FROM THE QUANTUM HARMONIC OSCILLATOR TO THE ORNSTEIN-UHLENBECK PROCESS AND BACK

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Abstract

In this thesis, the relation between the generator of the Ornstein-Uhlenbeck process and the Hamiltonian of the quantum harmonic oscillator is used to derive a new understanding of the evolution of certain quantum states. More precisely, we transform the Hamiltonian with respect to the ground state and corresponding eigenvalue to find that it is equal to minus the generator of the Ornstein-Uhlenbeck process. Next, we use the knowledge of the evolution of distributions in the Ornstein-Uhlenbeck process to obtain the time evolution of corresponding quantum states. Specifically, we derived that the evolution of normal distributions in the Ornstein-Uhlenbeck process remain normally distributed with varying mean and variance. Furthermore, the ground state of the harmonic oscillator is equal to the square root of the reversible distribution of the Ornstein-Uhlenbeck process. Combining these results gives us the evolution of quantum states with an almost Gaussian wave function. If we confine one degree of freedom in the end result, we obtain the coherent states of the quantum harmonic oscillator. These are Gaussian wave packets, which means that the probability density is Gaussian with constant variance and oscillating mean. Coherent states most closely resemble classical particles in the harmonic oscillator and minimise Heisenberg's uncertainty principle.

Contents

1 Introduction

In the nineteenth century quantum theory did not yet exist. Until then Newton's mechanics, Maxwell's electrodynamics and Einstein's relativity were used to predict and describe the world around us. Classical mechanics deterministically describes position x and momentum p as a function of time, if the Hamiltonian is known. This view drastically changed when quantum theory was introduced. Quantum mechanics describes physical systems in a different way, through the system's wave function; $\Psi(x,t)$. The wave function, however, cannot tell us everything we would like to know about the state of a system. We can only use it to calculate the probability of getting a certain outcome to a measurement. The indeterminacy of the quantum world is also seen in the fact that certain pairs of observables cannot be known with certainty. A well-known uncertainty relation was introduced by Werner Heisenberg in 1927. He showed that for each system the standard deviation of the position times the standard deviation of the momentum is equal to or greater than $\frac{\hbar}{2}$, where $\hbar$ is the reduced Planck constant. This relation indicates that the more precise the position is known, the less precise the momentum can be known.

In classical mechanics Newton's laws are used to describe the motion of particles over time. In quantum mechanics, however, the time evolution of a system's wave functions is found by solving the Schrödinger equation, which was introduced by Erwin Schrödinger in 1926. We will be considering a physical system with quadratic potential $V(x) = \frac{1}{2}m\omega^2x^2$, which is called the quantum harmonic oscillator. It is a fundamental object in mechanics and approximately describes systems close to there equilibrium state (which is a minimum of the potential energy). We will derive that the energy of the quantum harmonic oscillator is quantised at energies $(n+\frac{1}{2})\hbar\omega$. This means that when measuring the energy you cannot obtain other values than $(n+\frac{1}{2})\hbar\omega$. Later on in this thesis, coherent states will be introduced. These are special states of the quantum harmonic oscillator that minimise Heisenberg's uncertainty relation and that best resemble the behaviour of classical particles in the harmonic oscillator.

The central idea in this thesis is that there exists a connection between quantum mechanics and Markov evolutions. Calculating the evolution of a quantum state comes down to applying an operator of the form e^{-itH} and for the expectation of a Markov evolution over time we apply the operator e^{tL}, where L is a Markov generator. Therefore, by going from real to imaginary time and transforming the Hamiltonian H in such a way that it equals a Markov generator L we can understand the quantum mechanical system by treating it as a Markovian evolution and vice versa. The main subject in this thesis is the relation between the quantum harmonic oscillator and the Ornstein-Uhlenbeck process which is an example of such a relation. We perform an alternative way of calculating the time evolution of states of the quantum harmonic oscillator by transforming the Hamiltonian with respect to its ground-state to find that this is equal to minus the generator of the Ornstein-Uhlenbeck process. Such a transformation is called a ground-state transformation. In order to understand this connection, an introduction to Markov semigroups and Markov generators is needed. The fact that Gaussian distributions are conserved under Ornstein-Uhlenbeck evolutions

can then be linked to the time evolution of coherent states.

The rest of this thesis is organised in six other chapters. We start with some mathematical preliminaries in chapter 2 (the reader familiar with Markov process theory can skip this section). Firstly, we introduce the definition of a Markov process together with some important properties followed by mathematical introductions to the Paley-Wiener integral, invariant measures and some Markov semigroup theory. In the latter, the Markov generator is defined, which will be of particular importance later on. The stochastic process of interest, the Ornstein-Uhlenbeck process, is introduced in chapter 3, whereafter its important properties will be derived. We calculate the evolution of normal distributions in the Ornstein-Uhlenbeck process and finalize with a calculation of the Markov generator.

The quantum mechanics starts in chapter 4 with an introduction to the Schrödinger equation and wave function followed by a derivation of the Heisenberg uncertainty principle. The harmonic oscillator is looked at, the classical case and the quantum case. For the quantum harmonic oscillator we find the energy eigenfunctions together with the quantised energy levels. Then, in chapter 5, we introduce the concept of coherent states of the quantum harmonic oscillator and show that they behave in a way closely connected to the classical harmonic oscillator. We use its definition to derive their wave functions explicitly and also find that these minimise the Heisenberg uncertainty principle.

In chapter 6, we perform the ground-state transformation to the Hamiltonian of the quantum harmonic oscillator. Then, we use our knowledge of how normal distributions evolve according to the Ornstein-Uhlenbeck process in order to deduce the time evolution of the corresponding quantum states in the quantum harmonic oscillator. This is done for one and more dimensions. We finalize with the results and observations in chapter 7.

This is a Bachelor's thesis of the bachelor programs Applied Mathematics and Applied Physics at the TU Delft.

2 Preliminaries

Firstly, we give an introduction to the theory behind the connection between the Ornstein-Uhlenbeck process and the quantum harmonic oscillator. In this section we introduce some basic background from Markov process theory.

2.1 Random Walk

We start with the definition of a stochastic process.

Definition 1.1 *Consider a probability space $(\Omega, \mathcal{F}, P)$. Then a* ***stochastic process*** $\{X_t, t \geq 0\}$ *is a collection of random variables indexed by time.*

A Markov process is a kind of stochastic process for which the probability on future states only depends on current state values and not on how it got there over time. This property is called the Markov Property. A time-homogeneous process is a process whose transition probability (density) between times t and $t + s$ only depends on the time difference s, and not on the precise time t. Mathematically and in discrete time, this translates as follows.

Definition 1.2 *Consider a probability space $(\Omega, \mathcal{F}, P)$ and let $\{X_t, t \geq 0\}$ be a stochastic process with natural filtration $\mathcal{F}_t = \sigma\{X_s, s \leq t\}$ then we call it* ***time-homogeneous Markov*** *if for all $t, s > 0$ and for all $f \in C_b(\Omega)$*

$$\mathrm{E}[f(X_{t+s})|\mathcal{F}_t] = \mathrm{E}[f(X_{t+s})|X_t] = \mathrm{E}_{X_t} f(X_s), \tag{1}$$

where

$$\mathrm{E}_x f(X_s) = \mathrm{E}[f(X_s)|X_0 = x]. \tag{2}$$

A simple example of a time-homogeneous Markov process is the evolution of a particle's position over time in the case that it can either move up or down with equal probability at integer times. The construction of such a process can be done by considering $Z_1, Z_2, \ldots, Z_n$ independent random variables such that for all $i = 1, \ldots, n$:

$$Z_i = \begin{cases} 1 & \text{with probability } \frac{1}{2}. \\ -1 & \text{with probability } \frac{1}{2}. \end{cases}$$

Let $\{X_k, 0 \leq k \leq n\}$ denote the particles position. Then X_k can be expressed as:

$$X_k = \sum_{i=1}^{k} Z_i.$$

It can easily be seen that the development of the particle's position over time is a Markov Process, since the probability distribution of future positions is only dependent on its current position and not on the further history. This example

is known as the (one-dimensional, discrete time) random walk. See Figure 1 for a plot of the random walk.

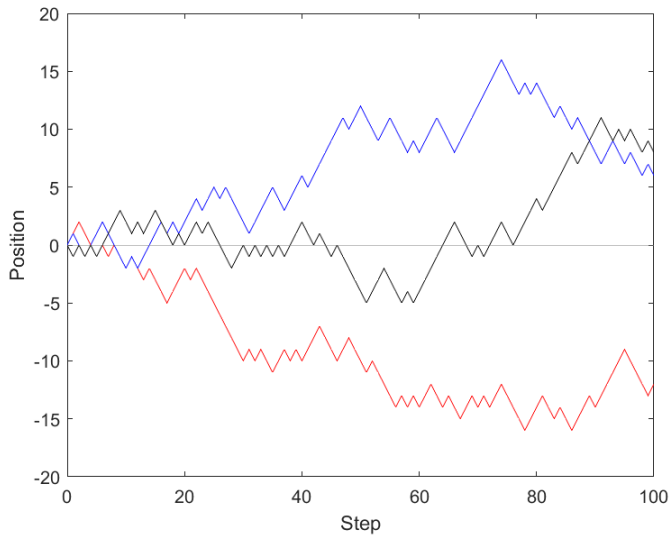

Figure 1. Three realizations of the random walk with 100 steps.

We give an example of a stochastic process which is not Markov. Consider independent and identically distributed random variables $Z_t \overset{d}{=} \mathcal{N}(0,1)$ for $t \in \mathbb{N}_0$. Let $X_0 = Z_0$, $X_1 = Z_1$ and for $t \geq 2$

$$X_t = X_{t-1} + X_{t-2} + Z_t.$$

Then X_{t+1} is not independent of X_{t-1} when conditioned on X_t. So clearly, the process $\{X_t, t \in \mathbb{N}_0\}$ is not Markov. Examples of more interesting stochastic processes are the self-avoiding random walk, which avoids visiting the same point more than once, and the reinforced random walk, where probability of crossing an interval depends on the amount of crossings it has had in total.

2.2 Wiener Process

2.2.1 Definition

A more interesting example of a time-homogeneous Markov process is the Wiener process. This is a fundamental object in probability theory and is defined below. In the definition we use the notation $\overset{d}{=}$ for equal in distribution.

Definition 1.3 *The Wiener process $\{W_t, t \geq 0\}$ is the stochastic process such that it satisfies the following properties:*

1. $W_0 = 0$,

2. *W_t has independent increments, i.e. if $0 \leq s_1 \leq t_1 \leq s_2 \leq t_2$ then $W_{t_1} - W_{s_1}$ and $W_{t_2} - W_{s_2}$ are independent random variables,*

3. *W_t has Gaussian increments with mean zero and variance equal to the time difference, i.e. for all $t, u \geq 0 : W_{t+u} - W_t \stackrel{d}{=} \mathcal{N}(0, u)$,*

4. *The map $t \to W_t$ is continuous.*

Proposition 1.1 The Wiener process is a time-homogeneous Markov process.

Proof. For $t, s > 0$ and $f \in C_b(\mathbb{R})$ we have

$$\mathrm{E}[f(W_{t+s})|\mathcal{F}_t] = \mathrm{E}[f(W_t + W_{t+s} - W_t)|\mathcal{F}_t].$$

Given $\mathcal{F}_t$, W_t is given and from the third property of definition 1.3, it follows that $W_{t+s} - W_t$ is independent of $\mathcal{F}_t$. Hence,

$$\begin{aligned}
&\mathrm{E}[f(W_t + W_{t+s} - W_t)|\mathcal{F}_t] = \mathrm{E}[f(W_t + \mathcal{N}(0, s))] = \\
&= \int_{-\infty}^{\infty} f(W_t + x) \frac{e^{-x^2/2s}}{\sqrt{2\pi s}} dx = \mathrm{E}[f(W_{t+s})|W_t] = \\
&= \mathrm{E}_{W_t} f(W_s).
\end{aligned}$$

□

2.2.2 Constructing the Wiener Process

The construction of the Wiener process can be done in a number of ways. The most straightforward one is done by starting off with the random walk. We consider a random walk with n steps evenly spaced in time that are done in a time interval $[0, T]$. Then, for the time step we have $\Delta t = T/n$, the space step we set to $\Delta x = \sqrt{\Delta t}$. The resulting stochastic process is known as the n-step Wiener walk and its value at time t_k is expressed as:

$$w^n(t_k) = \sum_{i=1}^{n} Z_i \Delta x.$$

Note that the probability density of the Wiener walk is binomial. The values in between steps are found through linear interpolation, which allows the Wiener walk to be in continuous time instead of discrete time. At each instance in time the expectation of the Wiener walk is equal to zero. When calculating the variance, we find

$$\begin{aligned}
\mathrm{Var}\left[w^n(T)\right] = \mathrm{E}\left[w^n(T)^2\right] &= \mathrm{E}\left[\left(\sum_{i=1}^{n} Z_i \Delta x\right)^2\right] = \\
&= \mathrm{E}\left[\sum_{i=1}^{n} \left(\Delta x Z_i\right)^2\right] = \Delta x^2 \sum_{i=1}^{n} \mathrm{E}\left[Z_i^2\right] = \\
&= \Delta x^2 n = T.
\end{aligned}$$

Now the claim is that by taking the limit $n \to \infty$ the Wiener process on the bounded interval $[0, T]$ is obtained [1]. It is obvious that the first and second property of definition 1.4 are satisfied. Furthermore, because of the central limit theorem we can conclude that the constructed process has indeed Gaussian increments with zero mean and variance equal to the time difference [2]. Because the obtained path is a limit of continuous functions, the fourth property seems plausible. However, sequences of continuous functions do not necessarily converge to continuous functions. Therefore, we should have given some more explanation to properly show that the fourth property is also satisfied. Now, we have constructed the Wiener process on a bounded interval, the unbounded case can be formed out of a sequence of bounded intervals. See figure 2 for a plot of the Wiener process.

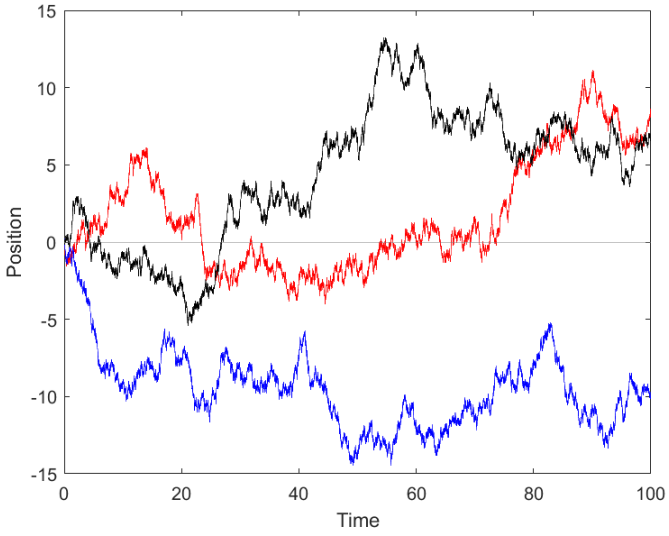

Figure 2. Three realizations of the Wiener process with a timespan of 100 seconds.

2.3 Paley-Wiener Integral

The Paley-Wiener integral is a stochastic variant of the Riemann-Stieltjes integral. The integrand is still a deterministic function but the integrator is now the Wiener process. Let $f \in C_b(\mathbb{R})$, we define a new stochastic process $\{Y_t, t \geq 0\}$ by

$$Y_t = \int_0^t f(s)dW_s := \lim_{n\to\infty} \sum_{j=1}^{n} f(t_{j-1})(W_{t_j} - W_{t_{j-1}}), \tag{3}$$

where the limit is with respect to the L^2-norm and $t_j = \frac{jt}{n}$. This is called a Paley-Wiener integral.

The third property of definition 1.3 states that increments of the Wiener process are distributed as normal distributions with variance equal to the time difference.

We have

$$\lim_{n\to\infty}\sum_{j=1}^{n} f(t_{j-1})\left(W_{t_j}-W_{t_{j-1}}\right) \overset{d}{=} \lim_{n\to\infty}\sum_{j=1}^{n} f(t_{j-1})\mathcal{N}_j\left(0,\frac{t}{n}\right)$$

where the $\mathcal{N}_j(0,\frac{t}{n})$'s are independent normal random variables with expectation 0 and variance $\frac{t}{n}$. Therefore, it follows that

$$\lim_{n\to\infty}\sum_{j=1}^{n} f(t_{j-1})\mathcal{N}_j\left(0,\frac{t}{n}\right) \overset{d}{=} \lim_{n\to\infty}\sum_{j=1}^{n} \mathcal{N}_j\left(0,f(t_{j-1})^2\frac{t}{n}\right) \overset{d}{=}$$
$$\overset{d}{=} \lim_{n\to\infty}\mathcal{N}\left(0,\sum_{j=1}^{n} f(t_{j-1})^2\frac{t}{n}\right) \overset{d}{=} \mathcal{N}\left(0,\lim_{n\to\infty}\sum_{j=1}^{n} f(t_{j-1})^2\frac{t}{n}\right) \overset{d}{=}$$
$$\overset{d}{=} \mathcal{N}\left(0,\int_0^t f(s)^2 ds\right).$$

Hence,

$$\int_0^t f(s)dW_s \overset{d}{=} \mathcal{N}\left(0,\int_0^t f(s)^2 ds\right). \tag{4}$$

Let $W_t = (W_{1,t}, W_{2,t}, \ldots, W_{n,t})$ be the n-dimensional Wiener process and $f:\mathbb{R}\to\mathbb{R}^n$ bounded and measurable. We define the multivariate analogue of the Paley-Wiener integral by

$$Y_t = \int_0^t f(s)dW_s, \tag{5}$$

where Y_t is the n-dimensional vector with i'th component equal to:

$$Y_{t,i} = \sum_{j=1}^{n}\int_0^t f_{ij}(s)dW_{j,s}. \tag{6}$$

In a similar way we can find the multivariate form of (4).

$$\int_0^t f(s)dW_s \overset{d}{=} \mathcal{N}\left(\mathbf{0},\int_0^t f(s)f(s)^T ds\right), \tag{7}$$

Here, $\mathcal{N}(\boldsymbol{\mu},\Sigma)$ stands for the multivariate normal distribution with mean $\boldsymbol{\mu}$ (column vector) and covariance matrix Σ.

2.4 Markov Semigroups

Consider a Markov process $\{X_t, t\geq 0\}$. We define $\{S_t, t\geq 0\}$ by

$$(S_t f)(x) := \mathrm{E}_x[f(X_t)] := \mathrm{E}[f(X_t)|X_0 = x] \tag{8}$$

for all $f\in C_b(\Omega)$.

Proposition 1.2 $\{S_t, t\geq 0\}$ satisfies the following properties:

1. Identity at time zero: $S_0 f = f$ for all f,
2. Normalization: $S_t 1 = 1$,
3. Right continuity: The map $t \to S_t$ is right continuous,
4. Semigroup property: for all $t, s > 0, f : S_{t+s} f = S_t(S_s f) = S_s(S_t f)$,
5. Positivity: $f > 0$ implies $S_t f > 0$,
6. Contraction: $\max_x |S_t f(x)| \leq \max_x |f(x)|$.

The properties 1,2,3,5 and 6 can be derived from the definition straightforwardly. We skip their proofs and restrict us to proving the semigroup property. We give the proof in discrete setting, i.e. for continuous time Markov chain on a finite set Ω.

Proof. We start by defining the transition probability function

$$p_t(x, y) = \mathbb{P}(X_t = y | X_0 = x).$$

We can write

$$S_{t+s} f(x) = \mathrm{E}[f(X_{t+s}) | X_0 = x] = \sum_{y \in \Omega} p_{t+s}(x, y) f(y).$$

Since $\{X_t, t \geq 0\}$ is Markov, we can apply the Chapman-Kolmogorov equation [3]:

$$p_{t+s}(x, y) = \sum_{z \in \Omega} p_t(x, z) p_s(z, y).$$

Combining these yields:

$$\begin{aligned} S_{t+s} f(x) &= \sum_{y \in \Omega} p_{t+s}(x, y) f(y) \\ &= \sum_{y \in \Omega} \sum_{z \in \Omega} p_t(x, z) p_s(z, y) f(y) \\ &= \sum_{z \in \Omega} p_t(x, z) \sum_{y \in \Omega} p_s(z, y) f(y) \\ &= \sum_{z \in \Omega} p_t(x, z) S_s f(z) \\ &= S_t(S_s f)(x). \end{aligned}$$

□

Semigroups like $\{S_t, t \geq 0\}$ are called Markov semigroups. Each Markov semigroup corresponds to an underlying Markov process [4]. For these semigroups we define a so-called Markov generator L:

$$Lf = \lim_{t \to 0} \frac{S_t f - f}{t} \tag{9}$$

for $f \in D(L)$, i.e. all $f \in C_b(\Omega)$ for which this limit exists. This is called the domain of L and is dense in $C_b(\Omega)$. In the case that Ω is infinite (e.g.

$\Omega = \mathbb{R}$) L is an unbounded operator with dense domain, and the limit has to be interpreted in sup-norm sense. These operators can also be linked back to Markov semigroups [5] [6].

Theorem 1.1 *If $f \in D(L)$, then $S_t f \in D(L)$ and the following holds:*

$$\frac{d}{dt} S_t f = S_t L f = L S_t f \tag{10}$$

Moreover, $S_t f$ is the unique solution of the differential equation

$$\frac{d\psi_t}{dt} = L\psi_t \tag{11}$$

with initial condition $\psi_0 = f$.

For a proof of this theorem see [5] and [6].

2.5 Invariant Measures

Let $\{X_t, t \geq 0\}$ be a Markov process with corresponding semigroup $\{S_t, t \geq 0\}$ and let μ be a probability measure on the probability space $(\Omega, \mathcal{F}, P)$. If we let the process start from μ, then we denote μS_t for the measure evolved after time t. Hence, this is the unique probability measure such that:

$$\int_\Omega S_t f d\mu = \int_\Omega f d\mu S_t \tag{12}$$

for all $f \in C_b(\Omega)$.

Definition 1.7 *Consider a Markov process on probability space $(\Omega, \mathcal{F}, P)$ with corresponding semigroup S_t. Then a probability measure μ is called **invariant** if the following relation holds for all $t \geq 0$ and all f bounded and continuous:*

$$\int_\Omega S_t f d\mu = \int_\Omega f d\mu. \tag{13}$$

Theorem 1.2 A probability measure μ is invariant if and only if

$$\int_\Omega L f d\mu = 0 \tag{14}$$

for all $f \in D(L)$.

Proof. Suppose μ is invariant and let $f \in D(L)$, then

$$\int_\Omega L f d\mu = \lim_{t\to 0} \frac{1}{t} \int_\Omega S_t f - f d\mu = \lim_{t\to 0} \frac{1}{t} \left(\int_\Omega S_t f d\mu - \int_\Omega f d\mu \right) = 0.$$

Conversely, if (14) holds, we find for all $f \in D(L)$:

$$\begin{aligned} &\int_\Omega S_t f - f d\mu = \int_\Omega \int_0^t \frac{d}{ds} S_s f ds d\mu = \\ &= \int_\Omega \int_0^t (L S_s f) ds d\mu = \int_0^t \left(\int_\Omega (L S_s f) d\mu \right) ds = \\ &= 0 \end{aligned}$$

Hence,

$$\int_\Omega S_t f d\mu = \int_\Omega f d\mu.$$

Since $D(L)$ is dense in $C_b(\Omega)$, this extends to all $f \in C_b(\Omega)$. □

Definition 1.9 *Consider a Markov process $\{X_t, t \geq 0\}$ on probability space $(\Omega, \mathcal{F}, P)$ with corresponding semigroup S_t. Then a probability measure μ is called* ***reversible*** *if*

$$\int (S_t f) g d\mu = \int f (S_t g) d\mu \tag{15}$$

for all $f, g \in C_b(\Omega)$.

Proposition 1.3 Consider a probability space $(\Omega, \mathcal{F}, P)$ and a Markov process X_t with semigroup S_t and generator L.

1. A reversible measure is invariant
2. Let the process start from $X_0 = \mu$. Then, μ is reversible if and only if $\{X_t, X_s\}$ has the same distribution as its time reversal $\{X_{T-t}, X_{T-s}\}$ for all $t, s \in [0, T], T > 0$.
3. A measure μ is reversible if and only if

$$\int g L(f) d\mu = \int f L(g) d\mu \tag{16}$$

for all $f, g \in D(L)$.

Proof. 1. Let μ be a reversible measure. From definition 1.9 we find that for all $f \in C_b(\Omega)$

$$\int_\Omega S_t f d\mu = \int_\Omega f(S_t 1) d\mu = \int_\Omega f d\mu.$$

Hence, μ is invariant.

2. Let μ be a reversible measure and let the process start from $X_0 = \mu$. Because a reversible measure is invariant, we have that $X_t = \mu$ for all $0 \leq t \leq T$. Let $T > 0$, we denote the time reversed process by $Y_t = X_{T-t}$ for $0 \leq t \leq T$. It follows that for all $0 \leq t \leq T$ and all $f, g \in C_b(\Omega)$:

$$\mathrm{E}_\mu[f(Y_0) g(Y_t)] = \mathrm{E}_\mu[f(X_T) g(X_T - t)]$$

Because X_t is Markov, we can conclude that

$$\mathrm{E}_\mu[f(X_T) g(X_T - t)] = \mathrm{E}_\mu[f(X_t) g(X_0)] = \int_\Omega S_t f(x) g(x) d\mu$$

We use the definition of reversibility and find:

$$\int_\Omega S_t f(x) g(x) d\mu = \int_\Omega f(x) S_t g(x) d\mu = \mathrm{E}_\mu[f(X_0) g(X_t)].$$

Hence,

$$\mathrm{E}[f(Y_0) g(Y_t) | Y_0 = \mu] = \mathrm{E}[f(X_0) g(X_t) | X_0 = \mu].$$

Because X_t is time-homogeneous Markov, we can conclude that $\{X_t, X_s\}$ has the same distribution as its time reversal $\{X_{T-t}, X_{T-s}\}$ for all $t, s \in [0, T]$ and $T > 0$. Now we can simply read this proof inside out in order to proof the converse statement.

3. Let $f, g \in D(L)$ and μ be a reversible measure. We insert (9) and find:

$$\int_\Omega gL(f)d\mu = \int_\Omega g \lim_{t\to 0} \frac{1}{t}(S_t f - f)d\mu = \lim_{t\to 0} \frac{1}{t} \int_\Omega gS_t f - gf d\mu.$$

Since μ is reversible, we can interchange $gS_t f$ with $fS_t g$ inside the integral:

$$\lim_{t\to 0} \frac{1}{t} \int_\Omega gS_t f - gf d\mu = \lim_{t\to 0} \frac{1}{t} \int_\Omega fS_t g - gf d\mu = \int_\Omega fL(g)d\mu.$$

We have found that

$$\int_\Omega gL(f)d\mu = \int_\Omega fL(g)d\mu.$$

We can use the fact that $D(L)$ is dense in $C_b(\Omega)$ and then read this proof inside out to prove the converse statement.

□

Remark. We defined reversibility for Markov processes only, but if we would define it on a general stochastic, then the equivalent of item 2 should read:

The stochastic process $\{X_t, t \geq 0\}$ *is reversible if and only if* $\{X_t, 0 \leq t \leq T\} \stackrel{d}{=} \{X_{T-t}, 0 \leq t \leq T\}$ *for* $T > 0$.

For time-homogeneous Markov processes this relation will already hold when the joint distribution of just two instances in time is distributed equally to its time reversal.

3 Ornstein-Uhlenbeck Process

The stochastic process of interest is the Ornstein-Uhlenbeck process. In this section we discuss its definition and consider some of its properties. Later on, these properties will be used to calculate the evolution of quantum states in the harmonic oscillator.

3.1 Univariate Case

3.1.1 Definition and Explicit Solution

The Ornstein-Uhlenbeck process is another example of a Markov process. We define it through the following stochastic differential equation

$$dX_t = \theta(\mu - X_t)dt + \sigma dW_t, \tag{17}$$

where θ, μ and σ are parameters and W_t is the Wiener process. Intuitively we can describe this as the position of a particle experiencing thermal noise with variance σ^2 which wants to return to its mean value μ with rate θ. Such a process is called a noisy relaxation process. See figure 3 for a plot of the Ornstein-Uhlenbeck process.

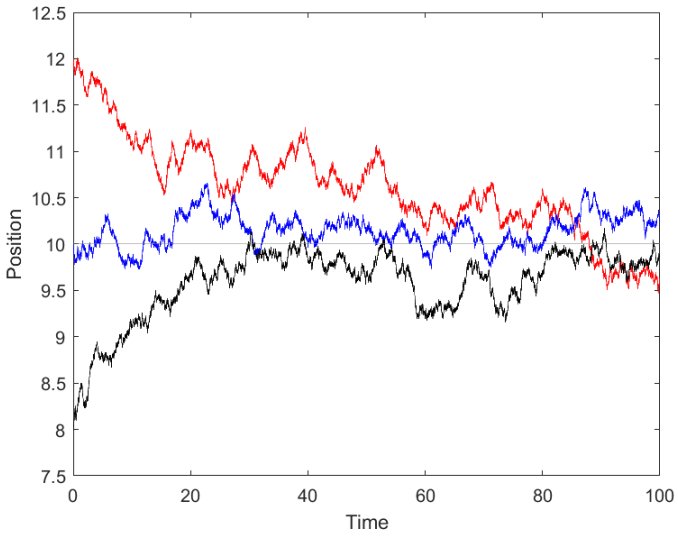

Figure 3. Plot of three realizations of the Ornstein-Uhlenbeck process with parameters $\mu = 10, \theta = 0.05, \sigma = 4$ and starting from positions 8, 10 and 12.

From now on we will limit our view to the case where the mean μ is equal to zero. For this case we want to calculate the explicit solution to (17). We start by introducing a change of variable:

$$Y_t = e^{\theta t} X_t.$$

We have:

$$\begin{aligned} dY_t &= \theta e^{\theta t} X_t dt + e^{\theta t} dX_t \\ &= \theta e^{\theta t} X_t dt + e^{\theta t} \left(-\theta X_t dt + \sigma dW_t\right) \\ &= \sigma e^{\theta t} dW_t \end{aligned}$$

Integrating from 0 to t yields

$$Y_t = Y_0 + \sigma \int_0^t e^{\theta s} dW_s,$$

where this is a Paley-Wiener integral as introduced in section 2.3. We reverse the change of variable to obtain the explicit solution to (17):

$$X_t = e^{-\theta t} Y_t = e^{-\theta t} X_0 + \sigma \int_0^t e^{-\theta(t-s)} dW_s. \tag{18}$$

If we start from an initial point, say $X_0 = x$, we find for its distribution after time t:

$$X_t = e^{-\theta t} x + \sigma \int_0^t e^{-\theta(t-s)} dW_s.$$

Using (4) we find

$$\int_0^t e^{-\theta(t-s)} dW_s \overset{d}{=} \mathcal{N}\left(0, \int_0^t e^{-2\theta(t-s)} ds\right) \overset{d}{=} \mathcal{N}\left(0, \frac{1}{2\theta}(1 - e^{-2\theta t})\right).$$

Hence,

$$X_t \overset{d}{=} e^{-\theta t} x + \mathcal{N}\left(0, \frac{\sigma^2}{2\theta}(1 - e^{-2\theta t})\right) \overset{d}{=} e^{-\theta t} x + \sqrt{1 - e^{-2\theta t}} \mathcal{N}(0, \frac{\sigma^2}{2\theta}). \tag{19}$$

We use this equation to find an expression for $S_t f(x)$:

$$S_t f(x) = \mathrm{E}[f(X_t) | X_0 = 0] = \int_{\mathbb{R}} f(e^{-\theta t} + \sqrt{1 - e^{-2\theta t}} y) \tilde{\mu}(y) dy, \tag{20}$$

where

$$\tilde{\mu} = \mathcal{N}(0, \frac{\sigma^2}{2\theta}). \tag{21}$$

The result of (20) is known as the Mehler formula [1].

3.1.2 Invariant and Reversible Measure

We want to calculate the time-invariant (or stationary) distribution from (19). We can do this by taking the limit $t \to \infty$, we find:

$$\lim_{t \to \infty} X_t \overset{d}{=} \lim_{t \to \infty} e^{-\theta t} X_0 + \sqrt{1 - e^{-2\theta t}} \mathcal{N}(0, \frac{\sigma^2}{2\theta}) \overset{d}{=} \mathcal{N}(0, \frac{\sigma^2}{2\theta}) \overset{d}{=} \tilde{\mu}. \tag{22}$$

This is the only invariant measure, since every initial distribution will converge towards this one. We will write the variance of the stationary distribution as $\sigma_*^2 = \frac{\sigma^2}{2\theta}$ and the distribution of the Ornstein-Uhlenbeck process starting from $\tilde{X}_0 = \tilde{\mu}$ as $\{\tilde{X}_t, t > 0\}$. Now the claim is that $\{\tilde{X}_t, t > 0\}$ is reversible. In order to proof this, we have to start by calculating the covariance between arbitrary times t and s. We have

$$\begin{aligned}\mathrm{Cov}(\tilde{X}_t, \tilde{X}_s) &= \mathrm{E}\left[\left(e^{-\theta t}\tilde{X}_0 + \sigma\int_0^t e^{-\theta(t-u)}dW_u)(e^{-\theta s}\tilde{X}_0 + \sigma\int_0^s e^{-\theta(s-u)}dW_u\right)\right] \\ &= \mathrm{E}\left[e^{-\theta(t+s)}\tilde{X}_0^2 + \sigma e^{-\theta(t+s)}\tilde{X}_0\int_0^s e^{\theta u)}dW_u\right. \\ &\left. + \sigma e^{-\theta(t+s)}\tilde{X}_0\int_0^t e^{\theta u}dW_u + \sigma^2 e^{-\theta(t+s)}\int_0^t e^{\theta u}dW_u\int_0^s e^{\theta u}dW_u\right].\end{aligned}$$

We can calculate the first term easily by inserting the distribution of $\tilde{X}_0$. For both the second and third term we know that the Paley-Wiener integrals are independent of $\tilde{X}_0$. Hence,

$$\mathrm{E}\left[\tilde{X}_0\int_0^r e^{\theta u}dW_u\right] = \mathrm{E}[\tilde{X}_0]\mathrm{E}\left[\int_0^r e^{\theta u}dW_u\right] = 0. \tag{23}$$

We rewrite the last term to

$$\begin{aligned}\int_0^t e^{\theta u}dW_u\int_0^s e^{\theta u}dW_u &= \int_{\min(s,t)}^{\max(s,t)} e^{\theta u}dW_u\int_0^{\min(s,t)} e^{\theta u}dW_u \\ &+ \int_0^{\min(s,t)} e^{\theta u}dW_u\int_0^{\min(s,t)} e^{\theta u}dW_u.\end{aligned}$$

The first part of this expression is the product of two independent random variables which both have an expectation of zero. Just as in (23) the expectation of their product will be equal to zero. For the expectation of the second part of the fourth term we find

$$\begin{aligned}&\mathrm{E}\left[\int_0^{\min(s,t)} e^{\theta u}dW_u\int_0^{\min(s,t)} e^{\theta u}dW_u\right] = \mathrm{Var}\left[\int_0^{\min(s,t)} e^{\theta u}dW_u\right] \\ &= \int_0^{\min(s,t)} e^{2\theta u}du = \frac{1}{2\theta}\left(e^{\min(s,t)} - 1\right).\end{aligned}$$

Combining these results yields

$$\mathrm{Cov}(\tilde{X}_t, \tilde{X}_s) = e^{-\theta(t+s)}\sigma_*^2 + e^{-\theta(t+s)}\sigma_*^2\left(e^{\min(s,t)} - 1\right) = \sigma_*^2 e^{-\theta|t-s|}. \tag{24}$$

Because $\mathrm{Cov}(\tilde{X}_t, \tilde{X}_s)$ is a function of $|t-s|$, we can conclude that the covariance matrix of the multivariate normal distributions $\{\tilde{X}_t, \tilde{X}_s\}$ and $\{\tilde{X}_{T-t}, \tilde{X}_{t-s}\}$ are equal for all $0 \leq t, s \leq T$ and $T > 0$. Therefore, $\{\tilde{X}_t, \tilde{X}_s\}$ and $\{\tilde{X}_{T-t}, \tilde{X}_{t-s}\}$ have the same distribution for all $0 \leq t, s \leq T$ and $T > 0$. From proposition 1.3 it follows that $\{\tilde{X}_t, t \geq 0\}$ is a reversible process.

3.1.3 Time Evolution of Normal Distributions

Normal distributions which diffuse according to the Ornstein-Uhlenbeck process will remain normally distributed (but with changing mean and variance). Let us start with initial distribution $X_0 = \mathcal{N}(\mu, \sigma_0^2)$, then for its time evolution X_t we get

$$\begin{aligned} X_t &= e^{-\theta t}\mathcal{N}(\mu, \sigma_0^2) + \sigma \int_0^t e^{-\theta(t-s)} dW_s \\ &\stackrel{d}{=} \mathcal{N}(\mu e^{-\theta t}, \sigma_0^2 e^{-2\theta t}) + \mathcal{N}(0, \sigma_*^2(1 - e^{-2\theta t})) \\ &\stackrel{d}{=} \mathcal{N}(\mu e^{-\theta t}, \sigma_0^2 e^{-2\theta t} + \sigma_*^2(1 - e^{-2\theta t})). \end{aligned} \tag{25}$$

3.1.4 Generator

The generator of the Ornstein-Uhlenbeck process will be of particular interest. Before we can calculate it on smooth test functions, we must look at its semigroup first:

$$S_t f(x) = \mathrm{E}_x[f(X_t)] = \mathrm{E}[f(xe^{-\theta t} + \mathcal{N}(0, \sigma_*^2(1 - e^{-2\theta t}))].$$

Taylor expanding f around $xe^{-\theta t}$ yields

$$\begin{aligned} S_t f(x) &= \mathrm{E}[f(xe^{-\theta t} + \mathcal{N}(0, \sigma_*^2(1 - e^{-2\theta t})) \\ &= \mathrm{E}\left[f(xe^{-\theta t})\right] + \mathrm{E}\left[f^{'}(xe^{-\theta t})\mathcal{N}(0, \sigma_*^2(1 - e^{-2\theta t}))\right] \\ &+ \mathrm{E}\left[\frac{f^{"}(xe^{-\theta t})}{2}\mathcal{N}(0, \sigma_*^2(1 - e^{-2\theta t}))^2 + \ldots\right] \\ &= f(xe^{-\theta t}) + \frac{f^{"}(xe^{-\theta t})}{2}\sigma_*^2(1 - e^{-2\theta t}) + \ldots \\ &= f(xe^{-\theta t}) - \frac{f^{"}(xe^{-\theta t})}{2}\sigma_*^2 \sum_{n=1}^{\infty} \frac{(-2\theta t)^n}{n!} + \ldots \\ &= f(xe^{-\theta t}) + \frac{f^{"}(xe^{-\theta t})}{2}\sigma^2 t + \ldots \end{aligned} \tag{26}$$

We insert this expression in the definition (9)

$$\begin{aligned} Lf(x) &= \lim_{t \to 0} \frac{S_t f(x) - f(x)}{t} \\ &= \lim_{t \to 0} \frac{f(xe^{-\theta t}) - f(x)}{t} + \frac{f^{"}(xe^{-\theta t})}{2}\sigma^2 \\ &= \lim_{t \to 0} \frac{f(x - x\frac{e^{\theta t} - 1}{e^{\theta t}}) - f(x)}{t} + \frac{f^{"}(xe^{-\theta t})}{2}\sigma^2. \end{aligned}$$

Lastly, we Taylor expand $f(x - x\frac{e^{\theta t}-1}{e^{\theta t}})$ around x to arrive at the final result:

$$\begin{aligned}
Lf(x) &= \lim_{t\to 0} \frac{f(x) - f'(x)x\frac{e^{\theta t}-1}{e^{\theta t}} + \ldots - f(x)}{t} + \frac{f^{"}(xe^{-\theta t})}{2}\sigma^2 \\
&= -xf'(x)\lim_{t\to 0}\frac{e^{\theta t}-1}{te^{\theta t}} + \frac{f^{"}(x)}{2}\sigma^2 \\
&= -xf'(x)\lim_{t\to 0}\frac{e^{\theta t}-1}{te^{\theta t}} + \frac{f^{"}(x)}{2}\sigma^2 \\
&= -xf'(x)\lim_{t\to 0}\frac{\theta e^{\theta t}}{e^{\theta t}+\theta t e^{\theta t}} + \frac{f^{"}(x)}{2}\sigma^2 \\
&= -\theta x f'(x) + \frac{\sigma^2}{2}f^{"}(x). \qquad (27)
\end{aligned}$$

Now that the generator is known, the stationary distribution can be derived from it too. We start by noting that the generator can be written in the following form:

$$Lf = Ce^{V(x)}\frac{d}{dx}\left(e^{-V(x)}\frac{df}{dx}\right), \qquad (28)$$

with $V(x) = \frac{\theta}{\sigma^2}x^2$ and $C = \frac{\sigma^2}{2}$. The claim is that when a generator can be written in this form, such that $V(x) \to \infty$ as $x \to \pm\infty$ and $\int_{\mathbb{R}} e^{-V}dx < \infty$, the stationary distribution is given by $\frac{e^{-V}}{Z}$, where Z is a normalization constant. We have for $f \in C_b^\infty$:

$$\begin{aligned}
\int_{\mathbb{R}} Lf d\mu &= \int_{-\infty}^{\infty}\frac{e^{-V}}{Z}Lf dx \\
&= \frac{C}{Z}\int_{-\infty}^{\infty}\frac{d}{dx}\left(e^{-V}\frac{df}{dx}\right)dx \\
&= \frac{C}{Z}\left[e^{-V}\frac{df}{dx}\right]_{-\infty}^{\infty} \\
&= 0.
\end{aligned}$$

Now the claim follows from theorem 1.2 and the fact that C_b^∞ is dense in C_b. The invariant measure is indeed equal to what we found earlier:

$$d\tilde{\mu} = \frac{e^{-V(x)}}{Z}dx = \sqrt{\frac{\theta}{\pi\sigma^2}}e^{\frac{\theta}{\sigma^2}x^2}dx = f_{\mathcal{N}(0,\sigma_*^2)}(x)dx.$$

We can also use the expression in (28) to prove that this is the reversible measure. We have for all $f, g \in C_b^\infty$:

$$\int_{\mathbb{R}} gL(f)d\tilde{\mu} = \frac{C}{Z}\int_{-\infty}^{\infty} g\frac{d}{dx}\left(e^{-V(x)}\frac{df}{dx}\right)dx.$$

Integration by parts yields:

$$\int_{\mathbb{R}} g\frac{d}{dx}\left(e^{-V(x)}\frac{df}{dx}\right)dx = \left[ge^{-V(x)}\frac{df}{dx}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{dg}{dx}e^{-V(x)}\frac{df}{dx}dx$$

The first term is zero, since $V(x) \to \infty$ as $x \to \pm\infty$. The remaining expression is symmetric in the roles of f and g. From interchanging them, we find:

$$\int_{\mathbb{R}} gL(f)d\tilde{\mu} = \int_{\mathbb{R}} fL(g)d\tilde{\mu}.$$

From the third statement of proposition 1.3 we can conclude that this measure is indeed the reversible measure.

3.2 Multivariate Case

3.2.1 Definition and Explicit Solution

The multivariate Ornstein-Uhlenbeck process is defined by the stochastic differential equation:

$$dX_t = BX_t + \Sigma dW_t, \tag{29}$$

where B and Σ are $n \times n$ matrices and W_t is the n-dimensional Wiener process. We consider the case where B is a symmetric, invertible matrix and $\Sigma = I$. Again, we want to calculate the explicit solution and start by introducing a change of variable:

$$Y_t = e^{Bt}X_t.$$

We have:

$$\begin{aligned} dY_t &= Be^{Bt}X_t dt + e^{Bt}dX_t \\ &= Be^{Bt}X_t dt + e^{Bt}\left(-BX_t dt + dW_t\right) \\ &= e^{Bt}dW_t. \end{aligned}$$

Integrating from 0 to t yields

$$Y_t = Y_0 + \int_0^t e^{Bs}dW_s,$$

where this is a multivariate Paley-Wiener integral as introduced in section 2.3. We reverse the change of variable to obtain the explicit solution to (29):

$$X_t = e^{-Bt}Y_t = e^{-Bt}X_0 + \int_0^t e^{-B(t-s)}dW_s. \tag{30}$$

3.2.2 Invariant and Reversible Measure

We want to calculate the invariant and reversible distribution. So we insert the Ornstein-Uhlenbeck process starting from $X_0 = 0$ in the explicit solution (30)

$$X_t = \int_0^t e^{-B(t-s)}dW_s.$$

By using the result for the multivariate Paley-Wiener integral, (7) we find

$$\int_0^t e^{-B(t-s)} dW_s \stackrel{d}{=} \mathcal{N}\left(\mathbf{0}, \int_0^t e^{-B(t-s)} e^{-B^T(t-s)} ds\right).$$

Since B is symmetric and invertible, we have

$$\begin{aligned}\mathcal{N}\left(\mathbf{0}, \int_0^t e^{-B(t-s)} e^{-B^T(t-s)} ds\right) &= \mathcal{N}\left(\mathbf{0}, \int_0^t e^{-2B(t-s)} ds\right) \\ &= \mathcal{N}\left(\mathbf{0}, \frac{1}{2} B^{-1}\left(1 - e^{-2Bt}\right)\right).\end{aligned}$$

Hence,

$$X_t \stackrel{d}{=} \mathcal{N}\left(\mathbf{0}, \frac{1}{2} B^{-1}\left(1 - e^{-2Bt}\right)\right). \tag{31}$$

By taking the limit $t \to \infty$ we find the invariant measure

$$\tilde{\mu} = \mathcal{N}\left(\mathbf{0}, \frac{1}{2} B^{-1}\right). \tag{32}$$

3.2.3 Time Evolution of Normal Distributions

Multivariate normal distributions also remain normally distributed while diffusing according to the multivariate Ornstein-Uhlenbeck process (with changing mean and variance). Let us start with initial distribution $X_0 = \mathcal{N}(\boldsymbol{\mu}, \Sigma_0)$, then for its time evolution X_t we get

$$\begin{aligned}X_t &= e^{-Bt}\mathcal{N}(\boldsymbol{\mu}, \Sigma_0) + \int_0^t e^{-B(t-s)} dW_s \\ &\stackrel{d}{=} \mathcal{N}\left(e^{-Bt}\boldsymbol{\mu}, e^{-Bt}\Sigma_0 e^{-B^T t}\right) + \mathcal{N}\left(\mathbf{0}, \int_0^t e^{-2B(t-s)} ds\right) \\ &\stackrel{d}{=} \mathcal{N}\left(e^{-Bt}\boldsymbol{\mu}, e^{-Bt}\Sigma_0 e^{-B^T t}\right) + \mathcal{N}\left(\mathbf{0}, \frac{1}{2} B^{-1}(1 - e^{-2Bt})\right) \\ &\stackrel{d}{=} \mathcal{N}\left(e^{-Bt}\boldsymbol{\mu}, e^{-Bt}\Sigma_0 e^{-Bt} + \frac{1}{2} B^{-1}(1 - e^{-2Bt})\right),\end{aligned} \tag{33}$$

where we have used that B is symmetric and invertible.

3.2.4 Generator

For the semigroup on smooth test functions we have

$$S_t f(\boldsymbol{x}) = \mathrm{E}_{\boldsymbol{x}}[f(X_t)] = \mathrm{E}[f(e^{-Bt}\boldsymbol{x} + \mathcal{N}(\mathbf{0}, \frac{1}{2} B^{-1}(1 - e^{-2Bt}))].$$

We Taylor expand f around $e^{-Bt}\boldsymbol{x}$ to obtain the multivariate equivalent of (26) [7] :

$$S_t f(\boldsymbol{x}) = f(e^{-Bt}\boldsymbol{x}) + \frac{1}{2}\nabla^2 f(e^{-Bt}\boldsymbol{x})t + \ldots \tag{34}$$

We insert this expression in the definition (9)

$$\begin{aligned} Lf(\boldsymbol{x}) &= \lim_{t\to 0} \frac{S_t f(\boldsymbol{x}) - f(\boldsymbol{x})}{t} \\ &= \lim_{t\to 0} \frac{f(e^{-Bt}\boldsymbol{x}) - f(\boldsymbol{x})}{t} + \frac{1}{2}\nabla^2 f(e^{-Bt}\boldsymbol{x}) \\ &= \lim_{t\to 0} \frac{f(\boldsymbol{x} - e^{-Bt}(e^{Bt}-1)\boldsymbol{x})) - f(\boldsymbol{x})}{t} + \frac{1}{2}\nabla^2 f(e^{-Bt}\boldsymbol{x}). \end{aligned}$$

Lastly, we Taylor expand $f(\boldsymbol{x} - e^{-Bt}(e^{Bt}-1)\boldsymbol{x})$ around $\boldsymbol{x}$ to arrive at the final result:

$$\begin{aligned} Lf(\boldsymbol{x}) &= \lim_{t\to 0} \frac{f(\boldsymbol{x}) - (e^{-Bt}(e^{Bt}-1)\boldsymbol{x})^T\nabla f(\boldsymbol{x}) + \ldots - f(\boldsymbol{x})}{t} + \frac{1}{2}\nabla^2 f(e^{-Bt}\boldsymbol{x}) \\ &= -\boldsymbol{x}^T \lim_{t\to 0}(\frac{1}{t}e^{-Bt}(e^{Bt}-1))^T\nabla f(\boldsymbol{x}) + \frac{1}{2}\nabla^2 f(\boldsymbol{x}) \\ &= -\boldsymbol{x}^T B^T\nabla f(\boldsymbol{x}) + \frac{1}{2}\nabla^2 f(\boldsymbol{x}) \\ &= -\boldsymbol{x}^T B\nabla f(\boldsymbol{x}) + \frac{1}{2}\nabla^2 f(\boldsymbol{x}). \end{aligned} \tag{35}$$

4 Harmonic Oscillator

Now that we have discussed the Ornstein-Uhlenbeck process, we will shift our view to some quantum mechanics. In this section we will turn our attention to the quantum harmonic oscillator. But before we start with the quantum mechanics, we first consider the classical version.

4.1 Classical Harmonic Oscillator

Consider a classical particle attached to a spring. If we pull the mass from its equilibrium position, it experiences a restoring force which is proportional to the magnitude, but opposite to the displacement. In this case the potential energy of the string is a quadratic function of the displacement. (Quantum) physical systems with a potential, quadratically dependent on position, are called the (quantum) harmonic oscillator. It is a fundamental system in mechanics and can model every system near an equilibrium configuration.

4.1.1 One-Dimensional Case

We start by considering the problem in one dimension for a particle of mass m. Applying Newton's second law for a potential $V(x)$ yields:

$$-\frac{dV}{dx} = F = m\ddot{x}.$$

By inserting a harmonic potential $V(x) = \frac{1}{2}m\omega^2 x^2$ we find:

$$\ddot{x} = -\frac{1}{m}\frac{dV}{dx} = -\omega^2 x.$$

The general solution to this differential equation is given by

$$x(t) = C\cos(\omega t + \phi), \tag{36}$$

where C and ϕ are constants depending on initial conditions. We have found that the position is an oscillating motion with angular frequency ω. The relative contributions of the kinetic and potential energy oscillate as well, with their sum being the constant total energy:

$$E = V(x) + \frac{p^2}{2m} = \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}m\dot{x}^2.$$

4.1.2 Multidimensional Case

First, we consider the n-dimensional harmonic oscillator with harmonic potentials along orthogonal axes. In this case the potential is of the form $V(\boldsymbol{x}) = \frac{1}{2}m\langle \boldsymbol{x}, D^2\boldsymbol{x}\rangle$, with

$$D^2 = \begin{bmatrix} \omega_1^2 & & & \\ & \omega_2^2 & & \\ & & \ddots & \\ & & & \omega_n^2 \end{bmatrix}.$$

This is simply the one-dimensional case in each direction. Hence,

$$\boldsymbol{x}(t) = \begin{bmatrix} C_1\cos(\omega_1 t + \phi_1) \\ C_2\cos(\omega_2 t + \phi_2) \\ \vdots \\ C_n\cos(\omega_n t + \phi_n) \end{bmatrix}. \tag{37}$$

Now we will look at the general case where the potential is of the form $V(\boldsymbol{x}) = \frac{1}{2}m\langle \boldsymbol{x}, A\boldsymbol{x}\rangle$ with A a positive definite real matrix, i.e. for each non-zero $\boldsymbol{x}$ the inner product $\langle \boldsymbol{x}, A\boldsymbol{x}\rangle$ is strictly positive. All eigenvalues of positive definite matrices are positive. We can rewrite $V(\boldsymbol{x})$ to a form where A is replaced by the symmetric matrix $\frac{1}{2}(A + A^T)$

$$\langle \boldsymbol{x}, A\boldsymbol{x}\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i A_{ij} x_j = \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{1}{2}x_i(A_{ij} + A_{ji})x_j = \langle \boldsymbol{x}, \frac{1}{2}(A + A^T)\boldsymbol{x}\rangle.$$

Therefore, we can consider $V(\boldsymbol{x}) = \frac{1}{2}m\langle \boldsymbol{x}, A\boldsymbol{x}\rangle$ with a symmetric, positive definite matrix A without loss of generality. Newton's second law yields the following equation of motion:

$$\ddot{\boldsymbol{x}} = -\frac{1}{m}\nabla V = -\frac{1}{2}\nabla\langle \boldsymbol{x}, A\boldsymbol{x}\rangle = -A\boldsymbol{x}. \tag{38}$$

Since A is real, symmetric and positive definite, it can be diagonalized by some orthogonal matrix Q such that[8]:

$$A = Q^{-1}D^2Q = Q^T D^2 Q. \tag{39}$$

Matrix A and D^2 have the same positive eigenvalues, say $\{\omega_1^2, \omega_2^2, \ldots, \omega_n^2\}$. The rows in Q correspond to the eigenvectors of these eigenfunctions. By substituting this relation in (38), we find:

$$\ddot{\boldsymbol{x}} = -A\boldsymbol{x} = -Q^T D^2 Q\boldsymbol{x}. \tag{40}$$

Hence,

$$\ddot{\tilde{\boldsymbol{x}}} = Q\ddot{\boldsymbol{x}} = -D^2 Q\boldsymbol{x} = -D^2\tilde{\boldsymbol{x}} \tag{41}$$

We can see that $\tilde{\boldsymbol{x}}$ has the same equation of motion as in the case with harmonic potentials along orthogonal axes. Therefore, we can use the solution of the orthogonal case (37) in order to conclude:

$$\boldsymbol{x}(t) = Q^T \tilde{\boldsymbol{x}}(t) = Q^T \begin{bmatrix} C_1 \cos(\omega_1 t + \phi_1) \\ C_2 \cos(\omega_2 t + \phi_2) \\ \vdots \\ C_3 \cos(\omega_n t + \phi_n) \end{bmatrix}. \tag{42}$$

4.2 Basics of Quantum Mechanics

4.2.1 Schrödinger Equation

In classical mechanics a particle's state is determined by knowing the position $x(t)$ at any given time t. All physical observables like velocity, momentum and kinetic energy can be derived from it. In quantum mechanics, however, a particle's state is described by its wave function $\Psi(x,t)$, whose interpretation will be discussed in the next subsection.

All quantum mechanical systems satisfy a single differential equation, the Schrödinger equation. We can use it to calculate the time evolution of quantum states, but solving the equation is not easy for most quantum states. In one dimension, the Schrödinger equation is given by [9]:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = H\Psi(x,t), \tag{43}$$

where $\hbar$ is the reduced Planck constant and the Hamiltonian operator H is given by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t). \tag{44}$$

Here m is the particle's mass. In quantum mechanics the bra-ket notation is standard notation for quantum states, the ket $|a\rangle$ stands for a column vector or eigenfunction, the bra $\langle a|$ is its hermitian conjugate and their inner product is denoted as $\langle a|a\rangle$. We use this notation to write down the more dimensional variant of the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle, \tag{45}$$

with

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x},t). \tag{46}$$

4.2.2 Interpretation of the Wave Function

In the preceding subsection, we introduced the concept of the wave function and how it's evolution over time can be calculated. But what does it actually mean and how can we interpret such a wave function. First of all, if a particle's

wave function is known, it can (mostly) not lead to an unambiguous prediction for the outcome of a measurement. For instance, the absolute value of the wave function squared is the probability distribution for measuring the particle at a certain point in space. Hence,

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1. \tag{47}$$

In quantum mechanics the value of a physical observable is (generally) not deterministic. Fundamentally, physical observables have a superposition of values. The observables are represented by linear operators and we can calculate the expectation value of such a measurement from it. For instance, the expectation of x is given by

$$\langle x \rangle = \langle \Psi(t) | x | \Psi(t) \rangle = \int_{-\infty}^{\infty} x |\Psi(x,t)|^2 dx.$$

After measuring an observable, the wave function changes its shape since it became an eigenfunction of that observable; the outcome of the measurement is equal to the corresponding eigenvalue. For instance, after measuring a particle at position $x = C$, $|\Psi(x,t)|^2$ becomes a delta function at $x = C$ and soon spreads according to the Schrödinger equation.

We calculate the momentum operator p. Consider a wave function Ψ, from the classical definition of momentum we have

$$\langle p \rangle = m \frac{d \langle x \rangle}{dt} = \int x \frac{\partial}{\partial t} (\Psi^* \Psi) dx.$$

We insert the Schrödinger equation:

$$\int x \frac{\partial}{\partial t} (\Psi^* \Psi) dx = -i\hbar \int x \frac{\partial^2}{\partial x^2} (\Psi^* \Psi) dx = -i\hbar \int x \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) dx.$$

This can be simplified using integration-by-parts and the fact that the wave function vanishes for $x \to \pm\infty$. This results in the following expression for $\langle p \rangle$:

$$\langle p \rangle = -i\hbar \int \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) dx.$$

We perform another integration-by-parts to arrive at the final result:

$$\langle p \rangle = -i\hbar \int \left(\Psi^* \frac{\partial \Psi}{\partial x} \Psi \right) dx = \langle \Psi | \frac{\hbar}{i} \frac{\partial}{\partial x} | \Psi \rangle \,. \tag{48}$$

Note that the momentum operator is hermitian. It turns out that all operators of physical observables are hermitian. This is because every eigenvalue of an operator can be an outcome of a measurement and measurements only give real values.

4.2.3 Heisenberg Uncertainty Principle

Some operators of observables do not commute. This results in a minimal insecurity up to which both observables can be known simultaneously. This principle is stated in the following theorem.

Theorem 2.1 *Consider a system with wave function* $|\Psi\rangle$ *and two physical observables* A *and* B*, then*

$$\sigma_A \sigma_B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right|, \tag{49}$$

where

$$\sigma_A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2} \tag{50}$$

$$\sigma_B = \sqrt{\langle B^2 \rangle - \langle B \rangle^2}. \tag{51}$$

This is called the uncertainty principle

Proof. If $\sigma_B \neq 0$, define the following operator for $\lambda \in \mathcal{R}$:

$$C := A - \langle A \rangle + i\lambda (B - \langle B \rangle).$$

We have

$$0 \leq \langle C\Psi | C\Psi \rangle = \langle \Psi | C^\dagger C | \Psi \rangle = \sigma_A^2 + \lambda^2 \sigma_B^2 + i\lambda \left\langle [A, B] \right\rangle.$$

This expression is real and has a minimum for the real-valued constant λ equal to

$$\lambda = -\frac{i \left\langle [A, B] \right\rangle}{2\sigma_B^2}.$$

This minimum is given by

$$\sigma_A^2 - \frac{i \left\langle [A, B] \right\rangle^2}{4\sigma_B^2} \geq 0,$$

which gives us the final result after rearranging:

$$\sigma_A \sigma_B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right|.$$

If $\sigma_B = 0$, then we can simply interchange the roles of A and B in this derivation. If both σ_A and σ_B are equal to zero, then we must have $[A, B] = 0$, which is also in accordance with the uncertainty principle. □

For the position x and momentum p we have:

$$\begin{aligned}
[x, p] |\Psi\rangle &= (xp - px) |\Psi\rangle \\
&= x \frac{\hbar}{i} \frac{\partial |\Psi\rangle}{\partial x} - \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) x |\Psi\rangle \\
&= x \frac{\hbar}{i} \frac{\partial |\Psi\rangle}{\partial x} + i\hbar |\Psi\rangle - x \frac{\hbar}{i} \frac{\partial |\Psi\rangle}{\partial x}. \\
&= i\hbar |\Psi\rangle .
\end{aligned} \tag{52}$$

Hence, $[x, p] = i\hbar$, which is known as the canonical commutation relation. Inserting this in the uncertainty principle (49) yields the following:

$$\sigma_x \sigma_p \geq \frac{1}{2} |\langle i\hbar \rangle| = \frac{\hbar}{2}. \tag{53}$$

This is known as Heisenberg's uncertainty principle. It states that the momentum and position of a quantum particle cannot be known simultaneously, but up to a certain insecurity.

4.3 Quantum Harmonic Oscillator

We consider the one-dimensional quantum harmonic oscillator with potential $V(x) = \frac{1}{2}m\omega^2 x^2$. The Schrödinger equation reads:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + \frac{1}{2} m\omega^2 x^2 \Psi(x,t). \tag{54}$$

We can see that the harmonic potential is time independent and therefore we can use separation of variables to solve the Schrödinger equation. We look for solutions of the form

$$\Psi(x,t) = \psi(x)\phi(t). \tag{55}$$

The time dependent part is solved by

$$\phi(t) = e^{-iEt/\hbar}$$

with E a separation constant. Now for $\phi(x)$ we have to solve the time independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi.$$

Therefore the solutions we are looking for are energy eigenstates of the harmonic oscillator. Rewriting this equation in terms of the momentum operator yields

$$H\psi = \frac{1}{2m}(p^2 + (m\omega x)^2)\psi = E\psi. \tag{56}$$

Definition 2.1 *The following operators are called* ***ladder operators***

$$a = \frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x) \tag{57}$$

$$a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x) \tag{58}$$

Here a is called the ***annihilation operator*** *and $a^\dagger$ is called the* ***creation operator****.*

Calculating the commutation relation of these ladder operators yields

$$\begin{aligned}[a, a^\dagger] &= \frac{1}{2\hbar m\omega}[m\omega x + ip, m\omega x - ip] \\ &= \frac{1}{2\hbar}\left([x, -ip] + [ip, x]\right) \\ &= -\frac{i}{2\hbar}([x, p] + [x, p]) \\ &= 1. \end{aligned} \tag{59}$$

We want to express the Hamiltonian operator in terms of the ladder operators. We use

$$aa^\dagger = \frac{1}{2\hbar m\omega}(p^2 + (m\omega x)^2) - \frac{i}{2\hbar}[x, p] = \frac{1}{\hbar\omega}H + \frac{1}{2},$$

which gives

$$H = \hbar\omega(aa^\dagger - \frac{1}{2}). \tag{60}$$

Hence,

$$[H, a] = \hbar\omega a[a^\dagger, a] = -\hbar\omega a \tag{61}$$

$$[H, a^\dagger] = \hbar\omega a^\dagger[a, a^\dagger] = \hbar\omega a^\dagger. \tag{62}$$

If we apply the lowering operator on a state $|\Psi\rangle$ that satisfies the time independent Schrödinger equation, we find:

$$Ha\,|\psi\rangle = (aH - \hbar\omega a)\,|\psi\rangle = (E - \hbar\omega)a\,|\psi\rangle\,. \tag{63}$$

Therefore, applying the lowering operator will lower the energy by $\hbar\omega$. As the name suggests, applying the raising operator will increase the energy by $\hbar\omega$:

$$Ha^\dagger\,|\psi\rangle = (aH + \hbar\omega a^\dagger)\,|\psi\rangle = (E + \hbar\omega)a^\dagger\,|\psi\rangle\,. \tag{64}$$

We denote the state with lowest energy by $|0\rangle$. The ground state must satisfy $a\,|0\rangle = 0$, because otherwise a state exists with lower energy due to (63). From this relation we can determine the ground state ψ_0

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \tag{65}$$

which has energy

$$E_0 = \frac{1}{2}\hbar\omega.$$

From the relations (63) and (64) it follows that the energy is quantised at energies:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega.$$

The corresponding eigenstates are found after applying the raising operator and normalizing:

$$|n\rangle = \frac{1}{\sqrt{n}}(a^\dagger)^n\,|0\rangle\,, \tag{66}$$

with

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{67}$$

$$a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{68}$$

It can be shown that these eigenfunctions form a complete orthonormal set of functions. See Figure 4 for an illustration of the first five energy eigenstates. They are plotted (at one instance in time) together with the harmonic potential at the height of their energies.

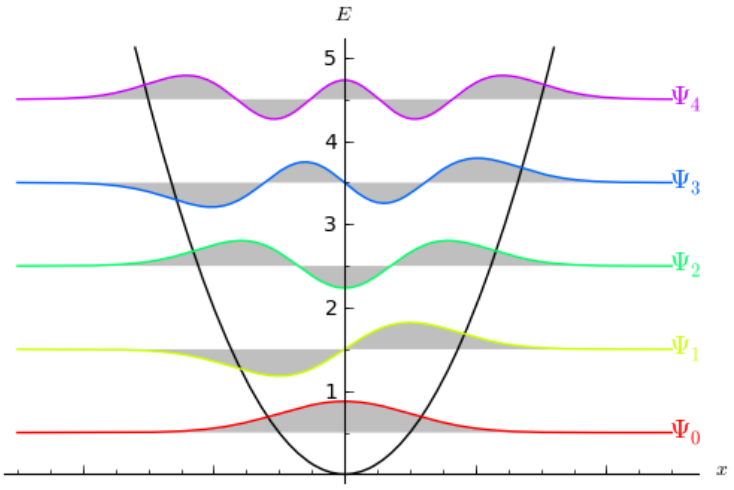

Figure 4. Plot of the first five energy eigenstates with the harmonic potential. The eigenstates are plotted at the height of their energies.

5 Coherent States

Coherent states are the states in the quantum harmonic oscillator that minimise Heisenberg's uncertainty principle and best resemble the behaviour of classical particles in the harmonic oscillator. In the field of quantum physics, coherent states are widely used. In this chapter coherent states in one dimension are considered.

5.1 Definitions and Properties

Definition 3.1 *A **coherent state** $|\alpha\rangle$ is defined as the eigenstate of the annihilation operator a with eigenvalues $\alpha \in \mathbb{C}$*

$$a\,|\alpha\rangle = \alpha\,|\alpha\rangle\,. \tag{69}$$

For the ground state we have $a\,|0\rangle = 0$. Therefore, $|0\rangle$ is a coherent state with eigenvalue 0. The relation in (66) shows that all energy eigenstates can be generated by applying the creation operator $a^\dagger$ on $|0\rangle$. The so-called displacement operator generates coherent states from $|0\rangle$ in a similar manner.

Definition 3.2 *The **displacement operator** $D(\alpha)$ is defined by*

$$D(\alpha) = e^{\alpha a^\dagger - \alpha^* a} \tag{70}$$

where $\alpha = |\alpha|e^{i\phi} \in \mathbb{C}$ is a complex number.

Lemma 3.1 The displacement operator satisfies the following:

1. $$D^\dagger(\alpha) = D^{-1}(\alpha) = D(-\alpha) \tag{71}$$

2. $$D^\dagger(\alpha) a D(\alpha) = a + \alpha \tag{72}$$

Proof. 1. This follows immediately from the definition of $D(\alpha)$ and the fact that $(a^\dagger)^\dagger = a$.

2. From item 1 it follows that

$$D^\dagger(\alpha) a D(\alpha) = e^{\alpha^* a - \alpha a^\dagger} a e^{\alpha a^\dagger - \alpha^* a} \tag{73}$$

We use the result from [10] to simplify this expression:

$$e^{\alpha^* a - \alpha a^\dagger} a e^{\alpha a^\dagger - \alpha^* a} = a + [\alpha^* a - \alpha a^\dagger, a].$$

This gives us the final result:

$$\begin{aligned} D^\dagger(\alpha) a D(\alpha) = e^{\alpha^* a - \alpha a^\dagger} a e^{\alpha a^\dagger - \alpha^* a} &= a + [\alpha^* a - \alpha a^\dagger, a] \\ &= a + \alpha^*[a, a] - \alpha[a^\dagger, a] = a + \alpha. \end{aligned}$$

□

This knowledge allows us to generate coherent states from $|0\rangle$.

Theorem 3.1 The coherent state $|\alpha\rangle$ is generated from the vacuum $|0\rangle$ by applying the displacement operator $D(\alpha)$

$$|\alpha\rangle = D(\alpha)\,|0\rangle\,. \tag{74}$$

Proof. By applying both equalities of lemma 4.1, we find

$$aD(-\alpha)\,|\alpha\rangle = D(-\alpha)D^{\dagger}(-\alpha)aD(\alpha)\,|\alpha\rangle = D(-\alpha)(a-\alpha)\,|\alpha\rangle$$

From the definition of coherent states, we have

$$(a-\alpha)\,|\alpha\rangle = 0.$$

Hence, we must have

$$D(-\alpha) = |0\rangle \implies D(\alpha)\,|0\rangle = |\alpha\rangle\,.$$

□

5.2 Decomposition of Coherent States

We want to decompose the coherent state $|\alpha\rangle$ in terms of the energy eigenstates $|n\rangle$

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle\,. \tag{75}$$

Inserting (67) yields

$$a\,|\alpha\rangle = \sum_{n=0}^{\infty} c_n\sqrt{n}\,|n-1\rangle\,.$$

By substituting these results in (69) we find

$$\sum_{n=0}^{\infty} c_n\sqrt{n}\,|n-1\rangle = \sum_{n=0}^{\infty} c_n\alpha\,|n\rangle\,, \tag{76}$$

which brings us the following relations

$$c_{n+1}\sqrt{n+1} = c_n\alpha$$

Hence,

$$c_n = \frac{\alpha}{\sqrt{n}}c_{n-1} = \frac{\alpha^2}{\sqrt{n(n-1)}}c_{n-2} = \frac{\alpha^n}{\sqrt{n!}}c_0.$$

We can find c_0 by using the normalization condition

$$\sum_{n=0}^{\infty}\left|\frac{\alpha^n}{\sqrt{n!}}c_0\right|^2 = 1 \implies |c_0|^2\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{n!} = 1.$$

By noting that

$$e^{|\alpha|^2} = \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!}$$

we find

$$c_0 = e^{\frac{-|\alpha|^2}{2}}$$

and the decomposition of the coherent state $|\alpha\rangle$ becomes

$$|\alpha\rangle = e^{\frac{-|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle . \tag{77}$$

5.3 Explicit Calculation of the Wave Function of a Coherent State

We want to derive the explicit form of the wave function of these coherent states. In order to do so, we start with the result we found for the time evolution of the energy eigenstates in section 4.3:

$$\Psi_n(x,t) = \psi_n(x) e^{(n+\frac{1}{2})i\omega t}.$$

We insert this in (77) to obtain the time evolutions of the coherent states.

$$\Psi_\alpha(x,t) = e^{\frac{-|\alpha|^2}{2}} e^{-\frac{1}{2}i\omega t} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} \psi_n(x) = \psi_{\alpha(t)}(x) e^{-\frac{1}{2}i\omega t}, \tag{78}$$

where $\alpha(t) = \alpha e^{-i\omega t} = |\alpha| e^{i\phi} e^{-i\omega t}$. Then, applying theorem 3.1 yields the following expression for the time evolution

$$\Psi_\alpha(x,t) = e^{-\frac{1}{2}i\omega t} D(\alpha(t)) \psi_0(x). \tag{79}$$

To simplify calculations, we write the annihilation and creation operator in terms of a new dimensionless variable $\xi = x\sqrt{\frac{m\omega}{\hbar}} = \frac{x}{x_0}$:

$$a = \frac{1}{\sqrt{2}}(\xi + \frac{d}{d\xi}) \tag{80}$$

$$a^\dagger = \frac{1}{\sqrt{2}}(\xi - \frac{d}{d\xi}). \tag{81}$$

We insert these expressions in the exponent of the displacement operator and find

$$\begin{aligned} \alpha a^\dagger - \alpha^* a &= \frac{\alpha(t)}{\sqrt{2}}(\xi - \frac{d}{d\xi}) - \frac{\alpha^*(t)}{\sqrt{2}}(\xi + \frac{d}{d\xi}) \\ &= \frac{\xi}{\sqrt{2}}(\alpha(t) - \alpha^*(t)) - \frac{1}{\sqrt{2}}\frac{d}{d\xi}(\alpha(t) + \alpha^*(t)) \\ &= \sqrt{2} i \,\mathrm{Im}(\alpha(t))\xi - \sqrt{2}\,\mathrm{Re}(\alpha(t))\frac{d}{d\xi}. \end{aligned} \tag{82}$$

Filling in this result in (79) yields:

$$\Psi_\alpha(x,t) = \left(\frac{1}{x_0^2\pi}\right)^{1/4} e^{-\frac{1}{2}i\omega t} e^{\sqrt{2}i\,\mathrm{Im}(\alpha(t))\xi - \sqrt{2}\,\mathrm{Re}(\alpha(t))\frac{d}{d\xi}} e^{\frac{-\xi^2}{2}}.$$

This expression is not explicit just yet, but it can be rewritten to the explicit solution. First we state the final result:

$$\Psi_\alpha(x,t) = \left(\frac{1}{x_0^2\pi}\right)^{1/4} e^{-\frac{1}{2}i\omega t} e^{\sqrt{2}\alpha(t)\xi - \frac{\xi^2}{2} - \mathrm{Re}(\alpha(t))\alpha(t)}, \tag{83}$$

which is derived below.

Proof. For this proof we follow the approach of [11]. We start by writing

$$\mathcal{D} = \sqrt{2}i\,\mathrm{Im}(\alpha(t))\xi - \sqrt{2}\,\mathrm{Re}(\alpha(t))\frac{d}{d\xi}.$$

In order to calculate

$$e^{\mathcal{D}} e^{-\frac{\xi^2}{2}} = (1 + \mathcal{D} + \frac{1}{2!}\mathcal{D}^2 + \dots) e^{-\frac{-\xi^2}{2}}, \tag{84}$$

we start by considering the linear and quadratic term in the operator expansion. For the linear term, we have

$$\begin{aligned}
\mathcal{D}e^{-\frac{\xi^2}{2}} &= \left(\sqrt{2}i\,\mathrm{Im}(\alpha(t))\xi - \sqrt{2}\,\mathrm{Re}(\alpha(t))\frac{d}{d\xi}\right) e^{-\frac{\xi^2}{2}} \\
&= \left(\sqrt{2}i\,\mathrm{Im}(\alpha(t))\xi + \sqrt{2}\,\mathrm{Re}(\alpha(t))\xi\right) e^{-\frac{\xi^2}{2}} \\
&= \sqrt{2}\alpha(t)\xi e^{-\frac{\xi^2}{2}},
\end{aligned}$$

and for the quadratic term

$$\begin{aligned}
\mathcal{D}^2 e^{-\frac{\xi^2}{2}} &= \sqrt{2}\alpha(t)\mathcal{D}\xi e^{-\frac{\xi^2}{2}} \\
&= \sqrt{2}\alpha(t)\left(\sqrt{2}i\,\mathrm{Im}(\alpha)\xi - \sqrt{2}\,\mathrm{Re}(\alpha(t))\frac{d}{d\xi}\right)\xi e^{-\frac{\xi^2}{2}} \\
&= (2\alpha(t)i\,\mathrm{Im}(\alpha(t))\xi^2 - 2\alpha(t)\,\mathrm{Re}(\alpha(t)) + 2\alpha(t)\,\mathrm{Re}(\alpha(t))\xi^2) e^{-\frac{\xi^2}{2}} \\
&= (2\alpha(t)^2\xi^2 - 2\alpha(t)\,\mathrm{Re}(\alpha(t))) e^{-\frac{\xi^2}{2}}.
\end{aligned}$$

Inserting both results into (84) yields

$$e^{\mathcal{D}} e^{-\frac{\xi^2}{2}} = (1 + \sqrt{2}\alpha(t)\xi - \mathrm{Re}(\alpha(t))\alpha(t) + \frac{2\alpha(t)^2\xi^2}{2!} + \dots) e^{-\frac{\xi^2}{2}}, \tag{85}$$

which shows the linear term and the first part of the quadratic term in the end result of the expansion. Hence, the result of (83) is obtained by rewriting this expansion to an exponential. □

From the result of (83) we can see that coherent states have almost Gaussian wave functions. For the probability density of coherent states over time, we find:

$$\begin{aligned}
|\Psi_\alpha(x,t)|^2 &= \Psi_\alpha(x,t)\Psi_\alpha^*(x,t) \\
&= \frac{1}{x_0\sqrt{\pi}} e^{\sqrt{2}(\alpha(t)+\alpha^*(t))\xi - \xi^2 - \mathrm{Re}(\alpha(t))(\alpha(t)+\alpha^*(t))} \\
&= \frac{1}{x_0\sqrt{\pi}} e^{2\sqrt{2}\,\mathrm{Re}(\alpha(t))\xi - \xi^2 - 2\,\mathrm{Re}(\alpha(t))^2} \\
&= \frac{1}{x_0\sqrt{\pi}} e^{-(\xi - \sqrt{2}\,\mathrm{Re}(\alpha(t)))^2} \\
&= \frac{1}{x_0\sqrt{\pi}} e^{-(\xi - \sqrt{2}|\alpha|\cos(\omega t - \phi))^2} \\
&= \frac{1}{x_0\sqrt{\pi}} e^{-\frac{(x - \sqrt{2}|\alpha| x_0 \cos(\omega t - \phi))^2}{x_0^2}}.
\end{aligned} \tag{86}$$

This is a Gaussian distribution with constant variance $\frac{1}{2}x_0^2$ and oscillating mean $\sqrt{2}|\alpha|x_0\cos(\omega t - \phi)$. Wave functions of this form are called Gaussian wave packets. The oscillating behaviour closely resembles the behaviour of classical particles in the harmonic oscillator as in (36).

5.4 Minimum Uncertainty Relation

It was already stated that coherent states minimise Heisenberg's uncertainty relation. We consider a coherent state $|\alpha\rangle$ and verify this explicitly. First, we calculate

$$\begin{aligned}
\langle x\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\,\langle\alpha|a + a^\dagger|\alpha\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\alpha + \alpha^*) \\
\langle p\rangle &= -i\sqrt{\frac{\hbar m\omega}{2}}\,\langle\alpha|a - a^\dagger|\alpha\rangle = -i\sqrt{\frac{\hbar m\omega}{2}}(\alpha - \alpha^*) \\
\langle x^2\rangle &= \frac{\hbar}{2m\omega}\,\langle\alpha|(a + a^\dagger)(a + a^\dagger)|\alpha\rangle = \frac{\hbar}{2m\omega}((\alpha + \alpha^*)^2 + 1) \\
\langle p^2\rangle &= -\frac{\hbar m\omega}{2}\,\langle\alpha|(a - a^\dagger)(a - a^\dagger)|\alpha\rangle = -\frac{\hbar m\omega}{2}((\alpha - \alpha^*)^2 - 1).
\end{aligned}$$

We use this to calculate the uncertainties of x and p:

$$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{\hbar}{2m\omega} \tag{87}$$

$$\sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2 = \frac{\hbar m\omega}{2}. \tag{88}$$

Hence,

$$\sigma_x\sigma_p = \frac{\hbar}{2}. \tag{89}$$

6 From the Ornstein-Uhlenbeck Process to the Quantum Harmonic Oscillator and Back

We will now focus on the relation between the Ornstein-Uhlenbeck process and the quantum harmonic oscillator. The main idea here is that the Hamiltonian can be transformed, by a ground-state transformation, to the Markov generator of a diffusion process. There are other examples of this kind for discrete quantum spin systems and associated discrete state space Markov chains, but we will limit ourselves to the correspondence between the quantum harmonic oscillator and the Ornstein-Uhlenbeck process. We will use our knowledge about the time evolution of normal distributions in the Ornstein-Uhlenbeck process as a tool to calculate the evolution of the corresponding quantum states in the harmonic oscillator.

6.1 Ground-State Transformation

The relation between the quantum harmonic oscillator and the Ornstein-Uhlenbeck process is best seen when we look at the Schrödinger equation from a different point of view. The problem of finding solutions can also be viewed as applying an operator to the initial wave function to obtain its time evolution. First, we consider the one-dimensional Schrödinger equation with initial condition $\Psi(x,0) = \Psi(x)$:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \Psi(x,t). \tag{90}$$

We rewrite this to a new form and take $\frac{\hbar}{m} = 1$ for simplicity:

$$\frac{\partial \Psi(x,t)}{\partial t} = -i\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\omega^2 x^2\right]\Psi(x,t) = -iH_s\Psi(x,t), \tag{91}$$

where we define the term in brackets as the Schrödinger operator H_s. In this form it is evident that the solution is given by:

$$\Psi(x,t) = \left(e^{-itH_s}\Psi\right)(x). \tag{92}$$

Now an easy way to switch from quantum mechanics to the field of diffusion and Markov theory is by simply replacing it by t, i.e. going from real time to imaginary time:

$$\Psi(x,t) = \left(e^{-tH_s}\Psi\right)(x). \tag{93}$$

We see that the resulting equation is of the same form as (11). Therefore, if H_s would be a Markov generator, the unique solution to (93) would be given by the corresponding semigroup and the initial Ψ. Unfortunately in our case, H_s is not a Markov generator yet. For a Markov generator L we must have $L1 = 0$. In order to satisfy this property we transform H_s in the following way:

$$(H_s - \lambda_0)(\psi_0 1) = 0.$$

For proper normalization we also have to divide by ψ_0. The claim is that this so-called ground-state transformation is equal to minus the generator of the Ornstein-Uhlenbeck process. We transform H_s into:

$$\begin{aligned}
\frac{1}{\psi_0}\left(H_s-\lambda_0\right)\left(\psi_0 f\right) &= \frac{1}{\psi_0}\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}\omega^2x^2-\frac{1}{2}\omega\right)\left(\psi_0 f\right)\\
&= -\frac{1}{2\psi_0}\frac{\partial^2(\psi_0 f)}{\partial x^2}+\frac{1}{2}\omega^2x^2f-\frac{1}{2}\omega f\\
&= -\frac{1}{2}\frac{\partial^2 f}{\partial x^2}-\frac{1}{\psi_0}\frac{\partial\psi_0}{\partial x}\frac{\partial f}{\partial x}-\frac{1}{2\psi_0}\frac{\partial^2\psi_0}{\partial x^2}f+\frac{1}{2}\omega^2x^2f-\frac{1}{2}\omega f\\
&= -\frac{1}{2}\frac{\partial^2 f}{\partial x^2}+\omega x\frac{\partial f}{\partial x}-\frac{1}{2}\omega^2x^2f+\frac{1}{2}\omega f+\frac{1}{2}\omega^2x^2f-\frac{1}{2}\omega f\\
&= -\left(-\omega x\frac{\partial}{\partial x}+\frac{1}{2}\frac{\partial^2}{\partial x^2}\right)f,
\end{aligned}$$

which is the generator L of the Ornstein-Uhlenbeck process with parameters $\theta=\omega$ and $\sigma^2=1$. Hence,

$$\frac{1}{\psi_0}\left(H_s-\lambda_0\right)\left(\psi_0 f\right) = -Lf. \tag{94}$$

By using this relation we can rewrite the operator solution in (93) to:

$$\left(e^{-tH_s}\Psi\right)(x) = \left(\psi_0 e^{t(L-\frac{1}{2}\omega)}\frac{1}{\psi_0}\Psi\right)(x). \tag{95}$$

From theorem 1.1 it follows that

$$S_t f = e^{tL}f,$$

where S_t is the semigroup of the Ornstein-Uhlenbeck process. Therefore we can calculate the time evolution of certain quantum states by knowing the time evolution of the corresponding distributions in the Ornstein-Uhlenbeck process. Consider for example the time evolution of $\Psi(x)=\psi_0(x)$. We can calculate this relatively easy since we know the time evolution of the constant function 1. We have

$$\begin{aligned}
\left(e^{-tH_s}\Psi\right)(x) &= \left(\psi_0 e^{t(L-\frac{1}{2}\omega)}\frac{1}{\psi_0}\psi_0\right)(x)\\
&= \psi_0(x)e^{-\frac{1}{2}\omega t}S_t 1\\
&= \psi_0(x)e^{-\frac{1}{2}\omega t},
\end{aligned}$$

after which we change back to real time to obtain its time evolution

$$\Psi_0(x,t) = \psi_0(x)e^{-i\frac{1}{2}\omega t}. \tag{96}$$

This example is a bit cumbersome, but it shows that by knowing the time evolution of distributions in the Ornstein-Uhlenbeck process, time evolutions of the corresponding quantum states can be calculated. Information about

the quantum harmonic oscillator can also be used to derive properties of the semigroup of the Ornstein-Uhlenbeck process. For instance, consider the higher energy eigenfunctions ψ_n. We know their time evolution from (66) and insert these in equation (95) to obtain:

$$\left(\psi_0 e^{t(L-\frac{1}{2}\omega)}\frac{1}{\psi_0}\psi_n\right)(x) = \psi_n(x)e^{-(n+\frac{1}{2})\omega t},$$

from which it follows that:

$$S_t\left(\frac{\psi_n}{\psi_0}\right) = \left(\frac{\psi_n}{\psi_0}\right)e^{-n\omega t}. \tag{97}$$

6.2 Invariant Distribution

The ground-state transformation described in (94) can be used to derive that the stationary distribution is equal to ψ_0^2. We have for $f \in D(L)$

$$\begin{aligned}\int Lf d\mu &= \int \psi_0^2 Lf dx \\ &= -\int \psi_0^2 \frac{1}{\psi_0}(H_s - \lambda_0)(f\psi_0)dx \\ &= -\int \psi_0 (H_s - \lambda_0)(f\psi_0)dx.\end{aligned}$$

Because the Schrödinger operator H_s is self adjoint, we find

$$\int \psi_0(H_s - \lambda_0)(f\psi_0)dx = \int f\psi_0(H_s - \lambda_0)\psi_0 dx.$$

Finally, we use the fact that $H_s\psi_0 = \lambda_0\psi_0$:

$$\int Lf d\mu = -\int f\psi_0(H_s - \lambda_0)\psi_0 dx = 0.$$

From theorem 1.2 we can now conclude that ψ_0^2 is the invariant distribution. Recall that

$$\psi_0(x)^2 = \sqrt{\frac{\omega}{\pi}}e^{-\omega x^2}.$$

6.3 Quantum State Time Evolution

Consider a distribution μ and a function g, then

$$\int g d\mu S_t = \int S_t g d\mu = \int S_t g \frac{d\mu}{d\tilde{\mu}} d\tilde{\mu},$$

where $\tilde{\mu}$ is the reversible distribution. Therefore we can interchange the roles of $\frac{d\mu}{d\tilde{\mu}}$ and g in order to obtain:

$$\int g d\mu S_t = \int S_t g \frac{d\mu}{d\tilde{\mu}} d\tilde{\mu} = \int g S_t \left[\frac{d\mu}{d\tilde{\mu}}\right] d\tilde{\mu}.$$

Hence,

$$\frac{d\mu S_t}{d\tilde{\mu}} = S_t \left[\frac{d\mu}{d\tilde{\mu}}\right]. \tag{98}$$

Recall that the behaviour of normal distributions under the Ornstein-Uhlenbeck process is known from section 3.1.3. For $d\mu = f_{\mathcal{N}(\mu,\sigma_0^2)}(x)dx$ we have:

$$d\mu St = f_{\mathcal{N}(\mu e^{-\omega t}, \sigma_0^2 e^{-2\omega t} + \sigma_*^2(1-e^{-2\omega t}))}(x)dx. \tag{99}$$

Combining (98) and (99) gives us the following relation:

$$S_t \left[\frac{f_{\mathcal{N}(\mu,\sigma_0^2)}}{f_{\mathcal{N}(0,\sigma_*^2)}}\right] = \frac{f_{\mathcal{N}(\mu e^{-\omega t}, \sigma_0^2 e^{-2\omega t} + \sigma_*^2(1-e^{-2\omega t}))}}{f_{\mathcal{N}(0,\sigma_*^2)}}. \tag{100}$$

This equation gives us enough information to be able to calculate the time evolution for wave functions of the form $\Psi(x,0) = C\frac{f_{\mathcal{N}(\mu,\sigma_0^2)}}{\psi_0}$, where C is a constant such that $\Psi(x,0)$ satisfies the normalization condition stated in (47). We use this condition to calculate C:

$$\begin{aligned}
\int_{-\infty}^{\infty} |\Psi(x,0)|^2 \, dx &= \int_{-\infty}^{\infty} |C|^2 \, \frac{f_{\mathcal{N}(\mu,\sigma_0^2)}^2}{\psi_0^2} dx \\
&= |C|^2 \, \frac{\sigma_*}{\sqrt{2\pi}\sigma_0^2} \int_{-\infty}^{\infty} e^{-\frac{1}{\sigma_0^2}(x-\mu)^2 + \frac{1}{2\sigma_*^2}x^2} \, dx \\
&= |C|^2 \, \frac{\sigma_*}{\sqrt{2\pi}\sigma_0^2} \sqrt{\frac{2\pi}{\frac{2}{\sigma_0^2} - \frac{1}{\sigma_*^2}}} e^{\frac{\mu^2}{2\sigma_*^2 - \sigma_0^2}} \\
&= 1.
\end{aligned}$$

For a converging integral we must have $\sigma_0^2 < 2\sigma_*^2$. For C we find:

$$C = \sqrt[4]{\frac{2\sigma_0^2}{\sigma_*^2} - \frac{\sigma_0^4}{\sigma_*^4}} e^{-\frac{\mu^2}{4\sigma_*^2 - 2\sigma_0^2}}. \tag{101}$$

Thus for a wave function

$$\Psi(x,0) = C\frac{f_{\mathcal{N}(\mu,\sigma_0^2)}}{\psi_0} = \sqrt[4]{\frac{1}{\pi\sigma_0^2} - \frac{1}{2\pi\sigma_*^2}} e^{-\frac{1}{2\sigma_0^2}(x-\mu)^2 + \frac{1}{4\sigma_*^2}x^2 - \frac{\mu^2}{4\sigma_*^2 - 2\sigma_0^2}}, \tag{102}$$

we calculate its time evolution in imaginary time:

$$\begin{aligned}
\left(e^{-tH_s}\Psi\right)(x) &= \left(\psi_0 e^{t(L-\frac{1}{2}\omega)} C \frac{1}{\psi_0} \frac{f_{\mathcal{N}(\mu,\sigma_0^2)}}{\psi_0}\right)(x) \\
&= C\psi_0 e^{-\frac{1}{2}\omega t} S_t \left[\frac{f_{\mathcal{N}(\mu,\sigma_0^2)}}{f_{\mathcal{N}(0,\sigma_*^2)}}\right] \\
&= C\frac{f_{\mathcal{N}(\mu e^{-\omega t}, \sigma_0^2 e^{-2\omega t} + \sigma_*^2(1-e^{-2\omega t}))}}{\psi_0} e^{-\frac{1}{2}\omega t}.
\end{aligned}$$

Changing back to real time gives us the final result:

$$\Psi(x,t) = C\frac{f_{\mathcal{N}(\mu e^{-i\omega t},\sigma_0^2 e^{-2i\omega t}+\sigma_*^2(1-e^{-2i\omega t}))}}{\psi_0}e^{-\frac{1}{2}i\omega t}. \tag{103}$$

We rewrite this as

$$\Psi(x,t) = C\frac{\sqrt[4]{2\pi\sigma_*^2}}{\sqrt{2\pi\sigma_t^2}}e^{-\frac{(x-\mu e^{-i\omega t})^2}{2\sigma_t^2}+\frac{x^2}{4\sigma_*^2}-\frac{1}{2}i\omega t} \tag{104}$$

with

$$\sigma_t^2 = \sigma_0^2 e^{-2i\omega t} + \sigma_*^2(1-e^{-2i\omega t}). \tag{105}$$

6.4 Multidimensional Case

6.4.1 Harmonic Potentials along Orthogonal Axes

In this section, we will look at the quantum harmonic oscillator in higher dimensions. Firstly, the case where all potentials along orthogonal axes are of the harmonic form is considered. Then, the Schrödinger operator H_s is

$$H_s = -\frac{1}{2}\nabla^2 + \frac{1}{2}\sum_{i=1}^{n}\omega_i^2 x_i^2. \tag{106}$$

The ground state of the time-independent Schrödinger equation is then simply given by the product of the individual ground state functions $\psi_{x_i,0}$ of each coordinate x_i. The corresponding energy is equal to the sum of the individual energies.

$$\psi_0(\boldsymbol{x}) = \prod_{i=1}^{n}\psi_{x_i,0} = \prod_{i=1}^{n}\left(\frac{\omega_i}{\pi}\right)^{1/4}e^{-\frac{\omega_i}{2}x_i^2} \tag{107}$$

with

$$E_0 = \frac{1}{2}\hbar\sum_{i=1}^{n}\omega_i. \tag{108}$$

As in the one dimensional case the ground state $\psi_0(\boldsymbol{x})$ is the square root of a (multivariate) normal distribution

$$\psi_0(\boldsymbol{x}) = \sqrt{\frac{1}{(2\pi)^{n/2}|\Sigma_*|^{1/2}}e^{-\frac{1}{2}\boldsymbol{x}^T\Sigma_*^{-1}\boldsymbol{x}}}, \tag{109}$$

with covariance matrix

$$\Sigma_* = \begin{bmatrix}\sigma_{*,1}^2 & & & \\ & \sigma_{*,2}^2 & & \\ & & \ddots & \\ & & & \sigma_{*,n}^2\end{bmatrix}. \tag{110}$$

The determinant of a matrix A is denoted by $|A|$.

We perform the same transformation as in the one-dimensional case, but with the new Schrödinger operator H_s, lowest eigenfunction ψ_0 and corresponding eigenvalue λ_0. In this case we find:

$$\begin{aligned}
\frac{1}{\psi_0}\left(H_s-\lambda_0\right)\left(\psi_0 f\right) &= \frac{1}{\psi_0}\left(-\frac{1}{2}\nabla^2+\frac{1}{2}\sum_{i=1}^{n}\omega_i^2x_i^2-\frac{1}{2}\sum_{i=1}^{n}\omega_i\right)\left(\psi_0 f\right)\\
&= -\frac{1}{2\psi_0}\nabla^2(\psi_0 f)+\frac{1}{2}f\sum_{i=1}^{n}\omega_i^2x_i^2-\frac{1}{2}f\sum_{i=1}^{n}\omega_i\\
&= -\frac{1}{2}\nabla^2 f-\frac{1}{\psi_0}\sum_{i=1}^{n}\frac{\partial\psi_0}{\partial x_i}\frac{\partial f}{\partial x_i}-\frac{1}{2\psi_0}f\nabla^2\psi_0\\
&+\frac{1}{2}f\sum_{i=1}^{n}\omega_i^2x_i^2-\frac{1}{2}f\sum_{i=1}^{n}\omega_i\\
&= -\frac{1}{2}\nabla^2 f+\sum_{i=1}^{n}\omega_i x_i\frac{\partial f}{\partial x_i}-\frac{1}{2}f\sum_{i=1}^{n}\omega_i^2x_i^2+\frac{1}{2}f\sum_{i=1}^{n}\omega_i\\
&+\frac{1}{2}f\sum_{i=1}^{n}\omega_i^2x_i^2-\frac{1}{2}f\sum_{i=1}^{n}\omega_i\\
&= -\sum_{i=1}^{n}\left(-\omega_i x_i\frac{\partial}{\partial x_i}+\frac{1}{2}\frac{\partial^2}{\partial x_i^2}\right)f.
\end{aligned}$$

This is equal to the generator L of the multivariate Ornstein-Uhlenbeck process. Hence,

$$\frac{1}{\psi_0}\left(H_s-\lambda_0\right)\left(\psi_0 f\right) = -\left(-\boldsymbol{x}^T D\nabla+\frac{1}{2}\nabla^2\right)f = -Lf, \tag{111}$$

where D is the diagonal matrix

$$D=\begin{bmatrix}\omega_1 & & & \\ & \omega_2 & & \\ & & \ddots & \\ & & & \omega_n\end{bmatrix}. \tag{112}$$

Since $\Sigma_* = \frac{1}{2}D^{-1}$, it follows from (32) that $\psi_0(\boldsymbol{x})^2$ is (again) the stationary and reversible distribution. In a similar manner, we find the multivariate equivalent to (100):

$$S_t\left[\frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{f_{\mathcal{N}(\mathbf{0},\Sigma_*)}}\right] = \frac{f_{\mathcal{N}(e^{-Dt}\boldsymbol{\mu},e^{-Dt}\Sigma_0e^{-Dt}+\Sigma_*(1-e^{-2Dt}))}}{f_{\mathcal{N}(\mathbf{0},\Sigma_*)}}. \tag{113}$$

Therefore, we can evaluate the time evolution for a wave function of the form

$$\Psi(\boldsymbol{x},0) = C\frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{\psi_0}.$$

We use the normalization condition to calculate C:

$$\begin{aligned}
\int_{\mathbb{R}^n} |\Psi(x,0)|^2 \, d\boldsymbol{x} &= \int_{\mathbb{R}^n} |C|^2 \, \frac{f^2_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{\psi_0^2} \\
&= \frac{|C|^2 \sqrt{|\Sigma_*|}}{(2\pi)^{n/2} \, |\Sigma_0|} \int_{\mathbb{R}^n} e^{-(\boldsymbol{x}-\boldsymbol{\mu})^T \Sigma_0^{-1} (\boldsymbol{x}-\boldsymbol{\mu}) + \frac{1}{2} \boldsymbol{x}^T \Sigma_*^{-1} \boldsymbol{x}} d\boldsymbol{x} \\
&= \frac{|C|^2 \sqrt{|\Sigma_*|}}{(2\pi)^{n/2} \, |\Sigma_0|} e^{-\frac{1}{2} \boldsymbol{\mu}^T \Sigma_*^{-1} \boldsymbol{\mu}} \\
&\int_{\mathbb{R}^n} e^{-\frac{1}{2} \boldsymbol{x}^T (2\Sigma_0^{-1} - \Sigma_*^{-1}) \boldsymbol{x} - \boldsymbol{\mu}^T \Sigma_0^{-1} \boldsymbol{\mu} + 2 \boldsymbol{\mu}^T \Sigma_0^{-1} \boldsymbol{x}} d\boldsymbol{x} \\
&= \frac{|C|^2}{|\Sigma_0|} \sqrt{\frac{|\Sigma_*|}{\left|2\Sigma_0^{-1} - \Sigma_*^{-1}\right|}} e^{-\boldsymbol{\mu}^T \Sigma_0^{-1} \boldsymbol{\mu} + 2 \boldsymbol{\mu}^T \Sigma_*^{-1} (2\Sigma_0^{-1} - \Sigma_*^{-1})^{-1} \Sigma_*^{-1} \boldsymbol{\mu}} \\
&= \frac{|C|^2}{\sqrt{\left|2\Sigma_0 \Sigma_*^{-1} - \Sigma_0^2 \Sigma_*^{-2}\right|}} e^{-\boldsymbol{\mu}^T \Sigma_0^{-1} \boldsymbol{\mu} + 2 \boldsymbol{\mu}^T (2\Sigma_0^{-1} \Sigma_*^2 - \Sigma_*)^{-1} \boldsymbol{\mu}} \\
&= 1.
\end{aligned}$$

In order to have a converging integral, we must have that $\Sigma_0^{-1} - \frac{1}{2}\Sigma_*^{-1}$ is positive definite. For C we find

$$C = \sqrt[4]{\left|2\Sigma_0 \Sigma_*^{-1} - \Sigma_0^2 \Sigma_*^{-2}\right|} e^{\frac{1}{2} \boldsymbol{\mu}^T \Sigma_0^{-1} \boldsymbol{\mu} - \boldsymbol{\mu}^T (2\Sigma_0^{-1} \Sigma_*^2 - \Sigma_*)^{-1} \boldsymbol{\mu}}. \tag{114}$$

Then, in imaginary time we have

$$\begin{aligned}
\left(e^{-tH_s} \Psi\right)(\boldsymbol{x}) &= \left(\psi_0 e^{t(L - \frac{1}{2}|D|)} \frac{1}{\psi_0} C \frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{\psi_0} \right)(\boldsymbol{x}) \\
&= C \psi_0 e^{-\frac{1}{2}|D|t} S_t \left[\frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{f_{\mathcal{N}(\mathbf{0},\Sigma_*^2)}} \right] \\
&= C e^{-\frac{1}{2}|D|t} \frac{f_{\mathcal{N}(e^{-Dt}\boldsymbol{\mu}, e^{-Dt}\Sigma_0 e^{-Dt} + \Sigma_*(1 - e^{-2Dt}))}}{\psi_0}.
\end{aligned}$$

Changing back to real time gives us the final result:

$$\Psi(\boldsymbol{x},t) = C e^{-\frac{1}{2} i |D| t} \frac{f_{\mathcal{N}(e^{-iDt}\boldsymbol{\mu}, e^{-iDt}\Sigma_0 e^{-iDt} + \Sigma_*(1 - e^{-2iDt}))}}{\psi_0} \tag{115}$$

$$= C e^{-\frac{1}{2} i |D| t} \frac{\sqrt[4]{|\Sigma_*|}}{\sqrt{(2\pi)^{n/2} |\Sigma_t|}} e^{\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu}(t))^T \Sigma_t^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) + \frac{1}{4} \boldsymbol{x}^T \Sigma_*^{-1} \boldsymbol{x}}, \tag{116}$$

where

$$\Sigma_t = e^{-iDt} \Sigma_0 e^{-iDt} + \Sigma_*(1 - e^{-2iDt}) \tag{117}$$

and

$$\boldsymbol{\mu}(t) = e^{-iDt} \boldsymbol{\mu}. \tag{118}$$

Note that if Σ_0 is a diagonal matrix, then the obtained result is the product of n one dimensional solutions. This result is quite straightforward, since the Hamiltonian and the initial condition are simply the product of n one-dimensional cases.

6.4.2 Harmonic Potentials in Arbitrary Directions

If we have harmonic potentials in arbitrary directions, then we consider the Schrödinger operator in its general form:

$$H_s = -\frac{1}{2}\nabla^2 + \frac{1}{2}\langle \boldsymbol{x}, A\boldsymbol{x}\rangle, \tag{119}$$

where A is a real, positive definite matrix. Note that in the preceding section we looked at the case where A was a diagonal matrix with eigenvalues ω_i^2. As was explained in section 4.1.2, we can consider A to be symmetric without loss of generality. Since A is symmetric and positive definite, it has strictly positive eigenvalues, say $\{\omega_1^2, \omega_2^2 \ldots, \omega_n^2\}$. Furthermore, it can be diagonalised by some orthogonal matrix Q:

$$A = Q^{-1}D^2Q = Q^TD^2Q, \tag{120}$$

with

$$D = \begin{bmatrix} \omega_1 & & & \\ & \omega_2 & & \\ & & \ddots & \\ & & & \omega_n \end{bmatrix}. \tag{121}$$

The rows in Q correspond to the eigenvectors of these eigenvalues. We define

$$B = Q^TDQ. \tag{122}$$

Note that B is again real and symmetric with eigenvalues $\{\omega_1, \omega_2 \ldots, \omega_n\}$ and $B^2 = A$. By substituting (120) in $\langle x, Ax\rangle$, we find

$$\langle \boldsymbol{x}, A\boldsymbol{x}\rangle = \langle \boldsymbol{x}, Q^TD^2Q\boldsymbol{x}\rangle = (Q\boldsymbol{x})^TD^2Q\boldsymbol{x} = \langle Q\boldsymbol{x}, D^2Q\boldsymbol{x}\rangle. \tag{123}$$

Let $g : \mathbb{R}^n \to \mathbb{R}^n$ be the function given by $g(\boldsymbol{x}) = Q\boldsymbol{x}$, then $g^{-1}(\boldsymbol{x}) = Q^T\boldsymbol{x}$. We use

$$f(\boldsymbol{x}) = (f \circ g^{-1} \circ g)(\boldsymbol{x}) = (f \circ g^{-1})(Q\boldsymbol{x}), \tag{124}$$

together with (123) to rewrite the Schrödinger operator in (119) to:

$$H_sf(\boldsymbol{x}) = -\frac{1}{2}\nabla^2(f\circ g^{-1})(Q\boldsymbol{x}) + \frac{1}{2}\langle Q\boldsymbol{x}, D^2Q\boldsymbol{x}\rangle(f\circ g^{-1})(Q\boldsymbol{x}) = \tilde{H}_s\tilde{f}(\tilde{\boldsymbol{x}}), \tag{125}$$

where

$$\begin{aligned} \tilde{\boldsymbol{x}} &= Q\boldsymbol{x} \\ \tilde{f} &= (f \circ g^{-1}) \\ \tilde{H}_s &= -\frac{1}{2}\nabla^2 + \frac{1}{2}\langle \tilde{\boldsymbol{x}}, D^2\tilde{\boldsymbol{x}}\rangle. \end{aligned}$$

The Laplacian is invariant under orthogonal transformations [12]. Hence,

$$\tilde{H}_s = -\frac{1}{2}\tilde{\nabla}^2 + \frac{1}{2}\langle \tilde{\boldsymbol{x}}, D^2\tilde{\boldsymbol{x}}\rangle, \tag{126}$$

where

$$\tilde{\nabla}^2 = \sum_{i=1}^{n} \frac{\partial}{\partial \tilde{x}_i^2}.$$

The resulting operator $\tilde{H}_s$ is identical to the H_s in (106), where we took the harmonic potentials to be along orthogonal axes. The ground state ψ_0 is defined analogously:

$$\begin{aligned}
\psi_0(\boldsymbol{x}) = \tilde{\psi_0}(\tilde{\boldsymbol{x}}) &= \sqrt{\frac{1}{(2\pi)^{n/2}|\Sigma_*|^{1/2}} e^{-\frac{1}{2}\tilde{\boldsymbol{x}}^T \Sigma_*^{-1} \tilde{\boldsymbol{x}}}} \\
&= \sqrt{\frac{1}{(2\pi)^{n/2}|\frac{1}{2}D^{-1}|^{1/2}} e^{-\frac{1}{2}(P\boldsymbol{x})^T (\frac{1}{2}D^{-1})^{-1} (P\boldsymbol{x})}} \\
&= \sqrt{\frac{1}{(2\pi)^{n/2}|\frac{1}{2}B^{-1}|^{1/2}} e^{-\frac{1}{2}\boldsymbol{x}^T (\frac{1}{2}B^{-1})^{-1} \boldsymbol{x}}} \\
&= \sqrt{f_{\mathcal{N}(0,\frac{1}{2}B^{-1})}(\boldsymbol{x})}.
\end{aligned} \tag{127}$$

We perform the same transformation to obtain:

$$\begin{aligned}
\frac{1}{\psi_0(\boldsymbol{x})} \left(H_s - \lambda_0\right) \left(\psi_0 f\right)(\boldsymbol{x}) &= \frac{1}{\tilde{\psi_0}(\tilde{\boldsymbol{x}})} \left(\tilde{H}_s - \lambda_0\right) \left(\tilde{\psi_0} \tilde{f}\right)(\tilde{\boldsymbol{x}}) \\
&= -\left(-\tilde{\boldsymbol{x}}^T D \tilde{\nabla} + \frac{1}{2}\tilde{\nabla}^2\right) \tilde{f}(\tilde{\boldsymbol{x}}) \\
&= -\left(-\boldsymbol{x}^T Q^T D Q \nabla + \frac{1}{2}\nabla^2\right) f(\boldsymbol{x}) \\
&= -\left(-\boldsymbol{x}^T B \nabla + \frac{1}{2}\nabla^2\right) f(\boldsymbol{x}).
\end{aligned}$$

We found that the transformed operator is again equal to minus the generator L of the multivariate Ornstein-Uhlenbeck process, but in this case L contains the non-diagonal, symmetric matrix B:

$$\frac{1}{\psi_0(\boldsymbol{x})} \left(H_s - \lambda_0\right) \left(\psi_0 f\right)(\boldsymbol{x}) = -\left(-\boldsymbol{x}^T B \nabla + \frac{1}{2}\nabla^2\right) f(\boldsymbol{x}) = -Lf(\boldsymbol{x}). \tag{128}$$

From (127) and (32) it follows that $\psi_0(\boldsymbol{x})$ is again the reversible distribution. Hence, we find the following equation in a similar manner as for the orthogonal case stated in (113):

$$S_t \left[\frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{f_{\mathcal{N}(\mathbf{0},\frac{1}{2}B^{-1})}}\right] = \frac{f_{\mathcal{N}(e^{-Bt}\boldsymbol{\mu}, e^{-Bt}\Sigma_0 e^{-Bt} + \frac{1}{2}B^{-1}(1-e^{-2Bt}))}}{f_{\mathcal{N}(\mathbf{0},\frac{1}{2}B^{-1})}}. \tag{129}$$

Therefore, we can evaluate the time evolution for a wave function of the form

$$\Psi(\boldsymbol{x}, 0) = C \frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{\psi_0}.$$

In order to have a converging integral in the normalization condition, we must have that $\Sigma_0^{-1} - B$ is positive definite. For C we find

$$C = \sqrt[4]{|4\Sigma_0 B - 4\Sigma_0^2 B^2|} e^{\frac{1}{2}\boldsymbol{\mu}^T \Sigma_0^{-1} \boldsymbol{\mu} - 2\boldsymbol{\mu}^T (\Sigma_0^{-1} B^{-2} - B^{-1})^{-1} \boldsymbol{\mu}}. \tag{130}$$

Then, in imaginary time we have

$$\begin{aligned}
\left(e^{-tH_s}\Psi\right)(\boldsymbol{x}) &= \left(\psi_0 e^{t(L-\frac{1}{2}\lambda_0)} \frac{1}{\psi_0} C \frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{\psi_0}\right)(\boldsymbol{x}) \\
&= C\psi_0 e^{-\frac{1}{2}|B|t} S_t \left[\frac{f_{\mathcal{N}(\boldsymbol{\mu},\Sigma_0)}}{f_{\mathcal{N}(\mathbf{0},\frac{1}{2}B^{-1})}}\right] \\
&= C e^{-\frac{1}{2}|B|t} \frac{f_{\mathcal{N}(e^{-Bt}\boldsymbol{\mu}, e^{-Bt}\Sigma_0 e^{-Bt} + \frac{1}{2}B^{-1}(1-e^{-2Bt}))}}{\psi_0}.
\end{aligned}$$

Changing back to real time gives us the final result:

$$\begin{aligned}
\Psi(\boldsymbol{x},t) &= C e^{-\frac{1}{2}i|B|t} \frac{f_{\mathcal{N}(e^{-iBt}\boldsymbol{\mu}, e^{-iBt}\Sigma_0 e^{-iBt} + \frac{1}{2}B^{-1}(1-e^{-2iBt}))}}{\psi_0} \\
&= C e^{-\frac{1}{2}i|B|t} \frac{\sqrt[4]{|\frac{1}{2}B^{-1}|}}{\sqrt{(2\pi)^{n/2}|\Sigma_t|}} e^{\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}(t))^T \Sigma_t^{-1}(\boldsymbol{x}-\boldsymbol{\mu}) + \frac{1}{4}\boldsymbol{x}^T \Sigma_*^{-1} \boldsymbol{x}},
\end{aligned} \tag{131}$$

where

$$\Sigma_t = e^{-iBt}\Sigma_0 e^{-iBt} + \frac{1}{2}B^{-1}(1 - e^{-2iBt}) \tag{132}$$

and

$$\boldsymbol{\mu}(t) = e^{-iBt}\boldsymbol{\mu}. \tag{133}$$

7 Conclusion

By performing a ground-state transformation on the Hamiltonian of the quantum harmonic oscillator and by going from real to imaginary time, we were able to calculate quantum state time evolutions from the evolutions of the corresponding distributions in the Ornstein-Uhlenbeck process (and vice versa), which in our case were Gaussian distributions.

7.1 One-Dimensional Case

In section 3.1.3 we have calculated that Gaussian distributions in the Ornstein-Uhlenbeck process remain normally distributed over time, but with changing mean and changing variance.

$$\mathcal{N}(\mu, \sigma_0) \xrightarrow{t} \mathcal{N}(\mu e^{-\theta t}, \sigma_0^2 e^{-2\theta t} + \sigma_*^2(1 - e^{-2\theta t})) \tag{134}$$

Hence, the mean will approach zero over time and the variance will converge to the invariant variance σ_*^2. In section 6.3 we found the time evolution of the one-dimensional quantum states that corresponded with these Gaussian distributions. The final result we obtained was

$$\Psi(x,t) = C\frac{\sqrt[4]{2\pi\sigma_*^2}}{\sqrt{2\pi\sigma_t^2}} e^{-\frac{(x-\mu e^{-i\omega t})^2}{2\sigma_t^2} + \frac{x^2}{4\sigma_*^2} - \frac{1}{2}i\omega t} \tag{135}$$

with

$$\sigma_t^2 = \sigma_0^2 e^{-2i\omega t} + \sigma_*^2(1 - e^{-2i\omega t}). \tag{136}$$

The value corresponding to the mean value of the Gaussian distribution is equal to $\mu e^{-i\omega t}$. This value is now circling around zero in the complex plane instead of converging to it. This follows from the switch made from real to imaginary time causing the exponential to be complex. Therefore, $|\Psi(x,t)|^2$ will show an oscillating, periodic behaviour from side to side with period $T = \frac{2\pi}{\omega}$. This is equal to the behaviour of the classical harmonic oscillator as in section 4.1.1. Likewise, the value of σ_t^2 is also now circling around the value of σ_*^2 in the complex plane. From (136) we have

$$\sigma_t^2 - \sigma_*^2 = (\sigma_0^2 - \sigma_*^2)e^{-2i\omega t}. \tag{137}$$

Therefore, $\lim_{T\to\infty} \frac{1}{T}\int_0^T (\sigma_t^2 - \sigma_*^2)dt = 0$. This type of convergence is called Cesaro convergence.

Because of the complex value of σ_t^2, evaluating the function $|\Psi(x,t)|^2$ analytically soon becomes really messy. In order to get a view of the function $|\Psi(x,t)|^2$ nonetheless, Matlab was used to plot it over time. In figure 5 the function $|\Psi(x,t)|^2$ is depicted for times $t = 0, t = \frac{T}{4}$ and $t = \frac{T}{2}$.

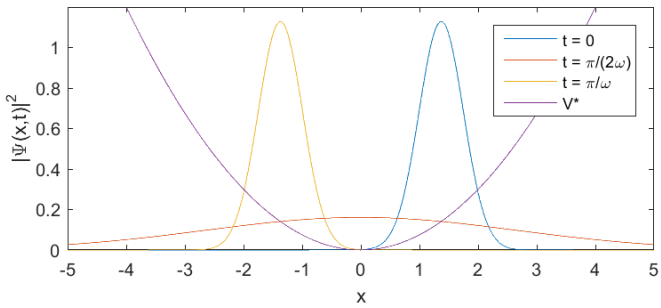

Figure 5. Plot of $|\Psi(x,t)|^2$ for times $t = 0, t = \frac{\pi}{2\omega}$ and $t = \frac{\pi}{\omega}$. The parameters were set to: $\mu = 1.2$ m, $\omega = 3$ rad s^{-1}, $\sigma_0 = \frac{1}{2}$ m and $\sigma_* = 1$ m. The harmonic potential is plotted as well, but scaled by a factor of $V* = V/(10\hbar)$.

7.2 Multidimensional Case

In section 3.2.3 we have calculated the multivariate analogue of 134. The matrix B in the definition of the multivariate Ornstein-Uhlenbeck was considered symmetric and invertible. We found

$$\mathcal{N}(\boldsymbol{\mu}, \Sigma_0) \xrightarrow{t} \mathcal{N}\left(e^{-Bt}\boldsymbol{\mu}, e^{-Bt}\Sigma_0 e^{-Bt} + \frac{1}{2}B^{-1}(1 - e^{-2Bt})\right) \tag{138}$$

Again, the mean converges to zero and the covariance matrix converges to the invariant covariance matrix $\frac{1}{2}B^{-1}$. For the case with harmonic potentials along orthogonal axes, the matrix B was equal to the (real) positive definite diagonal matrix D and for the case with harmonic potentials in arbitrary directions, B was more general, i.e. real, positive definite, invertible and symmetric. The final result we obtained was

$$\Psi(x,t) = Ce^{-\frac{1}{2}i|B|t}\frac{\sqrt[4]{|\frac{1}{2}B^{-1}|}}{\sqrt{(2\pi)^{n/2}|\Sigma_t|}}e^{\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}(t))^T\Sigma_t^{-1}(\boldsymbol{x}-\boldsymbol{\mu})+\frac{1}{4}\boldsymbol{x}^T\Sigma_*^{-1}\boldsymbol{x}}, \tag{139}$$

where

$$\Sigma_t = e^{-iBt}\Sigma_0 e^{-iBt} + \frac{1}{2}B^{-1}(1 - e^{-2iBt}) \tag{140}$$

and

$$\boldsymbol{\mu}(t) = e^{-iBt}\boldsymbol{\mu}. \tag{141}$$

Note that for the diagonal case we introduced $\Sigma_* = \frac{1}{2}D^{-1}$. We see that Σ_t and $\boldsymbol{\mu}(t)$ show the same behaviour as their one-dimensional analogues.

7.3 Coherent States

In chapter 5 we derived that coherent states are Gaussian wave packets with oscillating mean and constant variance. If we set $\sigma_0^2 = \sigma_*^2$, then the variance of the Gaussian in the Ornstein-Uhlenbeck process remains constant over time. Therefore, starting from this distribution we should expect to arrive at the time evolution of coherent states. We have

$$\Psi(x,t) = \frac{1}{\sqrt[4]{2\pi\sigma_*^2}} e^{-\frac{(x-\mu e^{-i\omega t})^2}{2\sigma_*^2} + \frac{x^2}{4\sigma_*^2} - \frac{1}{2}i\omega t - \frac{\mu^2}{2\sigma_*^2}}. \tag{142}$$

We rewrite this expression by substituting $\sigma_*^2 = \frac{1}{2\omega} = \frac{x^2}{2\xi^2} = \frac{1}{2}x_0^2$

$$\begin{aligned}
\Psi(x,0) &= \left(\frac{1}{x_0^2\pi}\right)^{1/4} e^{-\frac{1}{2}i\omega t} e^{-\frac{x^2 - 2\mu x e^{-i\omega t} + \mu^2 e^{-2i\omega t}}{2\sigma_*^2} + \frac{x^2}{4\sigma_*^2} - \frac{\mu^2}{2\sigma_*^2}} \\
&= \left(\frac{1}{x_0^2\pi}\right)^{1/4} e^{-\frac{1}{2}i\omega t} e^{-\frac{x^2}{4\sigma_*^2} + \frac{\mu x e^{-i\omega t}}{\sigma_*^2} - \frac{\mu^2}{2\sigma_*^2}(1 + e^{-2i\omega t})} \\
&= \left(\frac{1}{x_0^2\pi}\right)^{1/4} e^{-\frac{1}{2}i\omega t} e^{-\frac{\xi^2}{2} + \sqrt{2}\frac{\mu e^{-i\omega t}}{\sigma_*}\xi - \mathrm{Re}(\frac{\mu e^{-i\omega t}}{\sigma_*})\frac{\mu e^{-i\omega t}}{\sigma_*}},
\end{aligned}$$

where $\alpha(t) = \frac{\mu e^{-i\omega t}}{\sigma_*}$. The resulting expression is indeed equal to the time evolution of the coherent state with eigenvalue $\alpha = \frac{\mu}{\sigma_*}$ (83). For $|\Psi(x,t)|^2$ we find the following expression:

$$|\Psi(x,t)|^2 = \frac{1}{\sqrt{2\pi\sigma_*^2}} e^{-\frac{(x - 2\mu\cos(\omega t))^2}{2\sigma_*^2}}. \tag{143}$$

This is a Gaussian with oscillating mean $2\mu\cos(\omega t)$ and constant variance σ_*^2.

Substituting $\Sigma_0 = \Sigma_*$ and $\Sigma_0 = \frac{1}{2}B^{-1}$ in the orthogonal case and non-orthogonal case respectively gives us the multidimensional analogue of the coherent states defined in chapter 5. The probability densities are multivariate Gaussian distributions with oscillating means $\boldsymbol{\mu}(t)$ and $Q^T\boldsymbol{\mu}(t)$ (and constant covariance matrices). Here

$$\boldsymbol{\mu}(t) = \begin{bmatrix} 2\mu_1\cos(\omega_1 t) \\ 2\mu_2\cos(\omega_2 t) \\ \vdots \\ 2\mu_n\cos(\omega_n t) \end{bmatrix}. \tag{144}$$

7.4 Overview

An overview of the conclusions for the one-dimensional case is given in table 1. The same overview for the multidimensional case does not bring us new insights.

Table 1. Overview of some corresponding concepts and corresponding properties of the Ornstein-Uhlenbeck process and the quantum harmonic oscillator.

Ornstein-Uhlenbeck process	$\leftrightarrow$	Quantum harmonic oscillator
Generator		Hamiltonian
e^{tL}		e^{-itH}
Evolution of distributions		Quantum state time evolutions
$\mathcal{N}(\mu, \sigma_0) \xrightarrow{t} \mathcal{N}(\mu e^{-\theta t}, \sigma_t)$		General result of (135)
$\mathcal{N}(\mu, \sigma_*) \xrightarrow{t} \mathcal{N}(\mu e^{-\theta t}, \sigma_*)$		Coherent state time evolution
$\mu \xrightarrow{t} \mu e^{-\theta t}$		Oscillating behaviour of $\lvert\Psi(x,t)\rvert^2$
σ_t^2 converges to σ_*^2		σ_t^2 Cesaro converges to σ_*^2

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