes and their formal time derivatives, $dW_k^0(t)/dt = b_k(t) + b_k^\dagger(t)$, are quantum analogues of the classical white noises. If one takes $\mathcal{Z} = \mathbb{C}^d$, then $(W_1^0, W_2^0, \dots, W_d^0)$ is a collection of commuting processes and thus form a quantum analogue of d -dimensional classical Wiener process in the vacuum state. Moreover, one has $dW_i^0(t) dW_j^0(t) = \delta_{ij} dt$, which is the classical Itô correction formula for Wiener process. These results hold for a more general class of field observables:

Definition 8. Quantum Wiener processes. Let k be a positive integer. For $\theta_k \in \mathbb{R}$ (phase angle), we call the following operator-valued processes on the bosonic Fock space $\Gamma(\mathcal{H})$:

$$W_k^\theta(t) = e^{-i\theta_k} A_k(t) + e^{i\theta_k} A_k^\dagger(t). \quad (110)$$

quantum Wiener processes.

²⁸In the case where the integrands are unbounded operators, mathematically rigorous studies of these integrals are technically difficult. See, for instance, [46].

²⁹The trick to derive quantum Itô formula is to study product of quantum stochastic integrals sandwiched between coherent states by applying the properties of the fundamental field processes. All the basic ideas can be found in Section 25 of [123] or the seminal paper [72].

Quantum Wiener processes are quantum analogue of the classical Wiener processes and they satisfy the quantum Itô formula:

$$dW_i^\theta(t)dW_j^\theta(t) = \delta_{ij}dt,$$

for every $\theta \in \mathbb{R}$. Stochastic integrals with respect to the quantum Wiener processes can therefore be viewed as quantum analogues of the Itô stochastic integral in the classical theory. The classical Itô theory of stochastic calculus is included in the quantum calculus by using the Wiener-Segal identification of the bosonic Fock space with the L_2 space of Wiener process.

Remark 8. Following Remark 7, one can introduce the notion of quantum colored noise [16, 154]. For $k = 1, 2, \dots$, define

$$b_{g,k}^\dagger(t) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{b}_k^\dagger(\omega) e^{i\omega t} \hat{g}(\omega) d\omega, \quad b_{g,k}(t) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{b}_k(\omega) e^{-i\omega t} \overline{\hat{g}(\omega)} d\omega, \quad (111)$$

where $\hat{g}(\omega)$ and $\hat{b}_k(\omega)$ denote the Fourier transform of $g(t)$ and $b_k(t)$ respectively. Note that $b_{g,k}^\dagger(t)$ is the inverse Fourier transform of $\hat{b}_k^\dagger(\omega) \hat{g}(\omega)$ and so by the convolution theorem we have:

$$b_{g,k}^\dagger(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} g(t-s) b_k^\dagger(s) ds = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} g(t-s) dA_k^\dagger(s), \quad (112)$$

where the $A_k^\dagger(s)$ are creation processes. This is reminiscent of the formula for classical colored noise defined via filtering of white noise [98]:

$$\int_{\mathbb{R}} \gamma(t-s) 1_{\{s \leq t\}}(s) dB_s = \int_{-\infty}^t \gamma(t-s) dB_s, \quad (113)$$

where $\gamma(t)$ describes the filter and $B = (B_s)$ is a classical Wiener process. In the limit $g \rightarrow 1$ (flat spectrum limit), the $b_{g,k}^\dagger(t)$ converge to the fundamental noise process $b_k^\dagger(t) = dA_k^\dagger/dt$. Similar remarks apply to $b_{g,k}(t)$ and to appropriate linear combinations of $b_{g,k}(t)$ and $b_{g,k}^\dagger(t)$, which therefore deserve to be called quantum colored noise processes.

4 Open Quantum Systems

In reality, no quantum system is completely isolated from its surrounding. In other words, every quantum system (denoted S) is intrinsically in contact with its surroundings (environment or bath), denoted B , which usually has infinitely many degrees of freedom. This intrinsic openness of quantum systems is in contrast to classical systems. Similarly to the classical case, a popular approach to study open quantum systems are models of system-reservoir type. If \mathcal{H}_S denotes the Hilbert space associated with the system, and \mathcal{H}_B the Hilbert space associated with the bath, then the formal Hamiltonian for the total system, which takes into account the interaction between the system and bath, is

$$H = H_S \otimes I + I \otimes H_B + H_I \quad (114)$$

on the total space $\mathcal{H}_S \otimes \mathcal{H}_B$. In the above, H_S is the Hamiltonian describing the system, H_B is the Hamiltonian describing the bath, H_I is the Hamiltonian specifying their interaction, and I denotes identity operator on an understood space. The effective action of the reservoir on the system can often be modeled as a quantum noise. This line of thinking has been fruitful to study many concrete open quantum systems and has attracted increasing interest these days, particularly from researchers working in the field of quantum optics [51] and quantum information [118, 120]. Useful formalisms to study open quantum systems are fundamental, given the unprecedented³⁰ progress in the development of techniques to measure and manipulate quantum systems while keeping their essential quantum features.

Usually one is only interested in the dynamics of the open system which is, say, accessible for measurement. A variety of methods and formalisms has been developed and employed to study the open system. The standard formalism for the investigation of the dynamics of the open system is the *master equation*, which describes the evolution of the reduced density matrix of the open system, obtained by taking the partial trace over the degrees of freedom of the environment, i.e. the reduced density matrix is of the form $\rho_S(t) = \text{Tr}_B(\rho(t))$, where $\rho(t) = e^{-iHt/\hbar}(\rho_S \otimes \rho_B)e^{iHt/\hbar}$ is the density matrix of the total system and Tr_B denotes the partial trace. Note that the initial total density matrix, $\rho(0) = \rho_S \otimes \rho_B$, is in a factorized form and evolves unitarily, but the reduced density matrix $\rho_S(t)$ generally does not evolve unitarily.

³⁰For instance, Haroche and Wineland have developed an experiment to study the quantum mechanics of light trapped between two mirrors. They show that the quantum of light – the photon – can be controlled with atoms at an astonishing level of precision. Their work was recognized by a Nobel prize in 2012 [65]. Their experiments were explained using models and methods of open quantum systems in [136].

Early works in the open quantum systems literature focused on Markovian³¹ descriptions of an open quantum system. These descriptions provide approximate but reasonably accurate and tractable models for many open quantum systems. There are two approaches in such description: the axiomatic approach and the constructive approach.

In the constructive approach, one tries to derive the mathematically correct form of Markovian master equations from first principles. The starting point is a microscopic model of system-reservoir type described above. One obtains Markovian master equation as an approximation to the exact reduced dynamics of the open system. In the physical theory of open quantum systems, one often derives the so-called Born-Markov master equation for the reduced density operator of the system under uncontrolled approximations [139]. This leads to a breakdown of positivity of the density operator describing the state of the particle associated to a violation of the Heisenberg's uncertainty principle. In order to free of such problem, one naive remedy is to add a correction term, justifiable in certain parameter regimes, to bring the master equation into a physically correct Markovian form (the Lindblad form that we will discuss below) [92]. On the other hand, in the mathematical theory of open quantum systems, one derive the physically correct Markovian form from a microscopic model by taking well justified limits such as the weak coupling limits [57, 38] (or the stochastic limits [4]), repeated interaction limits [12], among others [22].

The axiomatic approach focus on deriving the mathematically correct form of Markovian master equations from the theory of completely positive maps [56]. Mathematical properties of the master equations and their solutions are studied. This leads to the theory of quantum dynamical semigroups and their dilations³².

We now briefly discuss the axiomatic³³ approach. A key observation is that any physically reasonable dynamical map, Λ , must map physical states to physical states, including those states of the system considered as part of a larger system. This is captured by the notion of complete positivity, which is stronger than mere positivity. For instance, the transpose map on matrices is positive but not completely positive. For precise definition, see [6]. Completely positive maps were studied already in the 50s and the celebrated Stinespring representation theorem leads to a general form of completely positive dynamical map, called the Kraus decomposition (or operator-sum representation):

$$\Lambda\rho = \sum_k W_k \rho W_k^*, \quad (115)$$

where ρ is a state (for instance the reduced density operator $\rho_S(t)$) and the W_k are (Kraus) operators such that $\sum_k W_k^* W_k = I$.

On the other hand, unity preservation of states is important to allow probabilistic interpretation. These lead to the notion of quantum dynamical semigroup (or quantum Markov semigroup), i.e. a dynamical map Λ_t which is completely positive and preserves the unity (trace-preserving) for all times $t \geq 0$. If Λ_t is continuous, then we can define its generator \mathcal{L}^* such that $\Lambda_t = e^{t\mathcal{L}^*}$ and write down the master equation for $\rho(t)$. The celebrated result of Lindblad [97] (and also of Gorini, Kossakowski and Sudarshan) provides the most general form of such master equations, called the *Lindblad master equations (LMEs)* with a bounded³⁴ generator:

$$\frac{d}{dt}\rho(t) = \mathcal{L}^*(\rho) = -\frac{i}{\hbar}[H_e, \rho] + \sum_k L_k \rho L_k^* - \frac{1}{2} \sum_k \{L_k^* L_k, \rho\}, \quad (116)$$

where $H_e = H_e^*$ and the L_k (*Lindblad operators*) are bounded operators. The right hand side of the LME above consists of three contributions. The term $-\frac{i}{\hbar}[H_e, \rho]$ gives the unitary contribution, the term $\sum_k L_k \rho L_k^*$ can be interpreted as quantum jumps and the term $\frac{1}{2} \sum_k \{L_k^* L_k, \rho\}$ represents dissipation. It is the dissipation term that make the solution of LME non-unitary. The choice of bounded operators H_e and the L_k is not unique and the sum over k can be replaced by an integral.

³¹Non-Markovian descriptions, in particular characterization and quantification of non-Markovianity, are equally important and in fact are topics of active research these days [37, 27].

³²It is well known from the theory of one-parameter semigroups that a one-parameter contraction semigroup on a Hilbert space can be expressed as a reduction of a unitary group [115]. This unitary group is called the dilation of the semigroup. This fact can be generalized to a quantum dynamical semigroup.

³³We refer to [134] for a nice mathematical introduction.

³⁴For open systems with infinite dimensional Hilbert spaces, the generators of the quantum dynamical semigroup are generally unbounded. However, in this case the Lindblad form often makes sense. Then the operators H_e and L_k can be unbounded and the sum over k can be replaced by an integral. To our knowledge, there is only one paper [142] that studies the case of unbounded generator.

The LME can be viewed as quantum analogue of the Fokker-Planck equation for transition probability density. The result of Lindblad³⁵ et. al. above says that the semigroup $\Lambda_t = e^{\mathcal{L}^* t}$, where \mathcal{L}^* is given in (116), is a quantum dynamical semigroup. Quantum dynamical semigroups are generalization of classical Markov semigroups to the quantum setting.

Hudson-Parthasarathy (H-P) theory of stochastic integration produces a dilation of quantum dynamical semigroups via their quantum stochastic differential equations (QSDEs). In contrast to closed quantum system's unitary evolution, interaction with an environment leads to randomness in the unitary evolution of an open quantum system. Using the quantum Itô formula, the general form of a unitary, reversible, Markovian evolution for a system interacting with an environment described by the fundamental noise processes can be deduced. The unitary evolution operator, $V(t)$, of the whole system, in the interaction picture with respect to the free field dynamics, is found to satisfy an Itô SDE of the following form:

$$dV(t) = \left[\left(-\frac{i}{\hbar} H_e - \frac{1}{2} \sum_k L_k^\dagger L_k \right) dt + \sum_k \left(L_k^\dagger dA_k(t) - L_k dA_k^\dagger(t) \right) \right] V(t), \quad (117)$$

$$V(0) = I, \quad (118)$$

associated to the system operators $(H_e, \{L_k\})$, where $H_e = H_e^\dagger$ is an effective Hamiltonian and the L_k are Lindblad coupling operators. It can be viewed as a noisy Schrodinger equation³⁶. The choice of the operators $(H_e, \{L_k\})$ depends on physical systems on hand.

The evolution of a noisy system observable, X , initially defined on \mathcal{H}_S , can also be obtained. By applying the quantum Itô formula, one can deduce that its evolution, $j_t(X) = V(t)^\dagger (X \otimes I) V(t)$ (Evans-Hudson flow), on \mathcal{F} is described by the following Heisenberg-Langevin equation³⁷:

$$dj_t(X) = j_t(\mathcal{L}(X))dt + \sum_k \left(j_t([X, L_k])dA_k^\dagger(t) + j_t([L_k^\dagger, X])dA_k(t) \right), \quad (119)$$

$$j_0(X) = X \otimes I, \quad (120)$$

where \mathcal{L} is the Lindblad generator:

$$\mathcal{L}(X) = \frac{i}{\hbar} [H_e, X] + \frac{1}{2} \sum_k ([L_k^\dagger, X]L_k + L_k^\dagger [X, L_k]). \quad (121)$$

One can also obtain the evolution of field observables in this way and study the relation between input and output field processes [51]. We call such equation for an observable a *quantum stochastic differential equation* (QSDE) and its solution is a *quantum stochastic process*, which is a noncommutative analogue of classical stochastic process.

To obtain the Lindblad master equation (LME) for reduced system density operator, $\rho_S(t)$, we first take the Fock vacuum conditional expectation of $j_t(X)$ to obtain the evolution of the reduced system observable, $T_t(X)$, defined via

$$\langle \psi | T_t(X) | \phi \rangle = \langle \psi \otimes e(u) | j_t(X) | \phi \otimes e(v) \rangle, \quad (122)$$

so that $dT_t(X) = T_t(\mathcal{L}(X))dt$, then the Lindblad master equation:

$$d\rho_S(t) = \mathcal{L}^*(\rho_S(t))dt \quad (123)$$

is obtained by duality. In this way, one sees that the Evans-Hudson flow is a dilation of the quantum dynamical semigroup. The equation for $T_t(X)$ above can be seen as quantum analogue of the backward Kolmogorov equation. Indeed, for simple instances, one sees that the restriction of \mathcal{L} to a commutative algebra coincides with infinitesimal generator of classical Markov processes (see Proposition 3.2 in [47]).

The next example illustrate how one can apply the above formalism to study models in quantum optics. For more examples, see the text [119] or the recent review paper [32].

Example 7. Two-level Atom Interacting with a Radiation Field [66]. Consider the small system to be a two-level atom, which is described by a Hilbert space $\mathcal{H}_S = \mathbb{C}^2$ and the Hamiltonian $H_e = \hbar\Omega\sigma_+\sigma_-$, where σ_+ and σ_- are the raising and lowering operator respectively. It interacts with a radiation field in equilibrium at a temperature T . The

³⁵It is remarkable that the Lindblad form can be derived in analogy with the classical Markovian conditions on the generator Q of the stochastic matrix e^{tQ} for classical Markov process, at least in finite dimensional systems. This was done by Kossakowski, who arrived at a set of equivalent conditions in the quantum case [134].

³⁶One can also derive SDEs for the wave function; see [124, 14].

³⁷This is often formulated in the so-called SLH framework in the quantum control and modeling literature [154].

evolution of the atom can be described effectively by two Lindblad operators $L_1 = \sqrt{\gamma(N+1)}\sigma_-$ and $L_2 = \sqrt{\gamma N}\sigma_+$, which describe the energy exchanges between the atom and the field. The first Lindblad operator describes the processes of spontaneous and stimulated emission, where the atom loses energy into the field, while the second one describes the absorption, where the atom gains energy from the field. Here γ is the rate at which the atom loses or gains energy when the radiation field is at the temperature T and N is the mean number of photons in the radiation field at the resonant frequency Ω . Using the above physical choice of H_e and L_k ($k = 1, 2$), one can write down an equation to describe evolution of dynamical variables of interest.

Example 8. A Lindblad model of damped quantum harmonic oscillator. Let X and P denotes the position and momentum operator on \mathcal{H}_S . Let $\gamma > 0$ be constant and $T > 0$ be the temperature. We take

$$H_e = \frac{P^2}{2M} + \frac{1}{2}kX^2 + \frac{\gamma}{M}\{X, P\}$$

and a single Lindblad operator

$$L = \frac{1}{\hbar}\sqrt{4k_B T \gamma}X + \frac{i}{M}\sqrt{\frac{\gamma}{4k_B T}}P.$$

Then we can write down the QSDE for $X_t = j_t(X)$ and $P_t = j_t(P)$, where I is identity operator on the boson Fock space \mathcal{F} :

$$dX_t = \frac{P_t}{M}dt - \frac{\hbar}{M}\sqrt{\frac{\gamma}{4k_B T}}dB_t^{(1)}, \quad (124)$$

$$dP_t = -kX_t dt - \frac{2\gamma}{M}P_t dt + \sqrt{4k_B T \gamma}dB_t^{(2)}, \quad (125)$$

where

$$B_t^{(1)} = A^\dagger(t) + A(t), \quad B_t^{(2)} = i(A^\dagger(t) - A(t))$$

are (noncommuting) quantum Wiener processes (recall $(A(t), A^\dagger(t))$ are the fundamental operator processes of Hudson-Parthasarathy). Therefore, our choice of (H_e, L) gives quantum analogue of the classical Langevin equation, modulo the appearance of a quantum noise term in the equation for X_t .

4.1 A Hamiltonian Model for Open Quantum Systems

Perhaps a straightforward model for open quantum system is a quantized version of the open system considered in the previous section, in which case the Hamiltonian (27) becomes an operator. We will see that indeed this is the case by studying the descriptions for a system, its environment and their interaction in the quantum mechanical setting. Basic references on these are [51, 26, 139] (for physics) and [11] (for mathematics).

Before we describe our model, we provide some physical motivations. An important class of open quantum systems is the *quantum Brownian motion (QBM)* [26, 51, 134]. In the standard form, the model for QBM consists of a particle moving in one spatial dimension and interacting linearly with an environment in thermal equilibrium. One candidate model for QBM is the Caldeira-Leggett model [28], a prototype of microscopic Hamiltonian model where the environment is modeled by a collection of non-interacting harmonic oscillators. Such model has been used widely to study decoherence [139] (a process in which quantum coherence is lost and the quantum system is brought into a classical state) and quantum dissipation phenomena [151]. A detailed study of QBM, in particular the memory effects and modeling of the environment by quantum noises, is important to understand, for instance, how one could exploit the interaction with the environment to design efficient quantum thermal machines [60] as well as to create entanglement and superpositions of quantum states [130, 86].

The original Caldeira-Leggett model is not realistic from experimental point of view, as it does not take into account the spatial inhomogeneity of the environment. Spatial inhomogeneity occurs, for instance, in the setup of a quantum impurity particle interacting with Bose-Einstein condensates (BECs) [108], where the inhomogeneity is due to a harmonic potential trapping the particle. One would like to have a generalized model that takes into account such inhomogeneity and studies in detail its quantum dynamics.

We consider an open system where the quantum Brownian particle is coupled to an equilibrium heat bath. The particle interacts with the heat bath via a coupling, which is a function that can be nonlinear in the system's position, in which case the particle is subject to inhomogeneous damping and diffusion [151, 108, 92]. The model can be viewed as a field version of the generalized Caldeira-Leggett model studied in [108, 92], a generalization of the spinless thermal Pauli-Fierz Hamiltonian with dipole type interactions [125, 39, 40], or a quantum analog of the classical Hamiltonian field model. It is a fundamental model which not only allows simple analytic treatments and provides physical insights, but also realistically models many open quantum systems — for instance, an atom in an electromagnetic field.

As the heat bath is an infinitely extended quantum system made up of identical particles on a bosonic Fock space, the formalism of second quantization is convenient for its description. The idea is that given an operator J from a Hilbert space \mathcal{H} to another Hilbert space \mathcal{K} , we can extend it naturally to an operator $\Gamma(J)$ from the boson Fock space $\Gamma(\mathcal{H})$ to the boson Fock space $\Gamma(\mathcal{K})$. More precisely, if J is the given operator on \mathcal{H} , so is $J^{\otimes n}$ on the n -particle space $\mathcal{H}^{\otimes n}$ for every n . Therefore, the operator $\Gamma(J)$, called the *second quantization* of J , defined by

$$\Gamma(J)(u_1 \circ \dots \circ u_n) = Ju_1 \circ \dots \circ Ju_n, \quad (126)$$

for $n \in \mathbb{N}$, or formally,

$$\Gamma(J) = I \oplus J \oplus J^{\otimes 2} \oplus \dots \oplus J^{\otimes n} \oplus \dots \quad (127)$$

on $\Gamma(\mathcal{H})$ is an operator satisfying $\Gamma(J)|e(u)\rangle = |e(Ju)\rangle$ for every $|u\rangle \in \mathcal{H}$. The identity-preserving correspondence $J \mapsto \Gamma(J)$ is called the *second quantization map* and satisfies:

$$\Gamma(J^*) = \Gamma(J)^*, \quad \Gamma(J_1 J_2) = \Gamma(J_1) \Gamma(J_2) \quad (128)$$

Therefore, $\Gamma(J)$ is a self-adjoint, positive, projection or unitary operator whenever J is. In particular, if $(U_t : t \in \mathbb{R})$ is a strongly continuous one-parameter group of unitary operators, then so is $(\Gamma(U_t) : t \in \mathbb{R})$. In this case, if $U_t = e^{-itH}$ for some self-adjoint operator H on \mathcal{H} , then $\Gamma(U_t) = e^{-it\Gamma(H)}$ is a strongly continuous unitary group on $\Gamma(\mathcal{H})$ generated by a self-adjoint operator $\Gamma(H)$. We denote its generator $\Gamma(H)$ as $d\Gamma(H)$ and call it the *differential second quantization* of H , whose action on the n -particles subspace is given by:

$$d\Gamma(H)(u_1 \circ \dots \circ u_n) = \sum_{k=1}^n u_1 \circ \dots \circ Hu_k \circ \dots \circ u_n. \quad (129)$$

In the special case when $H = I$ (identity operator), $d\Gamma(I)$ is called the number operator. Note that $\Gamma(e^{-itH}) = e^{-itd\Gamma(H)}$.

We describe the particle, the heat bath and their interaction in the model more precisely in the following. The Brownian particle is a quantum mechanical system, denoted \mathcal{S} , with energy operator H_S on the Hilbert space $\mathcal{H}_S := L^2(\mathbb{R})$. It is subjected to a confining, smooth potential $U(X)$. The infinite heat bath³⁸, denoted \mathcal{B} , is a field of mass-less bosons at a positive temperature. It is described by the triple $(\mathcal{H}_B, \rho_B, H_B)$, where $\mathcal{H}_B := \Gamma(L^2(\mathbb{R}^+))$, $\mathbb{R}^+ = [0, \infty)$, is the bosonic Fock space over $L^2(\mathbb{R}^+)$ (momentum space), H_B is the Hamiltonian of the heat bath defined on \mathcal{H}_B and $\rho_B = e^{-\beta H_B} / \text{Tr}(e^{-\beta H_B})$ is the Gibbs thermal state at an inverse temperature $\beta = 1/(k_B T)$. We take $H_B = d\Gamma(H_B^1)$, the differential second quantization of the energy operator H_B^1 which acts in the one-particle frequency space $L^2(\mathbb{R}^+)$ as:

$$(H_B^1 \phi)(w) = \epsilon(w) \phi(w), \quad (130)$$

where $\epsilon(w)$ is the energy of a boson with frequency $w \in \mathbb{R}^+$. The function $\epsilon(w)$ is the dispersion relation for the bath, which in our case, is a linear one, i.e. $\epsilon(w) = \hbar w$. The equilibrium frequency distribution of bosons at an inverse temperature β is given by the Planck's law:

$$\nu_\beta(w) = \frac{1}{\exp(\beta \epsilon(w)) - 1}. \quad (131)$$

The full dynamics of the model is described by the Hamiltonian:

$$H = H_S \otimes I + I \otimes H_B + H_I + H_{ren} \otimes I, \quad (132)$$

where H_S and H_B are Hamiltonians for the particle and the heat bath respectively, given by

$$H_S = \frac{P^2}{2m} + U(X), \quad H_B = \int_{\mathbb{R}^+} \hbar \omega b^\dagger(\omega) b(\omega) d\omega, \quad (133)$$

H_I is the interaction Hamiltonian given by

$$H_I = -f(X) \otimes \int_{\mathbb{R}^+} [c(\omega) b^\dagger(\omega) + \overline{c(\omega)} b(\omega)] d\omega, \quad (134)$$

and H_{ren} is the renormalization Hamiltonian given by

$$H_{ren} = \left(\int_{\mathbb{R}^+} \frac{|c(\omega)|^2}{\hbar \omega} d\omega \right) f(X)^2. \quad (135)$$

³⁸For a rigorous introduction to the heat bath (ideal quantum gas), we refer to the lecture notes [112]. We will not pursue the rigorous approach here.

Here X and P are the particle's position and momentum operators, m is the mass of the particle, $U(X)$ is a smooth confining potential, $b(\omega)$ and $b^\dagger(\omega)$ are the bosonic annihilation and creation operator of the boson of frequency ω respectively on $L^2(\mathbb{R}^+)$ and they satisfy the usual canonical commutation relations (CCR): $[b(\omega), b^\dagger(\omega')] = \delta(\omega - \omega')$, $[b(\omega), b(\omega')] = [b^\dagger(\omega), b^\dagger(\omega')] = 0$. We assume that the operator-valued function $f(X)$ is positive and can be expanded in a power series, and $c(\omega)$ is a complex-valued coupling function (form factor) that specifies the strength of the interaction with each frequency of the bath. It determines the spectral density of the bath and therefore the model for damping and diffusion of the particle. The heat bath is initially in the Gibbs thermal state, $\rho_\beta = e^{-\beta H_B} / \text{Tr}(e^{-\beta H_B})$, at an inverse temperature $\beta = 1/(k_B T)$. We will refer to the model specified by the above Hamiltonian as the *QBM model*.

The renormalization potential H_{ren} is needed to ensure that the bare potential acting on the particle is $U(X)$ and that the Hamiltonian can be written in a positively defined form: $H = H_S \otimes I + H_{B-I}$, where H_{B-I} is given by

$$H_{B-I} = \int_{\mathbb{R}^+} \hbar\omega \left(b(\omega) - \frac{c(\omega)}{\hbar\omega} f(X) \right)^\dagger \left(b(\omega) - \frac{c(\omega)}{\hbar\omega} f(X) \right) d\omega. \quad (136)$$

Lastly, we discuss the Gibbs thermal state ρ_β , in particular the derivation of quantum fluctuation-dissipation relation assuming that it is the initial state. Assume in the following that ρ_β is of trace class. In the case of thermodynamic limit (i.e. when the limit to an infinitely extended system with infinite volume and infinitely many degrees of freedom is already passed to), the ρ_β has infinite trace but the results derived below can still be made sense of [112].

Let A and B be two observables on \mathcal{H}_B . Denote $\tau_t(A) = A(t) = e^{iH_B t/\hbar} A e^{-iH_B t/\hbar}$ and similarly for $\tau_t(B)$. Then,

$$\langle A\tau_t(B) \rangle_\beta = \frac{\text{Tr}(A e^{iH_B t/\hbar} B e^{-(\hbar\beta + it)H_B/\hbar})}{\text{Tr}(e^{-\beta H_B})} = \frac{\text{Tr}(B e^{-(\hbar\beta + it)H_B/\hbar} A e^{iH_B t/\hbar})}{\text{Tr}(e^{-\beta H_B})}, \quad (137)$$

where we have used cyclicity of trace in the last line above. Taking the boundary value at $t = i\hbar\beta$, we have $\langle A\tau_t(B) \rangle_\beta|_{t=i\hbar\beta} = \langle BA \rangle_\beta$. This is the *Kubo-Martin-Schwinger (KMS) condition*, which completely characterizes the expectation $\langle \cdot \rangle_\beta$ and so gives an alternate definition of equilibrium states. In particular, setting $A = B = q$ (for instance, the position observable) and assuming $\langle q \rangle_\beta = 0$,

$$C^-(t) := \langle qq(t) \rangle_\beta = \langle q(t)q(i\hbar\beta) \rangle_\beta = \langle q(t - i\hbar\beta)q \rangle_\beta =: C^+(t - i\hbar\beta), \quad (138)$$

where we have used the time translation invariance of correlation function in the last line above. Taking the Fourier transform gives

$$\tilde{C}^-(\omega) = \tilde{C}^+(\omega) e^{-\hbar\omega\beta}, \quad (139)$$

where \tilde{F} denotes Fourier transform of F .

We now derive quantum fluctuation-dissipation relation of Callen and Welton [29]. Set $C^\pm(t) = S(t) + iA(t)$, where $S(t) = \langle \{q(t), q(0)\}/2 \rangle_\beta$ is the symmetric correlation function and $A(t) = -i\langle [q(t), q(0)]/2 \rangle_\beta$ is the anti-symmetric correlation function. Similarly, set $\tilde{C}^\pm(\omega) = \tilde{S}(\omega) + i\tilde{A}(\omega)$ for its Fourier transform.

Next we recall some notions from linear response theory. Define the response function (or generalized susceptibility) $\chi(t) = -2\theta(t)A(t)/\hbar$, where $\theta(t)$ is the step function specifying causality, and define the dynamical susceptibility, $\chi''(\omega)$, as the imaginary part of $\tilde{\chi}(\omega)$. Then $\chi''(\omega) = i\tilde{A}(\omega)/\hbar = (\tilde{C}^+(\omega) - \tilde{C}^-(\omega))/(2\hbar)$. Then using (139), we obtain the result of Callen-Welton:

$$\tilde{\chi}''(\omega) = \frac{1}{2\hbar} (1 - e^{-\hbar\omega\beta}) \tilde{C}^+(\omega). \quad (140)$$

This result implies that the symmetric correlation function the observable is related (in the Fourier domain) to the anti-symmetric correlation function as:

$$\tilde{S}(\omega) = i \coth(\hbar\omega\beta/2) \tilde{A}(\omega) = \hbar \coth(\hbar\omega\beta/2) \tilde{\chi}''(\omega). \quad (141)$$

4.2 Heisenberg-Langevin Equations

In this section, we derive the Heisenberg equations of motion for the QBM model and study the stochastic force term appearing in the equation. This will pave the way to model the action of the heat bath on the particle by appropriate quantum colored noises introduced in the next sections. Our final goal is the construction of dissipative non-Markovian Heisenberg-Langevin equations driven by appropriate thermal noises, which are built from H-P fundamental noise processes. From now on, I denotes identity operator on an understood space and 1_A denotes indicator function of the set A .

Recall that the particle's position evolves according to $\tau_t(X \otimes I) =: X(t)$ and momentum evolves according to $\tau_t(P \otimes I) =: P(t)$, where $\tau_t(O) = e^{iHt/\hbar} O e^{-iHt/\hbar}$ for an observable O of the total system. Define the particle's velocity, $V(t) = \frac{P(t)}{m}$ and note that $f'(X) = -i[f(X), P]/\hbar$. Let

$$b(\omega) = \sqrt{\frac{\omega}{2\hbar}} \left(x(\omega) + \frac{i}{\omega} p(\omega) \right), \quad b^\dagger(\omega) = \sqrt{\frac{\omega}{2\hbar}} \left(x(\omega) - \frac{i}{\omega} p(\omega) \right), \quad (142)$$

$$[x(\omega), p(\omega')] = i\hbar\delta(\omega - \omega')I, \quad (143)$$

where we have normalized the masses of all bath oscillators.

The Heisenberg equation of motion gives

$$\dot{X}(t) = \frac{i}{\hbar} [H, X(t)] = \frac{P(t)}{m}, \quad (144)$$

$$\begin{aligned} \dot{P}(t) &= \frac{i}{\hbar} [H, P(t)] \\ &= -U'(X(t)) + f'(X(t)) \int_{\mathbb{R}^+} d\omega c(\omega) \sqrt{\frac{2\omega}{\hbar}} x_t(\omega) - 2f(X(t))f'(X(t)) \int_{\mathbb{R}^+} r(\omega) d\omega, \end{aligned} \quad (145)$$

$$\dot{x}_t(\omega) = \frac{i}{\hbar} [H, x_t(\omega)] = p_t(\omega), \quad \omega \in \mathbb{R}^+, \quad (146)$$

$$\dot{p}_t(\omega) = \frac{i}{\hbar} [H, p_t(\omega)] = -\omega^2 x_t(\omega) + \sqrt{\frac{2\omega}{\hbar}} c(\omega) f(X(t)), \quad \omega \in \mathbb{R}^+, \quad (147)$$

where $r(\omega) = |c(\omega)|^2/(\hbar\omega)$ and $f'(X) = [f(X), P]/(i\hbar)$.

Next we eliminate the bath degrees of freedom from the equations for $X(t)$ and $P(t)$. Solving for $x_t(\omega)$, $\omega \in \mathbb{R}^+$, gives:

$$x_t(\omega) = \underbrace{x_0(\omega) \cos(\omega t) + p_0(\omega) \frac{\sin(\omega t)}{\omega}}_{x_t^0(\omega)} + \int_0^t \frac{\sin(\omega(t-s))}{\omega} \sqrt{\frac{2\omega}{\hbar}} c(\omega) f(X(s)) ds. \quad (148)$$

Substituting this into the equation for $P(t)$ results in:

$$\begin{aligned} \dot{P}(t) &= -U'(X(t)) + f'(X(t)) \int_{\mathbb{R}^+} d\omega c(\omega) \sqrt{\frac{2\omega}{\hbar}} x_t^0(\omega) \\ &\quad + \frac{2}{\hbar} f'(X(t)) \int_{\mathbb{R}^+} d\omega |c(\omega)|^2 \int_0^t ds \sin(\omega(t-s)) f(X(s)) - 2f(X(t))f'(X(t)) \int_{\mathbb{R}^+} d\omega r(\omega). \end{aligned} \quad (149)$$

Using integration by parts, we obtain

$$\int_0^t ds \sin(\omega(t-s)) f(X(s)) = \frac{f(X(t))}{\omega} - f(X) \frac{\cos(\omega t)}{\omega} - \int_0^t \frac{\cos(\omega(t-s))}{\omega} \frac{d}{ds} (f(X(s))) ds \quad (150)$$

and therefore,

$$\begin{aligned} \dot{P}(t) &= -U'(X(t)) + f'(X(t)) \underbrace{\int_{\mathbb{R}^+} d\omega c(\omega) (b_t^\dagger(\omega) + b_t(\omega))}_{\zeta(t)} \\ &\quad - f'(X(t)) \int_0^t ds \underbrace{\int_{\mathbb{R}^+} d\omega 2r(\omega) \cos(\omega(t-s))}_{\kappa(t-s)} \frac{d}{ds} (f(X(s))) \\ &\quad - f'(X(t)) f(X) \underbrace{\int_{\mathbb{R}^+} d\omega 2r(\omega) \cos(\omega t)}_{\kappa(t)}, \end{aligned} \quad (151)$$

where

$$\frac{d}{ds} (f(X(s))) = \frac{i}{\hbar} [H, f(X(s))] = \frac{\{f'(X(s)), P(s)\}}{2m}, \quad (152)$$

$b_t(\omega) = b(\omega)e^{-i\omega t}$, $b_t^\dagger(\omega) = b^\dagger(\omega)e^{i\omega t}$ and $\{\cdot, \cdot\}$ denotes anti-commutator.

Therefore, starting from the Heisenberg equations of motion and eliminating the bath variables, we obtain the following equations for the particle's observables:

$$\dot{X}(t) = V(t), \quad (153)$$

$$m\dot{V}(t) = -U'(X(t)) - f'(X(t)) \int_0^t \kappa(t-s) \frac{\{f'(X(s)), V(s)\}}{2} ds \\ + f'(X(t)) \cdot (\zeta(t) - f(X)\kappa(t)), \quad (154)$$

where

$$\kappa(t) = \int_{\mathbb{R}^+} d\omega \frac{2|c(\omega)|^2}{\hbar\omega} \cos(\omega t) = \int_{\mathbb{R}^+} d\omega \frac{2J(\omega)}{\omega} \cos(\omega t) \quad (155)$$

is the *memory kernel*,

$$\zeta(t) = \int_{\mathbb{R}^+} d\omega c(\omega) (b^\dagger(\omega)e^{i\omega t} + b(\omega)e^{-i\omega t}) \quad (156)$$

is a *stochastic force* whose correlation function depends on the coupling function, $c(\omega)$, and the distribution of the initial bath variables, $b(\omega)$ and $b^\dagger(\omega)$ – let us remind that we initially consider a thermal Gibbs state. The term $f'(X(t))f(X)\kappa(t)$ is the initial slip term. The initial position and velocity are given by X and V respectively.

The above equations are exact, non-Markovian and operator-valued. Note that in the damping term which is nonlocal in time, we have an anti-commutator, which does not appear in the corresponding classical equation or in the equation for the linear QBM model (where $f(X) = X$). The presence of the anti-commutator is thus a quantum feature of the inhomogeneous damping. The linear QBM model is exactly solvable. The properties of the solutions of the corresponding Heisenberg-Langevin equation³⁹ have been studied in standard references on open quantum systems.

The initial preparation of the total system, which fixes the statistical properties of the bath operators and of the system's degrees of freedom, turns the force $\zeta(t)$ into a stochastic one [73]. We specify a preparation procedure to fix the properties of the stochastic force. To this end, we absorb the initial slip term into the stochastic force, defining:

$$\xi(t) := \zeta(t) - f(X)\kappa(t). \quad (157)$$

With this, in the nonlinear coupling case, the equation for the particle's velocity is driven by the multiplicative noise $f'(X(t))\xi(t)$. From now on, we refer to $\xi(t)$ as the *quantum noise*. The statistics of $\xi(t)$ depends on the distributions of the initial bath variables ($b(\omega), b^\dagger(\omega)$) and the initial system variable $f(X)$.

The main difference between classical and quantum systems lie in the statistical nature of the noise. Denoting by E_β the expectation with respect to the thermal Gibbs state ρ_β at the temperature T , we have

$$E_\beta[(b^\dagger(\omega)e^{i\omega t} + b(\omega)e^{-i\omega t})(b^\dagger(\omega')e^{i\omega' s} + b(\omega')e^{-i\omega' s})] \\ = \left[(1 + \nu_\beta(\omega))e^{-i\omega(t-s)} + \nu_\beta(\omega)e^{i\omega(t-s)} \right] \delta(\omega - \omega'), \quad (158)$$

where $\nu_\beta(\omega)$ is given by the Planck's law

$$\nu_\beta(\omega) = \frac{1}{\exp(\beta\hbar\omega) - 1}. \quad (159)$$

Since we absorbed the initial slip term into the stochastic force, $\xi(t)$ no longer has a stationary correlation when averaged with respect to ρ_β [64]. However, $\xi(t)$ is stationary and Gaussian when conditionally averaged with respect to $\rho'_\beta = e^{-\beta H_{B-I}}/Tr(H_{B-I})$, where H_{B-I} is the quadratic Hamiltonian defined in (136) and the average is conditioned on the initial position variable X .

The statistical properties of the quantum noise is fully specified by its two-time correlation function with respect to ρ'_β , given by:

$$E'_\beta[\xi(t)\xi(s)] = \int_{\mathbb{R}^+} d\omega \hbar J(\omega) \left(\coth\left(\frac{\hbar\omega}{2k_B T}\right) \cos(\omega(t-s)) - i \sin(\omega(t-s)) \right) \quad (160)$$

$$=: D_1(t-s) - iD(t-s), \quad (161)$$

³⁹The rigorous study of the Heisenberg-Langevin equations, even in the case $f(X) = X$, is technically very difficult and there are only few works [36, 103] in the literature that treat them.

where D_1 is the noise kernel given by

$$D_1(t-s) := E'_\beta[\{\xi(t), \xi(s)\}/2], \quad (162)$$

i.e. the symmetric correlation function of $\xi(t)$ with respect to ρ'_β , and D is the dissipation kernel given by

$$D(t-s) := iE'_\beta[\{\xi(t), \xi(s)\}/2], \quad (163)$$

which is related to linear susceptibility. Expanding, one gets for small \hbar (or similarly, for large T), $E'_\beta[\xi(t)\xi(s)] = k_B T \kappa(t) + O(\hbar)$, which is the classical Einstein's relation. Therefore, (161) can be viewed as quantum analogue of the fluctuation-dissipation relation and a special case (and in time domain) of the quantum fluctuation-dissipation relation of Callen-Welton, since the noise kernel and dissipation kernel are related via:

$$\int_{\mathbb{R}} dt \cos(\omega t) D_1(t) = \hbar \coth(\hbar\omega\beta/2) \int_{\mathbb{R}} dt \sin(\omega t) D(t). \quad (164)$$

Therefore, the multiscale structure of the quantum noises is far richer than that of classical noises even in the simplest (Ornstein-Uhlenbeck type) model.

Remark 9. On zero temperature systems. For $T \rightarrow 0$ we have instead:

$$E'_\beta[\{\xi(t), \xi(s)\}/2] \rightarrow \frac{-\hbar\Lambda^2}{2\pi} (e^{-\Lambda(t-s)} \overline{Ei}(\Lambda(t-s)) + e^{\Lambda(t-s)} Ei(-\Lambda(t-s))), \quad (165)$$

where Ei is the exponential integral function defined as follows:

$$-Ei(-x) = \hat{\gamma}(0, x) = \int_x^\infty e^{-t}/t dt. \quad (166)$$

Here $\overline{Ei}(x) = \frac{1}{2}(Ei^+(x) + Ei^-(x))$, $Ei^+(x) = Ei(x + i0)$, $Ei^-(x) = Ei(x - i0)$. The symmetric correlation function obtained above can be interpreted as follows. As the temperature T decreases, the Matsubara frequencies ν_n get closer to each other, so at zero temperature all of them contribute and the sum may be replaced by an integral, which turns out to have expression in terms of the Ei functions [76]. In fact, in this case the symmetric correlation function decays polynomially for large times [79]. In other words, systems at zero temperature are strongly non-Markovian!

Remark 10. On stochastic modeling of the quantum noise. A natural approach to study the quantum noise is to model it as a quantum stochastic process which admits a QSDE representation, along the line in the classical case. The existence of such processes that satisfy the KMS condition was studied rigorously in [95], after the notions of quantum stochastic process and stationarity were defined there. However, to our knowledge no rigorous studies on their QSDE representation have been performed. Of interest to us is to study QSDE representations for the class of “quantum quasi-Markov” stationary Gaussian process, by mimicking the theory for classical quasi-Markov processes. However, this extension of the studies to the quantum setting is not too straightforward and one would need to deal with some technicalities, for instance in the construction of appropriate representation Hilbert space [8, 25, 24] for the quantum process.

4.3 The QBM Model with an Ohmic Spectral Density

We consider the coupling function:

$$c(\omega) = \sqrt{\frac{\hbar\omega}{\pi}} \frac{\Lambda^2}{\omega^2 + \Lambda^2}, \quad (167)$$

where Λ is a positive constant. The bath spectral density is given by:

$$J(\omega) := \frac{|c(\omega)|^2}{\hbar} = \frac{\omega}{\pi} \frac{\Lambda^2}{\omega^2 + \Lambda^2}, \quad (168)$$

which is the well-known Ohmic spectral density with a Lorentz-Drude cutoff [26].

Let us recall the Heisenberg-Langevin equation derived earlier. The equations for the particle's observables read:

$$\dot{X}(t) = V(t), \quad (169)$$

$$\begin{aligned} m\dot{V}(t) = & -U'(X(t)) - f'(X(t)) \int_0^t \kappa(t-s) \frac{\{f'(X(s)), V(s)\}}{2} ds \\ & + f'(X(t)) \cdot (\zeta(t) - f(X)\kappa(t)), \end{aligned} \quad (170)$$

where

$$\kappa(t) = \int_{\mathbb{R}^+} d\omega \frac{2|c(\omega)|^2}{\hbar\omega} \cos(\omega t) = \int_{\mathbb{R}^+} d\omega \frac{2J(\omega)}{\omega} \cos(\omega t) \quad (171)$$

is the *memory kernel*,

$$\zeta(t) = \int_{\mathbb{R}^+} d\omega c(\omega) (b^\dagger(\omega) e^{i\omega t} + b(\omega) e^{-i\omega t}) \quad (172)$$

is a *stochastic force*.

We will work in a *Fock vacuum representation* using the H-P quantum stochastic calculus approach. In particular, our goal is to describe the quantum noise as a quantum stochastic process satisfying certain QSDE such that the symmetric correlation function of the stochastic process with respect to the vacuum state on an enlarged Fock space coincides with that of $\xi(t)$ with respect to ρ'_β . As a preparation to achieve this goal, we study $E'_\beta[\xi(t)\xi(s)]$ in the following. Recall that:

$$E'_\beta[\xi(t)\xi(s)] = \int_{\mathbb{R}^+} d\omega \hbar J(\omega) \left(\coth\left(\frac{\hbar\omega}{2k_B T}\right) \cos(\omega(t-s)) - i \sin(\omega(t-s)) \right) \quad (173)$$

$$=: D_1(t-s) - iD(t-s), \quad (174)$$

where D_1 is the noise kernel given by

$$D_1(t-s) := E'_\beta[\{\xi(t), \xi(s)\}/2], \quad (175)$$

i.e. the symmetric correlation function of $\xi(t)$ with respect to ρ'_β , and D is the dissipation kernel given by

$$D(t-s) := iE'_\beta[[\xi(t), \xi(s)]]/2, \quad (176)$$

which is related to linear susceptibility.

For our choice of $c(\omega)$ (see (167)), the memory kernel, $\kappa(t)$, is exponentially decaying with decay rate Λ , i.e. $\kappa(t) = \Lambda e^{-\Lambda t}$. Moreover, one can compute, for $t > 0$:

$$D_1(t) = \frac{\hbar\Lambda}{2} \cot\left(\frac{\hbar\Lambda}{2k_B T}\right) \kappa(t) + \sum_{n=1}^{\infty} \frac{2k_B T \Lambda^2 \nu_n}{\nu_n^2 - \Lambda^2} e^{-\nu_n t}, \quad (177)$$

where $\nu_n = \frac{2\pi n k_B T}{\hbar}$ are the bath Matsubara frequencies [30]. Also, the dissipation kernel is

$$D(t) = \frac{\hbar\Lambda^3}{2} e^{-\Lambda t}. \quad (178)$$

In this paper, we consider the case $k_B T > \hbar\Lambda/\pi$, so that $\cot(\hbar\Lambda/2k_B T)$ and all the terms in the series in (177) are positive.

4.4 QSDE's for Quantum Noise

Guided by formula of the symmetric correlation function in (177) and the plan outlined in Section 4.2, we model the quantum noise by:

$$\sum_{k=0}^{\infty} \eta_k(t), \quad (179)$$

where the $\eta_k(t)$ are independent *quantum Ornstein-Uhlenbeck processes* (quantum analogue of the classical ones [35]), satisfying the SDEs:

$$d\eta_k(t) = -\alpha_k \eta_k(t) dt + \sqrt{\lambda_k} dW_k^\theta(t), \quad \eta_k(0) = \eta_k. \quad (180)$$

Here the W_k^θ are independent quantum Wiener processes defined earlier and the η_k are initial variables on a copy of Fock space. For a fixed θ , independence and commutation for these processes can be achieved by realizing the $\eta_k(t)$ on distinct copies of Fock space, i.e.

$$\sum_{k=0}^{\infty} \eta_k(t) = \eta_0(t) \otimes I \otimes I \otimes \cdots + I \otimes \eta_1(t) \otimes I \otimes \cdots + \cdots \quad (181)$$

on $\bigotimes_{k=0}^{\infty} \Gamma(L^2(\mathbb{R}^+)) = \Gamma(L^2(\mathbb{R}^+) \otimes \mathcal{K})$ where the multiplicity space \mathcal{K} is a sequence space whose elements are of the form (x_0, x_1, x_2, \dots) , with each $x_i \in \mathbb{C}$. From now on, each η_k is understood to be

$$\underbrace{I \otimes \dots \otimes I}_{k \text{ copies}} \otimes \eta_k \otimes I \otimes \dots \quad (182)$$

and similarly for each W_k^θ .

The formal solution to the SDE (180) is given by:

$$\eta_k(t) = \eta_k e^{-\alpha_k t} + \sqrt{\lambda_k} \int_0^t e^{-\alpha_k(t-s)} dW_k^\theta(s). \quad (183)$$

Since there is a unique stationary solution of the SDEs (180), for all k and $s \in [0, t]$:

$$E''_\infty[\eta_k^2] = \frac{\lambda_k}{2\alpha_k}, \quad E''_\infty[\eta_k W_k^\theta(s)] = E''_\infty[W_k^\theta(s) \eta_k] = 0, \quad (184)$$

where E''_∞ denotes expectation with respect to the vacuum state associated with $\Omega \otimes \Omega \otimes \dots$ on the enlarged Fock space $\Gamma(L^2(\mathbb{R}^+) \otimes \mathcal{K})$. Then, with the parameters α_n and λ_n defined by

$$\alpha_n = \nu_n 1_{\{n \geq 1\}} + \Lambda 1_{\{n=0\}} > 0 \quad (185)$$

and

$$\lambda_n = \frac{4\nu_n^2 \Lambda^2 k_B T}{\nu_n^2 - \Lambda^2} 1_{\{n \geq 1\}} + \hbar \Lambda^3 \cot\left(\frac{\hbar \Lambda}{2k_B T}\right) 1_{\{n=0\}} > 0, \quad (186)$$

it can be verified that

$$E''_\infty \left[\frac{\{\sum_k \eta_k(t), \sum_l \eta_l(s)\}}{2} \right] = D_1(t-s), \quad (187)$$

where D_1 is given in (177).

Equations (185) and (186) establish a link between the quantum noise as introduced in eqn. (179) and the physical model of Section 4.3. We remark that there is freedom in the above construction of quantum noise, as the driving noise process, (W_k^θ) , is a family of quantum Wiener processes parametrized by θ . On the one hand, the choice of the parameter should be fixed by physical considerations, i.e. by the nature of the field that the system couples to in the microscopic model. On the other hand, one would like to show that the quantum noises describe a Markovian system, so one should write the SDEs (180) in a H-P QSDE form.

To this end, let $\xi_k(t)$ and $\eta_k(t)$ be canonical conjugate bath observables that obey the commutation relation $[\xi_j(t), \eta_k(t)] = i\hbar \delta_{jk} I$ for all $t \geq 0$. Suppose that the evolution of each pair $(\xi_k(t), \eta_k(t))$ is Markovian and can be described by the H-P QSDEs associated with (H_k, L_k) , where

$$H_k = \frac{\eta_k^2}{2} + \frac{\alpha_k}{4} \{\xi_k, \eta_k\}, \quad L_k = \frac{\sqrt{\lambda_k}}{\hbar} \xi_k + i \frac{\alpha_k}{2\sqrt{\lambda_k}} \eta_k, \quad (188)$$

where α_k and λ_k are given as before. Therefore, they solve the H-P QSDEs:

$$d\xi_k(t) = \eta_k(t) dt + \frac{\hbar \alpha_k}{2\sqrt{\lambda_k}} dW_k^\pi(t), \quad (189)$$

$$d\eta_k(t) = -\alpha_k \eta_k(t) dt + \sqrt{\lambda_k} dW_k^{-\pi/2}(t), \quad (190)$$

where

$$W_k^\pi(t) = -(A_k(t) + A_k^\dagger(t)), \quad W_k^{-\pi/2}(t) = i(A_k(t) - A_k^\dagger(t)) \quad (191)$$

are noncommuting, conjugate quantum Wiener processes satisfying $[W_k^\pi(t), W_k^{-\pi/2}(s)] = 2i\delta(t-s)I$. Modulo the negative factor, one can view the formal time derivatives of the $W_k^\pi(t)$ and $W_k^{-\pi/2}(t)$ as the noises arising from the position and momentum field observables respectively. We fix the freedom in our construction by taking the Markovian system (189)-(190) as the model for noise. Therefore, we take $\sum_k \eta_k(t)$ to be the quantum colored noise that models the action of the heat bath on the evolution of the system's observables.

Physically, one can think of our quantum noise model as equivalent to a model of infinitely many non-interacting ancillas that convert the white noise to colored noise through a channel at each Matsubara frequency [153]. That one needs infinitely many ancillas is due to the fact that there are infinitely many transition (Bohr) energies, each of which equals the energy of a boson with a particular Matsubara frequency in the bath. According to our noise model, when a boson with the Matsubara frequency ν_k is created or annihilated, the energy transition does not occur instantaneously but happens on the time scale of $1/\alpha_k$ via a channel associated with ν_k .

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