A CLASSICAL AND QUANTUM NOISE MODEL

by

YEJUN YANG

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Date	Professor Leon Cohen Chair of Examining Committee
Date	Professor Steve Greenbaum Executive Officer

Professor Godfrey Gumbs

Professor Lou Massa

Professor Patrick Loughlin

Professor Viraht Sahni

Supervisory Committee

THE CITY UNIVERSITY OF NEW YORK

Abstract

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Yejun Yang

Adviser: Professor Leon Cohen

We develop detailed statistics of a noise model that consists of N independent harmonic oscillators where the total force is given by the sum of the individual forces. This model was first proposed in the paper by Ford, Kac, and Mazur that was aimed at deriving the Langevin equation from first principles. We extend the model and calculate relevant probability distributions and other statistical quantities such as the autocorrelation function. In the usual model one assumes that the initial position and momentum values are stochastic variables that determine the statistical features of the force by ensemble averaging over those quantities. We extend that by also treating the mass and frequency as statistical quantities. We consider both the equilibrium case, that is the canonical distribution for the initial positions and momenta, for the but we also consider other initial distributions and show that this leads to non-stationary autocorrelation functions. One of our basic aims is to also develop this model for the quantum case and compare the results with the classical case.

The general approach we use for the calculation of the statistical quantities is by way of the characteristic function. We use the characteristic function approach because the oscillators are independent of each other. However, the quantum characteristic function present unique difficulties because the initial momentum and position operators do not commute.

We use the Weyl correspondence to define the quantum characteristic function and we derive explicit expressions for both the pure case and mixtures. We show that many of the statistical quantities can be expressed in terms of the Wigner distribution.

In addition, we consider the time-frequency Wigner spectrum of momentum governed by the Langevin equation when the random driving term is quantum noise. We obtaine an explicit equation. The equation is solved exactly and includes both the transient and the stationary part. The time-dependent Wigner spectrum generalizes the result of Wang and Uhlenbeck wherein they showed that for the white noise driving force the power spectrum in the stationary state regime is Lorenzian. We show that our solution reduces to the classical solution when the parameters of the quantum noise are such that the white noise limit is approached and when the long time limit is taken.

Contents

Chapter 1

Introduction and Aims

One of the most general models for the study of noise is the independent harmonic oscillator model [1, 2]. This model encompasses many important physical problems because for those problems the equations can be transformed into the model [3]. The model consists of N independent harmonic oscillators where the total force is given by the sum of the individual forces. Such models originated in the classic paper by Ford, Kac, and Mazur [4] aimed at deriving the Langevin[5] equation from first principles and where the harmonic oscillators constitute a heat bath. Often such models are called FKM models.

We now briefly review the harmonic oscillator equations. For each harmonic oscillator the force, f_i, is

$$f_i = -k_i q_i \tag{1.1}$$

where i is used to distinguish between different oscillators in the bath. We assume all oscillators are attached to the origin via a spring constant k_i and the displacement of the oscillator is q_i. We also assume there are no other forces on the oscillator and therefore, the equation of motion for each oscillator is

$$\ddot{q}_i = \frac{f_i}{m_i} = -\frac{k_i}{m_i} q_i \tag{1.2}$$

were m_i is the mass of each oscillator. As standard, we use $k_i = m_i \omega_i^2$ giving

$$\ddot{q}_i = -\omega_i^2 q_i \tag{1.3}$$

The solution is

$$q_i(t) = q_i(0) \cos \omega_i t + \frac{\dot{q}_i(0)}{\omega_i} \sin \omega_i t \tag{1.4}$$

Defining p_i as usual,

$$p_i = m_i \dot{q}_i \tag{1.5}$$

we have

$$q_i(t) = q_i(0) \cos \omega_i t + \frac{p_i(0)}{m_i \omega_i} \sin \omega_i t \tag{1.6}$$

Substitute this result into Eq. (1.1) to obtain

$$f_i(t) = m_i \omega_i^2 q_i(t) = m_i \omega_i^2 q_i(0) \cos \omega_i t + \omega_i p_i(0) \sin \omega_i t \tag{1.7}$$

The force from an individual oscillator is independent of the other ones and is only a function of the initial conditions, the mass, m, and the spring constant or ω_i. That is it is a function of m_i, ω_i, $q_i(0)$ and $p_i(0)$.

The total force due to N oscillators, $F(t)$, is the sum of individual forces $f_i(t)$, and is given by

$$F(t) = \sum_{i=1}^{N} f_i(t) = \sum_{i=1}^{N} \left[m_i \omega_i^2 q_i(0) \cos \omega_i t + \omega_i p_i(0) \sin \omega_i t \right] \tag{1.8}$$

In our considerations we will use this model to study noise issues by taking m_i, ω_i, $q_i(0)$ and

$p_i(0)$ to be random variables. We will develop a general noise model where all the statistical properties of the force can be calculated exactly. This will allow one to test ideas regarding noise and examine the accuracy of statistical methods that have been proposed.

In particular our aim in this thesis is the following. If one considers the initial conditions as random variables we aim to obtain

a) The probability distribution of the force, $f_i(t)$.

b) For N oscillators we will find the probability distribution of the total force, $F(t)$

c) The corresponding autocorrelation functions

d) Other relevant random quantities.

e) In addition one of our basic aims is to also do the above for the quantum case and compare the results with the classical case. For the quantum case we define the total force operator, $\mathbf{F}(t)$, at time t, by

$$\mathbf{F}(t) = \sum_{j=1}^{N} m_j \omega_j^2 \left(\mathbf{q}_j(0) \cos \omega_j t + \mathbf{p}_j(0) \frac{\sin \omega_j t}{m_j \omega_j} \right) \tag{1.9}$$

$$= \sum_{j=1}^{N} \left(m_j \omega_j^2 \mathbf{q}_j(0) \cos \omega_j t + \mathbf{p}_j(0) \omega_j \sin \omega_j t \right) \tag{1.10}$$

where $\mathbf{q}_j(0)$ and $\mathbf{p}_j(0)$ are the initial position and momentum operators.

Also, we consider the time-frequency Wigner spectrum of momentum governed by the Langevin equation when the random driving term is quantum noise[6]. We will obtain an explicit equation for the Winger spectrum and we will solve it exactly[7]. Our solution will include both the transient and the stationary part. The time-dependent Wigner spectrum generalizes the result of Wang and Uhlenbeck wherein they showed that for the white noise driving force the power spectrum in the stationary regime is Lorenzian. We will show that our solution reduces to the classical solution when the parameters of the quantum noise are such that the white noise limit is approached and when the long time limit is taken.

Chapter 2

Characteristic Function Method

Since the total random force is a summation of independent random forces the standard method in probability theory is to calculate the probability of the force by way of the characteristic function [8]. In this chapter we explain the method for the classical case. Quantum characteristic functions [9] present unique features and we will treat them in a subsequent chapter. We first consider the one variable case. If we have a probability distribution, $P(x)$, the characteristic function, $M(\theta)$, is the Fourier transform of the density

$$M(\theta) \;=\; \int\; e^{i\theta x} P(x)\, dx \;=\; \langle\, e^{i\theta x}\,\rangle = E[e^{i\theta x}] \tag{2.1}$$

In Eq. (2.1) we have written $\langle\, e^{i\theta x}\,\rangle$ and $E[e^{i\theta x}]$ to mean the expectation value of $e^{i\theta x}$ since both notations will be used. The characteristic function is the average of $e^{i\theta x}$, where θ is a parameter. By expanding the exponential one has

$$M(\theta) \;=\; \int e^{i\theta x} P(x)\, dx \;=\; \int \sum_{i=1}^{\infty} \frac{(i\theta x)^n}{n!}\, P(x)\, dx \;=\; \sum_{i=1}^{\infty} \frac{i^n \theta^n}{n!} \langle\, x^n\,\rangle \tag{2.2}$$

which is a Taylor series in θ. Hence the moments are given by

$$\langle\, x^n \,\rangle \;=\; \frac{1}{i^n}\frac{\partial}{\partial\theta}M(\theta)\,\bigg|_{\theta\,=\,0} \tag{2.3}$$

There are two fundamental reasons for the use of the characteristic function. First, the moments are more easily calculated from the characteristic function since differentiation is easier than integration. The other is that often a characteristic function can be obtained from physical considerations without knowing the distribution and once that is done the probability distribution can be obtained by way of

$$P(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} M(\theta)e^{-i\theta x}d\theta \tag{2.4}$$

For the two variable case the characteristic function $M(\theta,\tau)$, is the average of $e^{i\theta x+i\tau y}$,

$$M(\theta,\tau) \;=\; \langle\, e^{i\theta x+i\tau y}\,\rangle \;=\; \iint\; e^{i\theta x+i\tau y}P(x,y)\,d\,x\,dy \tag{2.5}$$

and the distribution function is given by

$$P(x,y) \;=\; \frac{1}{4\pi^2}\iint M(\theta,\tau)\,e^{-i\theta x-i\tau y}\,d\theta\,d\tau \tag{2.6}$$

Further, by expanding the exponential in Eq. (2.5) one has

$$M(\theta,\tau) \;=\; \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{(i\theta)^n(i\tau)^m}{n!m!}\,\langle\, x^n y^m\,\rangle \tag{2.7}$$

and therefore

$$\langle\, x^n y^m\,\rangle \;=\; \frac{1}{i^n i^m}\quad\frac{\partial^{n+m}}{\partial\theta^n\partial\tau^m}\;M(\theta,\tau)\,\bigg|_{\theta,\tau\,=\,0} \tag{2.8}$$

We now explain the main idea that will be used for the calculation of the probability distribution of the random force. The basic idea is that the characteristic function method is that it can be used to calculate the probability distribution of a quantity when the quantity is the sum of individual quantities. Specifically, suppose $F(t)$ is the sum of individual quantities, $f_i(t)$,

$$F(t) = \sum_{i=1}^{N} f_i(t) \tag{2.9}$$

and that we know the statistical properties of $f_i(t)$ and we want to obtain the probability distribution of F. For example, we will want to calculate the probability distribution of force at a given time when

$$F(t) = \sum_{i=1}^{N} \left[m_i \omega_i^2 q_i(0) \cos \omega_i t + \omega_i p_i(0) \sin \omega_i t \right] \tag{2.10}$$

and where we are given the probability distribution of $q_i(0)$ and $p_i(0)$. (This will be done in the next chapter and here we just describe the general method). What one does is to calculate the characteristic function of F by way of

$$M_F(\theta; t) \ = \ \langle\, e^{i\theta F(t)} \,\rangle = \langle\, e^{i\theta \sum_{i=1}^{N} f_i(t)} \,\rangle \tag{2.11}$$

where

$$\langle\, e^{i\theta \sum_{i=1}^{N} f_i(t)} \,\rangle = \int \cdots \int e^{i\theta \sum_{i=1}^{N} f_i(t)} P_N(f_1, f_2 ... f_N; t) df_1 df_2 ... df_N \tag{2.12}$$

where $P_N(f_1, f_2 ... f_N; t)$ is the probability distribution of $(f_1, f_2 ... f_N)$. The probability distribution of F is then obtained from

$$P(F; t) \ = \ \frac{1}{2\pi} \int M_F(\theta; t) e^{-i\theta F} \, d\theta \tag{2.13}$$

However, if the joint probability is of the form

$$P_N(f_1, f_2 ... f_N; t) = \prod_{i=1}^{N} P(f_i, t) \tag{2.14}$$

in which case one has that

$$\langle \, e^{i\theta \sum_{i=1}^{N} f_i(t)} \, \rangle = \prod_{i=1}^{N} e^{i\theta f_i(t)} P(f_i, t) df_i \tag{2.15}$$

and therefore

$$M_F(\theta; t) \; = \; M_f^N(\theta) \tag{2.16}$$

The distribution is then

$$P(F; t) \; = \; \frac{1}{2\pi} \int \, M_f^N(\theta; t) \, e^{-i\theta F} \, d\theta \tag{2.17}$$

Also, if $M_f^N(\theta)$ is written as

$$M_f(\theta) = e^{K_f(\theta)} \tag{2.18}$$

one has

$$P(F; t) \; = \; \frac{1}{2\pi} \int \, e^{NK_f(\theta)} \, e^{-i\theta F} \, d\theta \tag{2.19}$$

We emphasize that often f is a function of random variables in which case the probability distribution $P(f, t)$ is just a symbolic way of expressing the probability distribution over those variables. For example, in Eq. (2.17) f is a function of the random variables position, $x_1, x_2 ... x_N$, and momentum, $p_1, p_2 ... p_N$, then by $P(f, t) \, df$ we shall mean that

$$P(f, t) \, df \; = P(x_1, x_2 ... x_N; p_1, p_2 ... p_N) dx_1, dx_2 ... dx_N, dp_1, dp_2 ... dp_N \tag{2.20}$$

The same idea will be used to calculate the joint distribution at two different times. One defines

$$F(t_1) = \sum_{i=1}^{N} f_i(t_1) \quad ; \quad F(t_2) = \sum_{i=1}^{N} f_i(t_2) \tag{2.21}$$

and we obtain the two variable characteristic function by way of

$$\begin{aligned} M_{F_1,F_2}(\alpha,\beta) &= \left\langle e^{i\alpha F(t_1)+i\beta F(t_2)} \right\rangle && (2.22)\\ &= \left\langle e^{i\alpha \sum_{i=1}^{N} f_i(t_1)+i\beta \sum_{i=1}^{N} f_i(t_2)} \right\rangle && (2.23)\\ &= \prod_{i=1}^{N} \left\langle e^{i\alpha f(t_1)+i\beta f(t_2)} \right\rangle && (2.24)\\ &= M^N_{f_1,f_2}(\alpha,\beta) && (2.25) \end{aligned}$$

where

$$M_{f_1,f_2}(\alpha,\beta) = \left\langle e^{i\alpha f(t_1)+i\beta f(t_2)} \right\rangle = \iint e^{i\alpha f_i(t_1)+i\beta f_i(t_2)} P(f_1,f_2;t_1,t_2) df_1 df_2 \tag{2.26}$$

The probability distribution at two different times is then

$$P(F_1,F_2;t_1,t_2) \;=\; \frac{1}{4\pi^2} \iint M^N_{f_1,f_2}(\alpha,\beta)\, e^{-i\alpha F_1 - i\beta F_2}\, d\alpha d\beta \tag{2.27}$$

Similarly, we will be able to calculate the N time joint probability distribution. We define

$$F(t_k) = \sum_{i=1}^{N} f_i(t_k) \tag{2.28}$$

and the N time characteristic function is then

$$M_{F_1,F_2\ldots F_K}(\alpha_1,\alpha_2,\ldots.\alpha_K) = \left\langle e^{i\sum_{k=1}^{K}\alpha_k \sum_{i=1}^{N} f_i(t_k)} \right\rangle \tag{2.29}$$

If we assume dependence as in Eq. (2.28) we have that

$$M_{F_1,F_2...F_K}(\alpha_1,\alpha_2,....\alpha_N) = \left\langle e^{i\alpha F(t_1)+i\beta F(t_2)}\right\rangle \tag{2.30}$$

$$= \left\langle e^{i\sum_{k=1}^{K}\alpha_k\sum_{i=1}^{N}f_i(t_k)}\right\rangle \tag{2.31}$$

$$= \prod_{i=1}^{N}\left\langle e^{i\sum_{k=1}^{K}\alpha_k f_i(t_k)}\right\rangle \tag{2.32}$$

The probability distribution at K different times is then

$$P(F_1,F_2...F_K;t_1,t_2...t_k) = \left(\frac{1}{2\pi}\right)^K \iint M_{F_1,F_2...F_N}(\alpha_1,\alpha_2,....\alpha_K)e^{-i\sum_{k=1}^{K}\alpha_k F_k} \tag{2.33}$$

$$d\alpha_1, d\alpha_2, ...d\alpha_K \tag{2.34}$$

These are the basic equations we will use but, of course, for the quantum case the situation is totally different and that will be considered in a subsequent chapter.

Chapter 3

Ensemble Averaging

The standard FKM harmonic oscillator models [4], assumes that $q_i(0)$ and $p_i(0)$ are stochastic variables that determine the statistical features of the force by ensemble averaging over those quantities. It treats m_i and ω_i as fixed variables. To make this problem more general, we treat all these four variables as stochastic variables with a joint distribution function $P_i(m_i, \omega_i, q_i(0), p_i(0))$. However, generally, we assume that

$$P_i(m_i, \omega_i, q_i(0), p_i(0)) = P(m_i, \omega_i) P_i(q_i(0), p_i(0) | m_i, \omega_i) \tag{3.1}$$

where $P_i(q_i(0), p_i(0)|m_i, \omega_i)$ is the conditional probability distribution of $(q_i(0), p_i(0)$ for a given m_i, ω_i and where $P(m_i, \omega_i)$ is the probability distribution of m_i, ω_i. We note that $P(m_i, \omega_i)$ is independent of $q_i(0), p_i(0)$.

Here we assume the conditional probability distribution of $q_i(0)$ and $p_i(0)$ satisfies the canonical distribution [8]

$$P_i(q_i(0), p_i(0)|m_i, \omega_i) = \frac{e^{-\frac{1}{kT} H_i(m_i, \omega_i, q_i(0), p_i(0))}}{\int e^{-\frac{1}{kT} H_i(m_i, \omega_i, q_i(0), p_i(0))} dq_i(0) dp_i(0))} \tag{3.2}$$

where k is the Boltzmann constant, T is temperature, and H_i is the Hamiltonian of an individual oscillator given by

$$H_i = \frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2 q_i^2}{2} \tag{3.3}$$

The integral inside Eq. (3.2) can be carried out

$$\int e^{-\frac{1}{kT} H_i(m_i,\omega_i,q_i(0),p_i(0))} dq_i(0) dp_i(0)) = \frac{2\pi kT}{\omega_i} \tag{3.4}$$

and therefore

$$P_i(q_i(0), p_i(0)|m_i, \omega_i) = \frac{\omega_i}{2\pi kT} e^{-\frac{1}{kT} H_i(m_i,\omega_i,q_i(0),p_i(0))} \tag{3.5}$$

For example, we can calculate the mean value and variance of individual force. For the mean we have that

$$\langle f_i \rangle = \int [m_i \omega_i^2 q_i(0) \cos \omega_i t + \omega_i p_i(0) \sin \omega_i t] P_i(m_i, \omega_i) e^{-\frac{1}{kT} H_i(m_i,\omega_i,q_i(0),p_i(0))} \tag{3.6}$$

$$dm_i d\omega_i dq_i(0) dp_i(0) \tag{3.7}$$

$$= 0 \tag{3.8}$$

and for the second moment,

$$< f_i^2 >= kT \int m_i \omega_i^2 P_i(m_i, \omega_i) dm_i d\omega_i \tag{3.9}$$

$$= kT < m_i \omega_i^2 > \tag{3.10}$$

In the next chapter we explicitly calculate the probability distribution function of the force.

Chapter 4

Probability Distribution of Force of One Oscillator

To obtain the probability distribution of force we first calculate the characteristic function. We substitute Eq. (2.10) into Eq. (2.2), to obtain

$$M_{f_i}(\theta) = \int e^{i\theta f_i} P_i(m_i, \omega_i, q_i(0), p_i(0)) dm_i d\omega_i dq_i(0) dp_i(0) \tag{4.1}$$

Here we again assume the initial condition $q_i(0)$ and $p_i(0)$ are in a thermal equilibrium state, so we use the probability distribution function, Eq. (3.2), as discussed in the previous chapter. Substituting Eq. (3.2) into Eq. (4.1) we have

$$M_{f_i}(\theta) = \int e^{i\theta f_i} \frac{\omega_i}{2\pi kT} e^{-\frac{1}{kT} H_i(m_i, \omega_i, q_i(0), p_i(0))} P_i(m_i, \omega_i) dm_i d\omega_i dq_i(0) dp_i(0) \tag{4.2}$$

where

$$H_i(m_i, \omega_i, q_i(0), p_i(0)) = \frac{1}{2} m_i \omega_i^2 q_i^2(0) + \frac{1}{2m_i} p_i^2(0) \tag{4.3}$$

Substituting for f_i, as given by Eq. (2.10), we have

$$M_{f_i}(\theta) = \frac{\omega_i}{2\pi kT} \int e^{i\theta(m_i\omega_i^2 q_i(0)\cos\omega_i t + \omega_i p_i(0)\sin\omega_i t) - \frac{1}{kT}H_i(m_i,\omega_i,q_i(0),p_i(0))} \tag{4.4}$$

$$P_i(m_i,\omega_i)dm_i d\omega_i dq_i(0)dp_i(0) \tag{4.5}$$

Integrating over $q_i(0)$ and $p_i(0)$ one obtains

$$M_{f_i}(\theta) = \iint e^{-\theta^2 kT m_i\omega_i^2/2} P_i(m_i,\omega_i)dm_i d\omega_i \tag{4.6}$$

This is the characteristic function of an individual oscillator. It is easy to see this will become Gaussian if the probability distribution function $P_i(m_i,\omega_i)$ is a delta function. That is, if

$$P_i(m_i,\omega_i) = \delta(m_i - m_i')\delta(\omega_i - \omega_i') \tag{4.7}$$

in which case we have

$$M_{f_i}(\theta) = e^{-\theta^2 kT m_i'\omega_i'^2/2} \tag{4.8}$$

which is the characteristic function of a Gaussian distribution.

Therefore under stochastic oscillator model, the probability distribution of a single force is not necessarily a Gaussian distribution. The probability distribution is given by

$$P_i(f_i) = \frac{1}{2\pi}\iiint e^{-i\theta f_i} e^{-\theta^2 kT m_i\omega_i^2/2} P_i(m_i,\omega_i)dm_i d\omega_i d\theta \tag{4.9}$$

$$= \frac{1}{\sqrt{2\pi kT}}\iint \frac{1}{\sqrt{m_i\omega_i^2}} e^{-\frac{f_i^2}{2kTm_i\omega_i}} P_i(m_i,\omega_i)dm_i d\omega_i \tag{4.10}$$

This, in general, is not a Gaussian distribution function unless $P_i(m_i,\omega_i)$ is a delta function as per Eq. (4.7).

We can calculate the mean and variance using Eq. (3.5) and compare to what we obtained in Eq. (3.8) and Eq. (3.10). For the average force we have

$$< f_i >= \int_{-\infty}^{\infty} f_i P(f_i) df_i \tag{4.11}$$

$$= \frac{1}{\sqrt{2\pi kT}} \int_{-\infty}^{\infty} f_i \frac{1}{\sqrt{m_i \omega_i^2}} e^{-\frac{f_i^2}{2kTm_i\omega_i}} P_i(m_i, \omega_i) dm_i d\omega_i df_i = 0 \tag{4.12}$$

and for the second moment we have

$$< f_i^2 >= \int_{-\infty}^{\infty} f_i^2 P(f_i) df_i \tag{4.13}$$

$$= \frac{1}{\sqrt{2\pi kT}} \int_{-\infty}^{\infty} f_i^2 \frac{1}{\sqrt{m_i \omega_i^2}} e^{-\frac{f_i^2}{2kTm_i\omega_i}} P_i(m_i, \omega_i) dm_i d\omega_i df_i \tag{4.14}$$

$$= kT \int m_i \omega_i^2 P_i(m_i, \omega_i) dm_i d\omega_i \tag{4.15}$$

$$= kT < m_i \omega_i^2 > \tag{4.16}$$

These are the same as Eq. (3.8) and (3.10).

An important property of the distribution of force, Eq. (4.9), is that it is time independent. The reason for this is because of the peculiar form of the distribution of initial velocities. In the next chapter we explicitly calculate the force with different initial distributions, that is other then Eq. (3.5) and explicitly show the time dependence.

Chapter 5

Classical Distribution with Non-Cononical Initial Distribution

We now take probability distributions other then Eq. (3.5). We do two different cases. For convenience we repeat Eq. (4.1) here

$$M_{f_i}(\theta) = \int e^{i\theta f_i} P_i(q_i(0), p_i(0)|m_i, \omega_i) P_i(m_i, \omega_i) dm_i d\omega_i dq_i(0) dp_i(0) \tag{5.1}$$

We take two different probability distributions for $P_i(q_i(0), p_i(0)|m_i, \omega_i)$ and call them case 1 and 2.

Case 1

We take the probability distribution of $q_i(0)$ to be uniformly distributed between $-Q$ and Q , and $p_i(0)$ to be normally distributed. In particular,

$$P_i(q_i(0), p_i(0)|m_i, \omega_i) = \frac{e^{-p_i^2(0)/\sigma^2(m_i,\omega_i)}}{2Q\sqrt{\pi\sigma^2(m_i, \omega_i)}} \tag{5.2}$$

For the characteristic function we have

$$M_{f_i}(\theta) = \int \frac{1}{2Q\sqrt{\pi\sigma^2(m_i,\omega_i)}} \int_{-\infty}^{\infty}\int_{-Q}^{Q} e^{i\theta(m_i\omega_i^2 q_i(0)\cos\omega_i t+\omega_i p_i(0)\sin\omega_i t)-p_i^2(0)/\sigma^2(m_i,\omega_i)} \tag{5.3}$$

$$dq_i(0)dp_i(0)P_i(m_i,\omega_i)dm_i d\omega_i \tag{5.4}$$

$$= \int \frac{1}{m_i Q\theta\omega_i^2} e^{-\frac{1}{4}\theta^2\omega_i^2\sin^2\omega_i t\sigma^2(m_i,\omega_i)} \sec\omega_i t \sin(m_i\omega_i^2 Q\theta\cos\omega_i t)P_i(m_i,\omega_i)dm_i d\omega_i \tag{5.5}$$

and hence the probability distribution is

$$P(f_i) = \frac{1}{2\pi}\int M_{f_i}(\theta)e^{-i\theta f_i}d\theta P_i(m_i,\omega_i)dm_i d\omega_i \tag{5.6}$$

$$= \int \frac{1}{4m_i\omega_i^2 Q\cos\omega_i t}\left[\mathrm{erf}\left(\frac{-f_i+m_i\omega_i^2 Q\cos\omega_i t}{|\sigma(m_i,\omega_i)\omega_i\sin\omega_i t|}\right)+\mathrm{erf}\left(\frac{f_i+m_i\omega_i^2 Q\cos\omega_i t}{|\sigma(m_i,\omega_i)\omega_i\sin\omega_i t|}\right)\right] \tag{5.7}$$

$$P_i(m_i,\omega_i)dm_i d\omega_i \tag{5.8}$$

where erf(z) is the error function,

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-x^2}dx \tag{5.9}$$

Note that the probability distribution is now not time independent.

For this case the mean and second moment are respectively

$$< f_i >= \int_{-\infty}^{\infty} f_i P(f_i)df_i = 0 \tag{5.10}$$

$$\left\langle f_i^2 \right\rangle = \int_{-\infty}^{\infty} f_i^2 P(f_i) df_i \tag{5.11}$$

$$= \int_{-\infty}^{\infty}\int_{-Q}^{Q} (m_i\omega_i^2 q_i \cos\omega_i at + \omega_i p_i \sin\omega_i at)^2 \frac{e^{-p_i^2/\sigma_i^2}}{2Q\sqrt{\pi\sigma_i^2}} P_i(m_i,\omega_i) dm_i d\omega_i dq dp \tag{5.12}$$

$$= \int \frac{\omega_i^2(2m_i^2Q^2\omega_i^2\cos^2\omega_i + 3\sigma^2\sin^2\omega_i at)}{6} P_i(m_i,\omega_i) dm_i d\omega_i \tag{5.13}$$

Case 2

We take

$$P_i(q_i(0), p_i(0)|m_i,\omega_i) = \frac{\sqrt{AB}}{\pi} e^{-Ap_i^2(0) - Bq_i^2(0)} \tag{5.14}$$

where A and B are positive constants and functions of m and ω. The characteristic function is

$$M_{f_i}(\theta) = \frac{\sqrt{AB}}{\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\theta(m_i\omega_i^2\cos\omega t + \omega q \sin\omega t) - Ap^2 - Bq^2} dp dq \tag{5.15}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{\theta^2\omega^2}{4}(\frac{\sin^2\omega t}{A} + \frac{m^2\omega^2\cos^2\omega t}{B})} P(m,\omega) dm d\omega \tag{5.16}$$

The probability is therefore

$$P(f_i) = \frac{1}{2\pi}\int_{-\infty}^{\infty} M_{f_i}(\theta) e^{-i\theta f_i} d\theta \tag{5.17}$$

$$= \iint \sqrt{\frac{AB}{Am_i^2\pi\omega_i^4\cos^2\omega_i t + B\pi\omega_i^2\sin^2\omega_i t}} \tag{5.18}$$

$$\exp\left[-\frac{AB}{Am_i^2\omega_i^4\cos^2\omega_i t + B\omega_i^2\sin^2\omega_i t} f_i^2\right] P(m_i,\omega_i) dm_i d\omega_i \tag{5.19}$$

Notice that again the solution is time dependent. If we take

$$B = Am_i^2\omega_i^2 \tag{5.20}$$

then the solution is independent of time and in particular we obtain

$$P(f_i) = \iint \sqrt{\frac{B}{m_i^2 \pi \omega_i^4}} \exp\left[-\frac{B}{m_i^2 \omega_i^4} f_i^2\right] P(m_i, \omega_i) dm_i d\omega_i \tag{5.21}$$

The mean and the second moment are

$$\langle f_i \rangle = 0 \tag{5.22}$$

$$\left\langle f_i^2 \right\rangle = \frac{\sqrt{AB}}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (m_i \omega_i^2 q_i \cos \omega_i at + \omega_i p_i \sin \omega_i at)^2 e^{-Ap^2 - Bq^2} dq dp \tag{5.23}$$

$$= \frac{\omega_i^2}{2} \left(\frac{A m_i^2 \omega_i^2 \cos^2 \omega_i at + B \sin^2 \omega_i at}{AB} \right) \tag{5.24}$$

The canonical distribution case, Eq. (3.5), is obtained when we set

$$A = \frac{1}{2 m_i kT} \qquad B = \frac{m_i \omega_i^2}{2kT} \tag{5.25}$$

in which case

$$\langle f_i \rangle = 0 \tag{5.26}$$

$$\left\langle f_i^2 \right\rangle = m \omega^2 kT \tag{5.27}$$

Chapter 6

Probability Distribution of Force Due to N Oscillators

If we assume there is no external field at the origin, the total force due to the bath is the sum of the individual forces. In the case where there are N oscillators connected to the origin and each one has its own distribution function of m_i and ω_i, the total force is

$$F = \sum_{i=1}^{N} f_i = \sum_{i=1}^{N} \left[m_i \omega_i^2 q_i(0) \cos \omega_i t + \omega_i p_i(0) \sin \omega_i t \right] \tag{6.1}$$

If we assume all the oscillators are independent of each other, the joint distribution function of all oscillators is the product of individual oscillator

$$P(m_1 ..., \omega_1 ..., q_i(0) ..., p_i(0)) = \prod_{i=1}^{N} P_i(m_i, \omega_i, q_i(0), p_i(0)) \tag{6.2}$$

Using Eq. (3.5) this becomes

$$P(m_1...,\omega_1...,q_i(0)...,p_i(0)) = \prod_{i=1}^{N} P_i(m_i,\omega_i)\frac{\omega_i}{2\pi kT}e^{-\frac{1}{kT}H_i(m_i,\omega_i,q_i(0),p_i(0))} \tag{6.3}$$

$$= \frac{1}{(2\pi kT)^N}e^{-\frac{1}{kT}\sum_{i=1}^{N}H_i(m_i,\omega_i,q_i(0),p_i(0))}\prod_{i=1}^{N}\omega_i P_i(m_i,\omega_i) \tag{6.4}$$

Because of the assumption that all oscillators are independent, we can treat the individual force as independent random variables. Therefore the characteristic function of the total force can be calculated by using Eq. (4.8)

$$M_F(\theta) = \prod_{i=1}^{N} M_{f_i}(\theta) = \prod_{i=1}^{N}\int e^{-\theta^2 kT m_i\omega_i^2/2}P_i(m_i,\omega_i)dm_i d\omega_i \tag{6.5}$$

We rewrite the product as a summation in the exponent to obtain

$$M_F(\theta) = \int e^{-\theta^2\frac{kT}{2}\sum_{i=1}^{N}m_i\omega_i^2}\prod_{i=1}^{N}P_i(m_i,\omega_i)dm_i d\omega_i \tag{6.6}$$

We now calculate the probability distribution function of the total force. Using Eq. (2.4) the probability distribution function is

$$P(F) = \frac{1}{2\pi}\int e^{-i\theta F}e^{-\theta^2\frac{kT}{2}\sum_{j=1}^{N}m_j\omega_j^2}\prod_{i=1}^{N}P_i(m_i,\omega_i)dm_i d\omega_i d\theta \tag{6.7}$$

The integral over θ can be carried out without explicitly knowing $P_i(m_i,\omega_i)$,

$$P(F) = \frac{1}{\sqrt{2\pi kT}}\int \frac{1}{\sqrt{\sum_{j=1}^{N}m_j\omega_j^2}}e^{-\frac{F^2}{2kT\sum_{j=1}^{N}m_j\omega_j^2}}\prod_{i=1}^{N}P_i(m_i,\omega_i)dm_i d\omega_i \tag{6.8}$$

From this result we can see that if

$$\sum_{i=1}^{N} m_i \omega_i^2 = \text{constant}, \tag{6.9}$$

the total force would be always be Gaussian function regardless of individual $P_i(m_i, \omega_i)$.

The probability distribution function of the total force can also be carried out by calculating the convolution of the probability functions of the individual forces. This is well known and is derived from the characteristic function. For simplicity we consider two forces. The probability function of summation of this two forces is

$$\begin{aligned} P(f) &= \int_{-\infty}^{\infty} P_1(f_1) P_2(f - f_1) df_1 && (6.10) \\ &= \int \frac{e^{-\frac{f^2}{2kT(m_1\omega_1^2 + m_2\omega_2^2)}}}{\sqrt{2\pi kT(m_1\omega_1^2 + m_2\omega_2^2)}} P_1(m_1, \omega_1) P(m_2, \omega_2) dm_1 d\omega_1 dm_2 d\omega_2 && (6.11) \end{aligned}$$

where we have used the fact that

$$\int_{-\infty}^{\infty} e^{-x^2/A} e^{-(y-x)^2/B} dx = \sqrt{\frac{\pi AB}{A+B}} e^{-\frac{y^2}{A+B}} \tag{6.12}$$

If we extend this method to N forces, the result is same as Eq. (6.4).

Chapter 7

Probability distribution of Force: Statistical Properties

In the last chapter we found the distribution function for the total force, Eq. (6.4). We now calculate the mean value and variance of the total force. We have

$$< F >= \frac{1}{\sqrt{2\pi kT}} \int_{-\infty}^{\infty} F \frac{1}{\sqrt{\sum_{j=1}^{N} m_j \omega_j^2}} e^{-\frac{F^2}{2kT \sum_{j=1}^{N} m_j \omega_j^2}} \prod_{i=1}^{N} P_i(m_i, \omega_i) dm_i d\omega_i dF \tag{7.1}$$

This is seen to be zero,

$$< F >= 0 \tag{7.2}$$

Now consider

$$< F^2 >= \frac{1}{\sqrt{2\pi kT}} \int_{-\infty}^{\infty} F^2 \frac{1}{\sqrt{\sum_{j=1}^{N} m_j \omega_j^2}} e^{-\frac{F^2}{2kT \sum_{j=1}^{N} m_j \omega_j^2}} \prod_{i=1}^{N} P_i(m_i, \omega_i) dm_i d\omega_i dF \tag{7.3}$$

Doing the integral results in

$$< F^2 >= kT \int \sum_{j=1}^{N} m_j \omega_j^2 \prod_{i=1}^{N} P_i(m_i, \omega_i) dm_i d\omega_i \tag{7.4}$$

Since $P_i(m_i, \omega_i)$ is a probability distribution function, we assume it is normalized

$$\int P_i(m_i, \omega_i) dm_i d\omega_i = 1 \tag{7.5}$$

and therefore, for each term when $i \neq j$, the integrals are equal to one. Hence,

$$\int m_j \omega_j^2 \prod_{i=1}^{N} P_i(m_i, \omega_i) dm_i d\omega_i = \int m_i \omega_i^2 P_i(m_i, \omega_i) dm_i d\omega_i \tag{7.6}$$

$$< F^2 >= kT \sum_{i=1}^{N} \int m_i \omega_i^2 P_i(m_i, \omega_i) dm_i d\omega_i \tag{7.7}$$

$$= kT \sum_{i=1}^{N} < m_i \omega_i^2 > \tag{7.8}$$

This result is the summation of individual forces since we assumed individual oscillators are independent.

We now assume that

$$\sum_{i=1}^{N} m_i \omega_i^2 = \text{constant=c=N} m_i \omega_i^2 = N < m_i \omega_i^2 > \tag{7.9}$$

This assumption is often used [1], in which case we have

$$P(F) = \frac{1}{\sqrt{2\pi kcT}} e^{-\frac{F^2}{2kTc}} \tag{7.10}$$

and we have that

$$< f_i >= \int_{-\infty}^{\infty} f_i P(f_i) df_i = 0 \tag{7.11}$$

$$< f_i^2 >= \int_{-\infty}^{\infty} f_i^2 P(f_i) df_i = kT < m_i \omega_i^2 > \tag{7.12}$$

Chapter 8

Joint Distribution Function for Force at Two Different Times and the Autocorrelation Function Due to N Oscillators

In the previous chapter we have calculated the probability distribution function of force due to one particle and total force due to N particles in the independent oscillator model. The result shows that the random force in this model is first-order stationary random process because the distribution function is time independent. To prove that this process is also second-order stationary, we need to show the joint distribution function of two forces at two different times only depends on the time interval.

Similar to the method used to obtain single force distribution function, we now calculate the joint distribution function by first calculating the characteristic function. Consider the two time characteristic function of $F(t)$. We write

$$F(t_1) = \sum_{i=1}^{N} f_i(t_1) \quad ; \quad F(t_2) = \sum_{i=1}^{N} f_i(t_2) \tag{8.1}$$

and the joint characteristic function is

$$M_{F_1,F_2}(\alpha,\beta) = \left\langle e^{i\alpha F(t_1)+i\beta F(t_2)} \right\rangle \tag{8.2}$$

$$= \left\langle e^{i\alpha \sum_{i=1}^{N} f_i(t_1)+i\beta \sum_{i=1}^{N} f_i(t_2)} \right\rangle \tag{8.3}$$

$$= \prod_{i=1}^{N} \left\langle e^{i\alpha f_i(t_1)+i\beta f_i(t_2)} \right\rangle \tag{8.4}$$

If all oscillators are independent of each other

$$M_{F_1,F_2}(\alpha,\beta) = M^N_{f_1,f_2}(\alpha,\beta) \tag{8.5}$$

where

$$M_{f_1,f_2}(\alpha,\beta) = \left\langle e^{i\alpha f(t_1)+i\beta f(t_2)} \right\rangle = \iint e^{i\alpha f(t_1)+i\beta f(t_2)} P(f_1,f_2;t_1,t_2) df_1 df_2 \tag{8.6}$$

The joint probability distribution of the force at two different times is therefore

$$P(F_1,F_2;t_1,t_2) \;=\; \frac{1}{4\pi^2} \iint M^N_{f_1,f_2}(\alpha,\beta)\, e^{-i\alpha F_1 - i\beta F_2}\, d\theta\, d\tau \tag{8.7}$$

We can simplify this further. Consider the two time characteristic function for a single oscillator. We have

$$\mathbf{f}(t_1) = qm\omega^2 \cos\omega t_1 + \omega p \sin\omega t_1 \tag{8.8}$$

$$\mathbf{f}(t_2) = qm\omega^2 \cos\omega t_2 + \omega p \sin\omega t_2 \tag{8.9}$$

and further

$$\alpha\mathbf{f}(t_1)+\beta\mathbf{f}(t_2) = \alpha(qm\omega^2\cos\omega t_1+\omega p\sin\omega t_1)+\beta qm\omega^2\cos\omega t_2+\omega p\sin\omega t_2 \tag{8.10}$$

$$= qm\omega^2(\alpha\cos\omega t_1+\beta\cos\omega t_2)+\omega p(\alpha\sin\omega t_1+\beta\sin\omega t_2) \tag{8.11}$$

Therefore, the characteristic function, $M_{f_1,f_2}(\alpha,\beta)$, is

$$M_{f_1,f_2}(\alpha,\beta) = \frac{\omega}{2\pi kT}\iint \exp \tag{8.12}$$

$$\left[-\frac{H(q,p)}{kT}+iqm\omega^2(\alpha\cos\omega t_1+\beta\cos\omega t_2)+i\omega p(\alpha\sin\omega t_1+\beta\sin\omega t_2)\right]dqdp \tag{8.13}$$

$$= \exp\left[-\frac{(m\omega^2)^2(\alpha\cos\omega t_1+\beta\cos\omega t_2)^2}{2\omega^2/mkT}-\frac{\omega^2(\alpha\sin\omega t_1+\beta\sin\omega t_2)^2}{2/mkT}\right] \tag{8.14}$$

$$= \exp\left[-\tfrac{1}{2}mkT\omega^2\left\{(\alpha\cos\omega t_1+\beta\cos\omega t_2)^2+(\alpha\sin\omega t_1+\beta\sin\omega t_2)^2\right\}\right] \tag{8.15}$$

$$= \exp\left[-\tfrac{1}{2}mkT\omega^2\left\{\alpha^2+\beta^2+2\alpha\beta(\cos\omega t_1\beta\cos\omega t_2+\sin\omega t_1\sin\omega t_2)\right\}\right] \tag{8.16}$$

$$= \exp\left[-\tfrac{1}{2}mkT\omega^2\left\{\alpha^2+\beta^2+2\alpha\beta\cos\omega(t_2-t_1)\right\}\right] \tag{8.17}$$

or

$$M_{f_1,f_2}(\alpha,\beta) \;=\; \exp\left[-\tfrac{1}{2}mkT\omega^2\left\{\alpha^2+\beta^2+2\alpha\beta\cos\omega(t_2-t_1)\right\}\right] \tag{8.18}$$

Now making the assumption that all the oscillators are independent of each other we use Eq. (8.4) to obtain

$$M_F(\alpha,\beta) = M_f^N(\alpha,\beta) \;=\; \exp\left[-\frac{1}{2}NmkT\omega^2\left\{\alpha^2+\beta^2+2\alpha\beta\cos\omega(t_2-t_1)\right\}\right] \tag{8.19}$$

The random variables are m_i,ω_i, $q_i(0)$ and $p_i(0)$ and hence

$$M(\alpha,\beta) = \int e^{i\alpha F(t_1)+i\beta F(t_2)} P_i(m_i,\omega_i,q_i(0),p_i(0)) dm_i d\omega_i dq_i(0) dp_i(0) \tag{8.20}$$

substitute for both forces from Eq. (8.1),

$$\begin{aligned} M_F(\alpha,\beta) = \int \exp[i \sum_{i=1}^{N} m_i\omega_i^2(\alpha\cos\omega_i t_1 + \beta\cos\omega_i t_2) q_i(0) \\ + i\sum_{i=1}^{N} \omega_i(\alpha\sin\omega_i t_1 + \beta\sin\omega_i t_2) p_i(0)] \qquad (8.21) \\ \prod_{i=1}^{N} P_i(m_i,\omega_i,q_i(0),p_i(0)) dm_i d\omega_i dq_i(0) dp_i(0) \qquad (8.22) \end{aligned}$$

The summation in the exponent can be rewritten as a product, giving

$$\begin{aligned} M_F(\alpha,\beta) = \prod_{i=1}^{N} \frac{\omega_i}{2\pi kT} \int \qquad (8.23) \\ \exp[i m_i\omega_i^2(\alpha\cos\omega_i t_1 + \beta\cos\omega_i t_2) q_i(0) + i\omega_i(\alpha\sin\omega_i t_1 + \beta\sin\omega_i t_2) p_i(0) \qquad (8.24) \\ - \frac{1}{kT} H_i(m_i,\omega_i,q_i(0),p_i(0))] P_i(m_i,\omega_i) dm_i d\omega_i dq_i(0) dp_i(0) \qquad (8.25) \end{aligned}$$

The integral over $q_i(0)$ and $p_i(0)$ yields

$$M_F(\alpha,\beta) = \prod_{i=1}^{N} \int e^{-\frac{kTm_i\omega_i^2}{2}[\alpha^2+\beta^2+2\alpha\beta\cos\omega_i(t_1-t_2)]} P_i(m_i,\omega_i) dm_i d\omega_i \tag{8.26}$$

We now rewrite the product as a summation in the following way,

$$M(\alpha,\beta) = \int e^{-\sum_{i=1}^{N}\frac{kTm_i\omega_i^2}{2}[\alpha^2+\beta^2+2\alpha\beta\cos\omega_i(t_1-t_2)]} \prod_{i=1}^{N} P_i(m_i,\omega_i) dm_i d\omega_i \tag{8.27}$$

This joint characteristic function is only a function of the difference in time, t_1- t_2, and therefore this is a second-order stationary random process.

The joint distribution function is

$$P(F_1, F_2) = \frac{1}{(2\pi)^2} \int M(\alpha, \beta) e^{-i\alpha F_1 - i\beta F_2} d\alpha d\beta \tag{8.28}$$

$$= \frac{1}{(2\pi)^2} \int e^{-\sum_{i=1}^{N} \frac{kTm_i\omega_i^2}{2}[\alpha^2+\beta^2+2\alpha\beta\cos\omega_i(t_1-t_2)]-i\alpha F_1-i\beta F_2} \prod_{i=1}^{N} P_i(m_i, \omega_i) dm_i d\omega_i d\alpha d\beta \tag{8.29}$$

We now rewrite this in terms of the standard 2-D joint Gaussian distribution,

$$P(x, y) = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-r^2}} e^{-\frac{1}{2(1-r^2)}\left[\frac{(x-a)^2}{\sigma_x^2}+\frac{(y-b)^2}{\sigma_y^2}-2r\frac{(x-a)(y-b)}{\sigma_x\sigma_y}\right]} \tag{8.30}$$

where r is correlation coefficient which satisfies $|r| < 1$, a and b are the mean value of x and y, and where σ_x and σ_y are the corresponding standard deviations. The characteristic function of this Gaussian distribution is

$$M(\alpha, \beta) = e^{ia\alpha+ib\beta-\frac{1}{2}(\sigma_x^2\alpha^2+2r\sigma_x\sigma_y\alpha\beta+\sigma_y^2\beta^2)} \tag{8.31}$$

Comparing the standard Gaussian characteristic function with the function inside our integral, Eq. (8.29), we have that

$$a = 0 \tag{8.32}$$

$$b = 0 \tag{8.33}$$

$$\sigma^2 = \sigma_x^2 = \sigma_y^2 = kT \sum_{i=1}^{N} m_i\omega_i^2 \tag{8.34}$$

$$r = \frac{\sum_{i=1}^{N} m_i\omega_i^2 \cos\omega_i(t_1 - t_2)}{\sum_{i=1}^{N} m_i\omega_i^2} \tag{8.35}$$

Using this result in our integral, the joint distribution function, Eq. (8.27) can be written as

$$P(F_1,F_2)=\int\frac{1}{2\pi\sigma^2\sqrt{1-r^2}}e^{-\frac{1}{2(1-r^2)\sigma^2}(F_1^2+F_2^2-2rF_1F_2)}\prod_{i=1}^{N}P_i(m_i,\omega_i)dm_id\omega_i \tag{8.36}$$

This distribution function has only two parameters σ and r.

Autocorrelation function.

We now calculate the the autocorrelation function, $< F_1F_2 >$, between the two forces

$$< F_1F_2 >=\int F_1F_2P(F_1,F_2)dF_1dF_2 \tag{8.37}$$

If we do the integral over F_1 and F_2 first, the result is similar autocorrelation function of two Gaussian correlated variable.

$$< F_1^2 >=\int r\sigma^2\prod_{i=1}^{N}P_i(m_i,\omega_i)dm_id\omega_i \tag{8.38}$$

$$< F_1F_2 >=kT\int\sum_{j=1}^{N}m_j\omega_j^2\cos\omega_j(t_1-t_2)\prod_{i=1}^{N}P_i(m_i,\omega_i)dm_id\omega_i \tag{8.39}$$

Because the $P_i(m_i,\omega_i)$ is a normalized probability distribution function, when $i\neq j$, the integral equals one, and we have that

$$< F_1F_2 >=kT\sum_{i=1}^{N}\int m_i\omega_i^2\cos\omega_i(t_1-t_2)P_i(m_i,\omega_i)dm_id\omega_i \tag{8.40}$$

$$=kT\sum_{i=1}^{N}< m_i\omega_i^2\cos\omega_i(t_1-t_2) > \tag{8.41}$$

This result is a summation of expected value of single oscillator autocorrelation. So the result is determined by what is summation and what is the expected value of $m_i\omega_i^2\cos\omega_i(t_1-$

t_2). Now we separate this problem into two different cases, where the result is only affected by one of these two calculations.

Case 1. The first case is that each individual oscillator has constant values of m'_i and ω'_i. Therefore the probability distribution function $P_i(m_i, \omega_i)$ is a delta function.

$$P_i(m_i, \omega_i) = \delta(\omega_i - \omega'_i)\delta(m_i - m'_i) \tag{8.42}$$

and the autocorrelation function is

$$< F_1 F_2 >= NkT \sum_{i=1}^{N} m'_i \omega'^2_i \cos \omega'_i (t_1 - t_2) \tag{8.43}$$

When N goes to infinity, this summation can be written as an integral. If we assume the density function of m'_i and ω'_i is $D(m, \omega)$ we have

$$< F_1 F_2 >= NkT \int D(m, \omega) m\omega^2 \cos \omega (t_1 - t_2) dm d\omega \tag{8.44}$$

Case 2. In the second case, we assume all the expected values of the individual oscillators have the same value, which means all individual oscillators have same distribution function $P_i(m_i, \omega_i)$ which we write as $P(m, \omega)$. The summation in Eq. (8.43) then becomes

$$\begin{aligned} < F_1 F_2 > &= NkT < m\omega^2 \cos \omega (t_1 - t_2) > && (8.45) \\ &= NkT \iint P(m, \omega) m\omega^2 \cos \omega (t_1 - t_2) dm d\omega && (8.46) \end{aligned}$$

Comparing Eq. (8.43) with Eq. (8.46), the above two cases would have the same autocorrelation function if $D(m, \omega)$ and $P(m, \omega)$ satisfies

$$D(m, \omega) = P(m, \omega) \tag{8.47}$$

White noise.

We now ask whether Eq. (8.46) can yield white noise. For white noise the autocorrelation function should be a delta function of $t_1 - t_2$. For that to be the case $P(m, \omega)m\omega^2$ should be a constant. We assume this constant is C and write

$$P(m, \omega) = \frac{C}{m\omega^2} \tag{8.48}$$

However this can be satisfied by the follwing condition on $P(m, \omega)$

$$\int P(m, \omega) dm d\omega = \int \frac{C}{m\omega^2} dm d\omega = \tag{8.49}$$

$$= 2C[\ln m_{max} - \ln m_{min}][\frac{1}{\omega_{min}} - \frac{1}{\omega_{max}}] = 1 \tag{8.50}$$

Therfore

$$C = \frac{1}{2[\frac{1}{\omega_{min}} - \frac{1}{\omega_{max}}][\ln m_{max} - \ln m_{min}]} \tag{8.51}$$

Hence we see ω can have no upper bound. When ω gooes to infinity

$$C = \frac{\omega_{min}}{2[\ln m_{max} - \ln m_{min}]} \tag{8.52}$$

Chapter 9

Statistical Properties

We now list some standard properties of two dimensional Gaussian distribution and apply them to our case as developed in the previous chapter. We repeat here the standard two dimensional Gaussian distribution

$$P(x,y) = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-r^2}} \exp\left[-\frac{1}{2(1-r^2)}\left\{\frac{(x-a)^2}{\sigma_x^2} + \frac{(y-b)^2}{\sigma_y^2} - 2r\frac{(x-a)(y-b)}{\sigma_x\sigma_y}\right\}\right] \tag{9.1}$$

In Eq. (9.1) r is the correlation coefficient and satisfies $|r| \leq 1$. The characteristic function of $P(x,y)$ is

$$M(\theta,\tau) \ = \exp\left[\, ia\theta + ib\tau - \tfrac{1}{2}(\sigma_x^2\theta^2 + 2r\sigma_x\sigma_y\theta\tau + \sigma_y^2\tau^2)\,\right] \tag{9.2}$$

and the marginals are

$$P(x) = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp\left[-\frac{(x-a)^2}{2\sigma_x^2}\right] \tag{9.3}$$

$$P(y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left[-\frac{(x-a)^2}{2\sigma_y^2}\right] \tag{9.4}$$

The conditional distribution, defined by

$$P(y|x) = \frac{P(x,y)}{P(x)} \tag{9.5}$$

is given by

$$P(y|x) = \frac{1}{\sqrt{2\pi\sigma_y^2}\sqrt{1-r^2}} \exp\left[-\frac{1}{2\sigma_y^2(1-r^2)}\left(y - b - r\frac{\sigma_y}{\sigma_x}(x-a)\right)^2\right] \tag{9.6}$$

In addition, we list some other standard properties,

$$E[(x-a)(y-b)) = r\sigma_x\sigma_y \tag{9.7}$$

$$E[y|x) = b + r\frac{\sigma_y}{\sigma_x}(x-a) \tag{9.8}$$

$$E[y^2|x) = \sigma_y^2(1-r^2) + \left\{b + r\frac{\sigma_y}{\sigma_x}(x-a)\right\}^2 \tag{9.9}$$

$$E[\sigma_y^2|x) = \sigma_y^2(1-r^2) \tag{9.10}$$

We now apply these formulas to our case. Comparing Eq. (8.17) with Eq. (9.2) we have that

$$P(F_1, F_2; t_1, t_2) = \frac{1}{2\pi\sigma^2\sqrt{1-r^2}} \exp\left[-\frac{1}{2(1-r^2)\sigma^2}\left(F_1^2 + F_2^2 - 2rF_1F_2\right)\right] \tag{9.11}$$

with

$$r = \cos\omega(t_2 - t_1) \tag{9.12}$$

$$\sigma^2 = NmkT\omega^2 \tag{9.13}$$

Eq. (9.11) can be written as

$$P(F_1, F_2; t_1, t_2) = \frac{1}{2\pi \left|\sin\omega(t_2 - t_1)\right| \sigma^2} \tag{9.14}$$

$$\exp\left\{-\frac{1}{2\left|\sin\omega(t_2 - t_1)\right|\sigma^2}\left[F_1^2 + F_2^2 - 2\cos\omega(t_2 - t_1)F_1F_2\right]\right\} \tag{9.15}$$

Also, we have that the conditional distribution is

$$E[F_2|F_1) = \cos\omega(t_2 - t_1)F_1 \tag{9.16}$$

and the autocorrelation function is

$$\langle F_1F_2\rangle = NmkT\omega^2\cos\omega(t_2 - t_1) \tag{9.17}$$

which shows that it is a stationary process. The conditional distribution is given by,

$$P(F_2|F_1) = \frac{1}{\sqrt{2\pi\sin^2\omega(t_2 - t_1)\sigma^2}}\exp\left[-\frac{1}{2\sigma^2\sin^2\omega(t_2 - t_1)}\left(F_2 - \cos\omega(t_2 - t_1)F_1\right)^2\right] \tag{9.18}$$

Chapter 10

Multi-Time Distribution for N Classical Oscillators

We now derive the multiple time distribution function. That is we aim at getting the joint probability distribution of force at K different times. We calculate the N force – K different time characteristic function defined by way of

$$M(\alpha) = E\left[\exp\left[i\sum_{k=1}^{K}\alpha_k F(t_k)\right]\right] \tag{10.1}$$

$$= \int e^{i\sum_{i=1}^{N} m_i\omega_i^2 \sum_k \alpha_k \cos\omega_i t_k q_i(0) + i\sum_{i=1}^{N}\sum_k \alpha_k \sin\omega_i t_k p_i(0)} \tag{10.2}$$

$$\prod_{i=1}^{N} P_i(m_i,\omega_i,q_i(0),p_i(0))dm_i d\omega_i dq_i(0)dp_i(0) \tag{10.3}$$

where α is a M dimension vector and α_k is component of it

$$M(\alpha) = \prod_{i=1}^{N} \frac{\omega_i}{2\pi kT} \int e^{aim_i\omega_i^2 \sum_k \alpha_k \cos\omega_i t_k q_i(0) + i\omega_i \sum_k \alpha_k \sin\omega_i t_k p_i(0) - \frac{1}{kT} H_i(m_i,\omega_i,q_i(0),p_i(0))} \tag{10.4}$$

$$P_i(m_i,\omega_i) dm_i d\omega_i dq_i(0) dp_i(0)$$

$$= \prod_{i=1}^{N} \int e^{-\frac{kTm_i\omega_i^2}{2}[(\sum_k \alpha_k \cos\omega_i t_k)^2 + (\sum_k \alpha_k \sin\omega_i t_k)^2]} P_i(m_i,\omega_i) dm_i d\omega_i \tag{10.5}$$

$$= \prod_{i=1}^{N} \int e^{-\frac{kTm_i\omega_i^2}{2}\sum_{k,l}\alpha_k\alpha_l \cos\omega_i(t_k - t_l)} P_i(m_i,\omega_i) dm_i d\omega_i \tag{10.6}$$

$$= \int e^{-\sum_i \frac{kTm_i\omega_i^2}{2}\sum_{k,l}\alpha_k\alpha_l \cos\omega_i(t_k - t_l)} \prod_{i=1}^{N} P_i(m_i,\omega_i) dm_i d\omega_i \tag{10.7}$$

This is the characteristic function of multivariate Gaussian distribution with Covariance matrix

$$\sigma_{k,l} = kT \sum_{i=1}^{N} m_i\omega_i^2 \cos\omega_i(t_k - t_l) \tag{10.8}$$

The distribution of multiple forces can be written as

$$P(f) = \int \frac{1}{(2\pi)^{M/2}|\sigma|^{1/2}} \exp(-\frac{1}{2} f^T \sigma^{-1} f) \prod_{i=1}^{N} P_i(m_i,\omega_i) dm_i d\omega_i \tag{10.9}$$

Chapter 11

Quantum Characteristic Function Method

The quantum case presents a number of new features [10, 11, 12, 13, 14, 15]. The fundamental issue is that we have operators instead of ordinary functions. That presents no problem when we have one variable, but presents significant difficulties for the two variable case when the operators do not commute. In such a case one uses the concept of quasi-probability distribution. In particular, for the quantum case the total force operator, $\mathbf{F}(t)$, at time t, is given by

$$\mathbf{F}(t) = \sum_{j=1}^{N} m_j \omega_j^2 \left(\mathbf{q}_j(0) \cos \omega_j t + \mathbf{p}_j(0) \frac{\sin \omega_j t}{m_j \omega_j} \right) \tag{11.1}$$

$$= \sum_{j=1}^{N} \left(m_j \omega_j^2 \mathbf{q}_j(0) \cos \omega_j t + \mathbf{p}_j(0) \omega_j \sin \omega_j t \right) \tag{11.2}$$

where $\mathbf{q}_j$ and $\mathbf{p}_j$ are the standard position and momentum operators that satisfy the commutation relation

$$[\mathbf{q}_j, \mathbf{p}_j] = i\hbar \tag{11.3}$$

where m_j and ω_j are the masses and frequencies. Many properties of the model have been developed and in particular the autocorrelation of the force has been obtained [4, 16, 17, 18].

First we discuss the general concept of a quantum characteristic function operator. If we have an operator, $\mathbf{A}$, then one defines the characteristic function operator by

$$\mathbf{M}(\theta) = e^{i\theta\mathbf{A}} \tag{11.4}$$

and the characteristic function is then the quantum mechanical expectation value

$$M(\theta) = \langle \mathbf{M}(\theta) \rangle = \int \ \psi^*(q) e^{i\theta\mathbf{A}} \psi(q) \ dq \tag{11.5}$$

The probability distribution is then given by

$$P(a) \ = \frac{1}{2\pi} \int \ M(\theta) \, e^{-i\theta a} \, da \tag{11.6}$$

Equivalently, of course, one can calculate $P(a)$ in the usual quantum mechanical procedure where the probability distribution is given by

$$P(a) = |\phi(a)|^2 \tag{11.7}$$

where

$$\phi(a) = \int \ u_a^*(x) \psi(x) dx \tag{11.8}$$

and where $u_a(x)$ are the eigenfunctions of the operator $\mathbf{A}$ with eigenvalues a,

$$\mathbf{A} u_a(x) = a u_a(x) \tag{11.9}$$

That the $P(a)$ given by Eq. (11.6) and Eq. (11.7) are the same is given in reference

[19]. Hence there is no difficulty for obtaining quantum distributions for a single quantum operator.

The difficulty comes in when we have one or more operators. For two variables one defines the characteristic function operator by [13, 10, 11, 15] way of

$$\mathbf{M}(\alpha,\beta) = e^{i\alpha\mathbf{A}+i\beta\mathbf{B}} \tag{11.10}$$

However, now, there are many other choices such as,

$$\mathbf{M}(\alpha,\beta) = e^{i\alpha\mathbf{A}}\ e^{i\beta\mathbf{B}} \tag{11.11}$$

$$\text{or } e^{i\beta\mathbf{B}}\ e^{i\alpha\mathbf{A}} \tag{11.12}$$

$$\text{or } e^{i\alpha\mathbf{A/2}}e^{i\beta\mathbf{B}}e^{i\alpha\mathbf{A/2}} \tag{11.13}$$

among many others. The characteristic function is then the expectation value of the characteristic function operator for $\mathbf{A}, \mathbf{B}$

$$M(\alpha,\beta) = \langle \mathbf{M}(\alpha,\beta)\rangle = \int\ \psi^*(q)\mathbf{M}(\alpha,\beta)\ \psi(q)\ dq \tag{11.14}$$

Each of the choices gives a different answer for the characteristic function and the distribution. Once a particular choice is explicitly obtained an infinite number of others can be obtained by way of [13, 10, 11, 15, 12]

$$P(a,b) = \frac{1}{4\pi^2}\iint \Phi(\alpha,\beta)M(\alpha,\beta)e^{-i\alpha a-i\beta b}d\alpha d\beta \tag{11.15}$$

where $\Phi(\alpha,\beta)$ is the kernel function [11]. In this thesis we consider the case given by Eq.

(11.10). The probability distribution is given by

$$P(a,b) = \frac{1}{4\pi^2} \iint M(\alpha,\beta) e^{-i\alpha a - i\beta b} d\alpha d\beta \tag{11.16}$$

where $M(\alpha,\beta)$ is given by Eq. (11.14).

Chapter 12

Quantum Characteristic Function and Distribution for $\mathbf{f}(t) = a(t)\mathbf{q} + b(t)\mathbf{p}$

Many of our subsequent calculations can be cast in the form where we have to find the characteristic function of

$$\mathbf{f}(t) = a(t)\mathbf{q} + b(t)\mathbf{p} \tag{12.1}$$

Different cases will involve taking particular forms for $a(t)$ and $b(t)$ and therefore we will do this general case first and specialize appropriately as needed. We want to calculate and simplify the quantum characteristic operator of $\mathbf{f}(t)$,

$$e^{i\theta \mathbf{f}(t)} = e^{i\theta\{a(t)\mathbf{q}+b(t)\mathbf{p}\}} \tag{12.2}$$

When two operators, **A** and **B** satisfy

$$[A,[A,B]] = [B,[A,B]] = 0 \tag{12.3}$$

one has that

$$e^{\mathbf{A}+\mathbf{B}} = e^{-\frac{1}{2}[\mathbf{A},\mathbf{B}]} e^{\mathbf{A}} e^{\mathbf{B}} \tag{12.4}$$

For our case we have

$$[A, B] = [i\theta a(t)\mathbf{q}, i\theta b(t)\mathbf{p}] = -\theta^2 a(t)b(t)[\mathbf{q}, \mathbf{p}] = -i\theta^2 a(t)b(t)\hbar \tag{12.5}$$

and hence the quantum characteristic operator for $\mathbf{f}(t)$ is

$$\mathbf{M}_f(\theta; t) = e^{i\theta\mathbf{f}(t)} = e^{i\theta^2 a(t)b(t)\hbar/2} e^{i\theta a(t)\mathbf{q}} e^{i\theta b(t)\mathbf{p}} \tag{12.6}$$

We note that $e^{i\theta b(t)\mathbf{p}}$ is the displacement operator

$$e^{i\theta b(t)\mathbf{p}} f(x) = f(x + \theta b(t)) \tag{12.7}$$

Now consider the characteristic function which is the expectation value of the characteristic function operator,

$$\begin{align}
M_f(\theta; t) &= \langle \mathbf{M}_f(\theta; t) \rangle \tag{12.8} \\
&= \int \psi^*(q) e^{i\theta\mathbf{f}(t)} \psi(q) dq \tag{12.9} \\
&= \int \psi^*(q)\, e^{i\theta^2 a(t)b(t)\hbar/2}\, e^{i\theta a(t)\mathbf{q}}\, e^{i\theta b(t)\mathbf{p}} \psi(q) dq \tag{12.10} \\
&= \int \psi^*(q)\, e^{i\theta^2 a(t)b(t)\hbar/2}\, e^{i\theta a(t)\mathbf{q}}\, \psi(q + \theta b(t)\hbar) dq \tag{12.11} \\
&= \int \psi^*(q - \theta b(t)\hbar/2)\; e^{i\theta a(t)\mathbf{q}}\, \psi(q + \theta b(t)\hbar/2) dq \tag{12.12}
\end{align}$$

The distribution of f is then

$$
\begin{aligned}
P(f;t) &= \frac{1}{2\pi}\int M_f(\theta;t)\, e^{-i\theta f}\, d\theta && (12.13)\\
&= \frac{1}{2\pi}\iint \psi^*(q-\theta b(t)\hbar/2)\; e^{i\theta a(t)\mathbf{q}}\, \psi(q+\theta b(t)\hbar/2)\, e^{-i\theta f}\, dqd\theta && (12.14)\\
&= \frac{1}{2\pi}\iint \psi^*(q-\theta b(t)\hbar/2)\; e^{-i\theta(f-a(t)\mathbf{q})}\, \psi(q+\theta b(t)\hbar/2)\, dqd\theta && (12.15)\\
&= \frac{1}{2\pi b(t)}\iint \psi^*(q-\theta\hbar/2)\; e^{-i\theta(f-a(t)q)/b(t)}\, \psi(q+\theta\hbar/2)\; dqd\theta && (12.16)
\end{aligned}
$$

This is the answer but we now show that it can be cast in an interesting way by the use of the Wigner distribution [20] which is defined by

$$
W(q,p) = \frac{1}{2\pi}\int \psi^*(q-\tfrac{1}{2}\hbar\tau)\, e^{-i\tau p}\psi(q+\tfrac{1}{2}\hbar\tau)d\tau \qquad (12.17)
$$

Comparing Eq. (12.16) with Eq. (12.17) we have that

$$
P(f;t) = \frac{1}{b(t)}\int W\left(q, \frac{f-a(t)q}{b(t)}\right) dq \qquad (12.18)
$$

Density matrix and mixtures

We point out that the Wigner distribution can be written in terms of the density matrix [21]. The density matrix in the coordinate representation is given by

$$
\rho(q,q') = \sum p_i \psi^*(q)\, \psi(q') \qquad (12.19)
$$

and the Wigner distribution is then

$$
W(q,p) = \frac{1}{2\pi}\int \rho(q-\tfrac{1}{2}\hbar\tau, q+\tfrac{1}{2}\hbar\tau)\, e^{-i\tau p}d\tau \qquad (12.20)
$$

The same derivation that has led to Eq. (12.16) can be used to show that Eq. (12.17) applies to Eq. (12.20). Hence, Eq. (12.18) applies to both pure cases and mixtures. Explicitly we have

$$P(f;t) = \frac{1}{b(t)} \int W\left(q, \frac{f - a(t)q}{b(t)}\right) dq \tag{12.21}$$

Chapter 13

Quantum Joint Distribution Function of Single Force at One Time for the Pure Case

The force is

$$\mathbf{F}(t) = \mathbf{q} m\omega^2 \cos\omega t + \mathbf{p}\omega \sin\omega t \tag{13.1}$$

and our aim is to find the characteristic function and the probability distribution of $\mathbf{F}(t)$. We repeat here the main results from the previous chapter. If

$$\mathbf{f}(t) = a(t)\mathbf{q} + b(t)\mathbf{p} \tag{13.2}$$

then the characteristic function is given by

$$M_f(\theta; t) = \int \psi^*(q - \theta b(t)\hbar/2)\ e^{i\theta a(t)\mathbf{q}}\, \psi(q + \theta b(t)\hbar/2) dq \tag{13.3}$$

and the distribution in terms of the wave function and Wigner distribution is, respectively,

$$P(f;t) = \frac{1}{2\pi b(t)}\iint \psi^*(q-\theta\hbar/2)\ e^{-i\theta(f-a(t)q)/b(t)}\ \psi(q+\theta\hbar/2)\ dqd\theta \tag{13.4}$$

$$= \frac{1}{b(t)}\int W\left(q,\frac{f-a(t)q}{b(t)}\right)dq \tag{13.5}$$

We now specialize to our case where. Comparing Eq.(13.1) with Eq.(13.2) it is clear that we have to take

$$a(t) = m\omega^2\cos\omega t \tag{13.6}$$

$$b(t) = \omega\sin\omega t \tag{13.7}$$

Therefore

$$M_f(\theta;t) = \int \psi^*(q-\theta b(t)\hbar/2)e^{i\theta a(t)\mathbf{q}}\ \psi(q+\theta b(t)\hbar/2)dq \tag{13.8}$$

$$= \int \psi^*(q-\theta\hbar/2\omega\sin\omega t)\ e^{i\theta q m\omega^2\cos\omega t}\ \psi(q+\theta\hbar/2\omega\sin\omega t)dq \tag{13.9}$$

and the distribution of force is

$$P(f;t) = \frac{1}{b(t)}\int W\left(q,\frac{f-a(t)q}{b(t)}\right)dq \tag{13.10}$$

$$= \frac{1}{|\omega\sin\omega t|}\int W\left(q,\frac{f-qm\omega^2\cos\omega t}{\omega\sin\omega t}\right)dq \tag{13.11}$$

In terms of the wave function we have

$$P(f;t) = \frac{1}{2\pi|\omega\sin\omega t|}\iint \psi^*(q-\theta\hbar/2)\ \exp\left[-i\theta\frac{(f-qm\omega^2\cos\omega t)}{\omega\sin\omega t}\right]\ \psi(q+\theta\hbar/2)\,dqd\theta \tag{13.12}$$

In the last section of this chapter we give an alternate derivation of these results.

We note that if all the algebra was done correctly the distribution should be automatically normalized. That is, we expect that for all time

$$\int P(f,t)df = 1 \tag{13.13}$$

To show that this is the case consider,

$$\int P(f,t)df = \frac{1}{2\pi|\omega \sin \omega t|}\iint \psi^*(q-\theta\hbar/2)\ \exp\left[-i\theta\frac{(f-qm\omega^2\cos\omega t)}{\omega\sin\omega t}\right]\ \psi(q+\theta\hbar/2)\,dqd\theta df \tag{13.14}$$

$$= \frac{1}{|\omega \sin \omega t|}\iint \psi^*(q-\theta\hbar/2)\ \delta(\theta\frac{1}{\omega\sin\omega t})\psi(q+\theta\hbar/2)\,dqd\theta \tag{13.15}$$

$$= \iint \psi^*(q-\theta\hbar/2)\ \delta(\theta)\psi(q+\theta\hbar/2)\,dqd\theta \tag{13.16}$$

$$= \int \psi^*(q)\ \ \psi(q)\,dq = 1 \tag{13.17}$$

It is also of interest to do it by way of the Wigner distribution, Eq.(12.20),

$$\int P(f,t)df = \iint \frac{1}{|\omega\sin\omega t|}W\left(q,\frac{f-qm\omega^2\cos\omega t}{\omega\sin\omega t}\right)dqdf \tag{13.18}$$

$$= \iint \frac{1}{|\omega\sin\omega t|}W\left(q,\frac{f}{\omega\sin\omega t}\right)dqdf \tag{13.19}$$

$$= \iint W\left(q,f\right)dqdf = 1 \tag{13.20}$$

The last step follows because the Wigner distribution is normalized to one if the wave function is.

We now calculate the first and second moment

$$\int fP(f,t)df = \iint \frac{f}{|\omega\sin\omega t|} W\left(q, \frac{f - qm\omega^2\cos\omega t}{\omega\sin\omega t}\right) dqdf \tag{13.21}$$

$$= \iint \frac{f + qm\omega^2\cos\omega t}{|\omega\sin\omega t|} W\left(q, \frac{f}{\omega\sin\omega t}\right) dqdf \tag{13.22}$$

$$= \iint (p\omega\sin\omega t + qm\omega^2\cos\omega t) W(q,p)\, dqdp \tag{13.23}$$

$$= \omega\sin\omega t \iint pW(q,p)\, dqdp + m\omega^2\cos\omega t \iint qW(q,p)\, dqdp \tag{13.24}$$

$$= \omega\sin\omega t < p > + m\omega^2\cos\omega t < q > \tag{13.25}$$

$$= 0 \tag{13.26}$$

$$\int f^2P(f,t)df = \iint \frac{f^2}{|\omega\sin\omega t|} W\left(q, \frac{f - qm\omega^2\cos\omega t}{\omega\sin\omega t}\right) dqdf \tag{13.27}$$

$$= \iint (p\omega\sin\omega t + qm\omega^2\cos\omega t)^2 W(q,p)\, dqdp \tag{13.28}$$

$$= \omega^2\sin^2\omega t \iint p^2W(q,p)\, dqdp \tag{13.29}$$

$$+ m^2\omega^4 \int\int q^2W(q,p)\, dqdp + 2m\omega^3\sin\omega t\cos\omega t \int\int pqW(q,p)\, dqdp \tag{13.30}$$

$$= \omega^2\sin^2\omega t < p^2 > + m^2\omega^4 < q^2 > \tag{13.31}$$

Alternate derivation of Eq. (13.5)

We now give an somewhat alternate derivation of Eq. (13.5). The force is

$$\mathbf{F}(t) = \sum_{j=1}^{N} \left(m_j\omega_j^2\mathbf{q}_j\cos\omega_j t + \mathbf{p}_j\omega_j\sin\omega_j t \right) \tag{13.32}$$

We first consider

$$\mathbf{f} = \mathbf{q}m\omega^2\cos\omega t + \omega\mathbf{p}\sin\omega t \tag{13.33}$$

The characteristic function operator is

$$\begin{aligned}\mathbf{M}_f(\theta;t) &= e^{i\theta\mathbf{f}} && (13.34)\\ &= e^{i\theta(\mathbf{q}m\omega^2\cos\omega t+\omega\mathbf{p}\sin\omega t)} && (13.35)\\ &= e^{i\theta^2 m\omega^3\cos\omega t\sin\omega t/2}e^{i\theta\mathbf{q}m\omega^2\cos\omega t}e^{i\theta\omega\mathbf{p}\sin\omega t} && (13.36)\end{aligned}$$

and the characteristic function is then

$$\begin{aligned}M_f(\theta,t) &= \int\psi^*(q)\mathbf{M}_f(\theta;t)\psi(q)\,dq && (13.37)\\ &= \int\psi^*(q)\,e^{i\hbar\theta^2 m\omega^3\cos\omega t\sin\omega t/2}e^{i\theta\mathbf{q}m\omega^2\cos\omega t}\psi(q+\theta\hbar\omega\sin\omega t)\,dq && (13.38)\\ &= \int\psi^*(q-\tfrac{1}{2}\hbar\theta\omega\sin\omega t)\,e^{i\theta qm\omega^2\cos\omega t}\psi(q+\tfrac{1}{2}\hbar\theta\omega\sin\omega t)\,dq && (13.39)\end{aligned}$$

where we have used the fact that

$$\begin{aligned}[\theta\mathbf{q}m\omega^2\cos\omega t,\theta\omega\mathbf{p}\sin\omega t] &= \theta^2 m\omega^3\cos\omega t\sin\omega[q,p] && (13.40)\\ &= i\hbar\theta^2 m\omega^3\cos\omega t\sin\omega && (13.41)\end{aligned}$$

The distribution is then given by

$$\begin{aligned}P(f,t) &= \frac{1}{2\pi}\int\ M_f(\theta,t)\,e^{-i\theta f}\,d\theta && (13.42)\\ &= \frac{1}{2\pi}\int\psi^*(q-\tfrac{1}{2}\hbar\theta\omega\sin\omega t)e^{-i\theta f}\ e^{i\theta qm\omega^2\cos\omega t}\psi(q+\frac{1}{2}\hbar\theta\omega\sin\omega t)\,dqd\theta && (13.43)\\ &= \frac{1}{2\pi}\int\psi^*(q-\tfrac{1}{2}\hbar\theta\omega\sin\omega t)\,e^{-i\theta(f-qm\omega^2\cos\omega t)}\psi(q+\tfrac{1}{2}\hbar\theta\omega\sin\omega t)\,dqd\theta && (13.44)\end{aligned}$$

Making the transformation

$$\tau = \theta\omega \sin \omega t \tag{13.45}$$

$$d\tau = \omega \sin \omega t d\theta \tag{13.46}$$

we have that

$$P(f,t) \; = \; \frac{1}{2\pi \left|\omega \sin \omega t\right|} \int \psi^*(q - \tfrac{1}{2}\hbar\tau) \, \exp\left[-i\tau \frac{f - qm\omega^2 \cos \omega t}{\omega \sin \omega t}\right] \psi(q + \tfrac{1}{2}\hbar\tau) \, dq d\tau \tag{13.47}$$

If we define the Wigner distribution in the usual way

$$W(q,p) = \frac{1}{2\pi} \int \psi^*(q - \tfrac{1}{2}\hbar\tau) \, e^{-i\theta p} \psi(q + \tfrac{1}{2}\hbar\tau) d\tau \tag{13.48}$$

then $P(f,t)$ can be written as

$$P(f,t) \; = \; \frac{1}{\left|\omega \sin \omega t\right|} \int W\left(q, \frac{f - qm\omega^2 \cos \omega t}{\omega \sin \omega t}\right) dq \tag{13.49}$$

Chapter 14

Density Matrix Approach and Mixtures

In the previous sections we have treated the pure case. We now address the case where we have a mixture characterized by a density matrix. We then specialize to a particular density matrix representing an ensemble of harmonic oscillators. The density matrix in the coordinate representation is

$$\rho(q,q') = \sum p_i \psi^*(q)\, \psi(q') \tag{14.1}$$

For the characteristic function we have

$$M_f(\theta;t) = \int \rho(q - \theta\hbar/2\omega\sin\omega t, q + \theta\hbar/2\omega\sin\omega t)\ e^{i\theta q m\omega^2\cos\omega t}\, dq \tag{14.2}$$

and for the distribution

$$P(f;t) = \frac{1}{2\pi|\omega\sin\omega t|}\iint \rho(q-\theta\hbar/2, q+\theta\hbar/2)\ \exp\left[-i\theta\frac{(f-qm\omega^2\cos\omega t)}{\omega\sin\omega t}\right]\ dq d\theta \tag{14.3}$$

We now take the following density matrix

$$\rho(x,x') = \sqrt{\frac{m\omega \tanh\left(\frac{\hbar\omega}{2kT}\right)}{\pi\hbar}} \exp\left[-\frac{m\omega}{4\hbar}((x-x')\coth\left(\frac{\hbar\omega}{2kT}\right) + (x+x')\tanh\left(\frac{\hbar\omega}{2kT}\right)\right] \tag{14.4}$$

This density matrix is well known and corresponds to the case of a harmonic oscillator heat bath. The corresponding Wigner distribution is also well known and is given by

$$\begin{aligned} W(x,p) &= \frac{1}{\pi\hbar}\int dy\rho(x-y,x+y)e^{2ipy/\hbar} && (14.5)\\ &= \frac{1}{\pi\hbar}\tanh\left(\frac{\hbar\omega}{2kT}\right)\exp\left[-\left(\frac{p^2}{m\hbar\omega}+\frac{m\omega^2x^2}{\hbar\omega}\right)\tanh\left(\frac{\hbar\omega}{2kT}\right)\right] && (14.6) \end{aligned}$$

For the sake of completeness we give a derivation of these results at the end of this chapter.

Distribution of force for a mixture

We now calculate the distribution of force for this Wigner distribution, Eq.(14.6). We rewrite Eq. (13.5)

$$P(f;t) \; = \frac{1}{b(t)}\int W\left(q, \frac{f-a(t)q}{b(t)}\right)dq \tag{14.7}$$

and substitute Eq.(14.4) for Eq.(14.3) to obtain

$$P(f,t) = \frac{1}{b(t)}\frac{1}{\pi\hbar}\tanh(\frac{\hbar\omega}{2kT})\int \exp[-\{\frac{m\omega}{\hbar}q^2 + \frac{(\frac{f-a(t))q}{b(t)})^2}{m\omega\hbar}\}\tanh\frac{\hbar\omega}{2kT}]dq \tag{14.8}$$

This integrates to

$$P(f,t) = \sqrt{\frac{m\omega\tanh\frac{\hbar\omega}{2kT}}{(a^2+b^2m^2\omega^2)\pi\hbar}}\exp\left[-\frac{m\omega\tanh\frac{\hbar\omega}{2kT}}{(a^2+b^2m^2\omega^2)\hbar}f^2\right] \tag{14.9}$$

and is seen to be a Gaussian distribution with mean zero and standard deviation given by

$$\sigma^2 = \frac{(a^2 + b^2 m^2 \omega^2) h}{2 m\omega \tanh \frac{\hbar\omega}{2kT}} \tag{14.10}$$

The corresponding characteristic function is

$$M(\theta, t) = \exp\left[\frac{(a^2 + b^2 m^2 \omega^2)\hbar}{4m\omega \tanh \frac{\hbar\omega}{2kT}}\theta\right] \tag{14.11}$$

For our case, as per Eq.(13.1), we have

$$a(t) = m\omega^2 \cos\omega t \tag{14.12}$$

$$b(t) = \omega \sin\omega t \tag{14.13}$$

and using the fact that

$$(a^2 + b^2 m^2 \omega^2) = ((m\omega^2 \cos\omega t)^2 + (\omega \sin\omega t)^2 m^2 \omega^2) = m^2 \omega^4 \tag{14.14}$$

we obtain

$$P(f, t) = \sqrt{\frac{\tanh \frac{\hbar\omega}{2kT}}{m\omega^3 \pi\hbar}} \exp\left[-\frac{\tanh \frac{\hbar\omega}{2kT}}{m\omega^3 \hbar} f^2\right] \tag{14.15}$$

If we substitute Eq. (14.15) into (2.1) we have for the characteristic function

$$M_f(\theta; t) = \sqrt{\frac{m\omega \tanh(\frac{\hbar\omega}{2kT})}{\pi\hbar}} e^{-\frac{m\omega}{4\hbar}\theta^2\omega^2 \sin^2\omega t \coth\frac{\hbar\omega}{2kT}} \int e^{i\theta m_i \omega_i^2 x \cos\omega_i t - \frac{m\omega}{\hbar} x^2 \tanh\frac{\hbar\omega}{kT}} dx \tag{14.16}$$

$$= e^{-\frac{m\omega}{4\hbar}\theta^2\omega^2 \sin^2\omega t \coth\frac{\hbar\omega}{2kT} - \frac{m\omega}{4\hbar}\theta^2\omega^2 \cos^2\omega t \coth\frac{\hbar\omega}{2kT}} \tag{14.17}$$

$$= e^{-\frac{m\omega}{4\hbar}\theta^2\omega^2 \coth\frac{\hbar\omega}{2kT}} \tag{14.18}$$

Classical limits

We now consider the classical limits. First, we point out the well known result that

$$\lim_{T\to\infty} \tan \frac{\hbar\omega}{2kT} \sim \frac{\hbar\omega}{2kT} \tag{14.19}$$

Applying this approximation to Eq.(14.9) we have

$$\lim_{T\to\infty} P(f,t) \sim e^{-\frac{m\omega^2}{2kT(a^2+b^2m^2\omega^2)}f^2} \sqrt{\frac{m\omega^2}{2\pi kT(a^2+b^2m^2\omega^2)}} \tag{14.20}$$

and for Eq.(14.15) we have

$$\lim_{T\to\infty} P(f,t) \sim \sqrt{\frac{1}{2\pi kTm\omega^2}}e^{-\frac{f^2}{2kTm\omega^2}} \tag{14.21}$$

This is seen to be the classical results as given by Eq.(6.4). Thus we have shown that the joint distribution function approach reduces to the classical results for $T \to \infty$ or for $\hbar \to 0$.

Derivation of density matrix and Wigner distribution for the harmonic oscillator bath

The density matrix and Wigner distribution for a harmonic oscillator heat bath have been derived by many in various ways. For the sake of completeness we give a derivation here. The most common derivation is to write a differential equation for the density matrix and solve it. Here we give an straightforward derivation. First, we list the main properties of the Harmonic oscillator. The eigenfunctions and eigenvalues are

$$u_n(x) = N_n e^{-\alpha^2x^2/2} H_n(\alpha x) \tag{14.22}$$

$$E_n = (n+\frac{1}{2})\hbar\omega \tag{14.23}$$

where

$$\alpha = \sqrt{\frac{m\omega}{\hbar}} = \left(\frac{mk}{\hbar^2}\right)^{1/4} \qquad \omega = \sqrt{\frac{k}{m}} \qquad N_n = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{1/2} \tag{14.24}$$

and H_n are the Hermit polynomials. We will be using Mahler's formula

$$\sum_{k=0}^{\infty} H_n(x)H_n(x')\frac{t^n}{2^n n!} = \frac{1}{\sqrt{1-t^2}} \exp\left[\frac{2txx' - t^2(x^2 + x'^2)}{1-t^2}\right] \tag{14.25}$$

Now, the density matrix is defined by way of

$$\rho(q, q') = \sum p_i \psi_i^*(q)\, \psi_i(q') \tag{14.26}$$

where

$$p_i = \frac{e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}} \tag{14.27}$$

and

$$\beta = \frac{1}{kT} \tag{14.28}$$

For the harmonic oscillator case we have

$$\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} \tag{14.29}$$

$$= \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} = \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} = \frac{1}{2\sinh\beta\hbar\omega/2} \tag{14.30}$$

and hence

$$p_i = 2\sinh(\beta\hbar\omega/2)e^{-\beta\hbar\omega(n+1/2)} \tag{14.31}$$

Therefore

$$\begin{aligned}
\rho(q,q') &= 2\sinh(\beta\hbar\omega/2)\sum_{k=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)}u_n(x)u_n(x') && (14.32)\\
&= 2\sinh(\beta\hbar\omega/2)\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)}N_n^2 e^{-\alpha^2(x^2+x'^2)/2}H_n(\alpha x)H_n(\alpha x') && (14.33)\\
&= 2\sinh(\beta\hbar\omega/2)\sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)}\frac{\alpha}{\sqrt{\pi}2^n n!}e^{-\alpha^2(x^2+x'^2)/2}H_n(\alpha x)H_n(\alpha x') && (14.34)\\
&= \frac{\alpha}{\sqrt{\pi}}2\sinh(\beta\hbar\omega/2)e^{-\beta\hbar\omega/2}e^{-\alpha^2(x^2+x'^2)/2}\sum_{k=0}^{\infty} e^{-\beta\hbar\omega n}\frac{1}{2^n n!}H_n(\alpha x)H_n(\alpha x') && (14.35)
\end{aligned}$$

Now in Mahler's formula, Eq. (14.25) put

$$t = e^{-\beta\hbar\omega} \tag{14.36}$$

to obtain

$$\sum_{k=0}^{\infty} H_n(\alpha x)H_n(\alpha x')\frac{e^{-\beta\hbar\omega n}}{2^n n!} = \frac{1}{\sqrt{1-e^{-2\beta\hbar\omega n}}}\exp\left[\alpha^2\frac{2e^{-\beta\hbar\omega n}xx' - e^{-2\beta\hbar\omega n}(x^2+x'^2)}{1-e^{-2\beta\hbar\omega n}}\right] \tag{14.37}$$

Hence,

$$\begin{aligned}
& e^{-\beta\hbar\omega/2}e^{-\alpha^2(x^2+x'^2)/2}\sum_{k=0}^{\infty} e^{-\beta\hbar\omega n}\frac{1}{2^n n!}H_n(\alpha x)H_n(\alpha x') && (14.38)\\
&= \frac{e^{-\beta\hbar\omega/2}e^{-\alpha^2(x^2+x'^2)/2}}{\sqrt{1-t^2}}\exp\left[\frac{2txx'\alpha^2 - t^2\alpha^2(x^2+x'^2)}{1-t^2}\right] && (14.39)\\
&= \frac{\sqrt{t}}{\sqrt{1-t^2}}e^{-\alpha^2(x^2+x'^2)/2}\exp\left[\frac{2txx' - t^2(x^2+x'^2)}{1-t^2}\alpha^2\right] && (14.40)\\
&= \frac{1}{\sqrt{1/t-t}}e^{-\alpha^2(x^2+x'^2)/2}\exp\left[\frac{2txx' - t^2(x^2+x'^2)}{1-t^2}\alpha^2\right] && (14.41)\\
&= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}}e^{-\alpha^2(x^2+x'^2)/2}\exp\left[\frac{2txx' - t^2(x^2+x'^2)}{1-t^2}\alpha^2\right] && (14.42)
\end{aligned}$$

$$= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\frac{2txx' - t^2(x^2 + x'^2)}{1 - t^2}\alpha^2 - \frac{\alpha^2(x^2 + x'^2)}{2}\right] \tag{14.43}$$

$$= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\frac{4txx' - 2t^2(x^2 + x'^2)}{2(1 - t^2)}\alpha^2 - \frac{\alpha^2(1 - t^2)(x^2 + x'^2)}{2(1 - t^2)}\right] \tag{14.44}$$

$$= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\alpha^2\frac{4txx' - (2t^2 + (1 - t^2))(x^2 + x'^2)}{2(1 - t^2)}\right] \tag{14.45}$$

$$= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\alpha^2\frac{4xx' - (2t + (1/t - t))(x^2 + x'^2)}{2(1/t - t)}\right] \tag{14.46}$$

$$= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\alpha^2\frac{4xx' - (2\cosh(\beta\hbar\omega))(x^2 + x'^2)}{4\sinh(\beta\hbar\omega)}\right] \tag{14.47}$$

$$= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\alpha^2\frac{4xx' - (2\cosh(\beta\hbar\omega))(x^2 + x'^2)}{4\sinh(\beta\hbar\omega)}\right] \tag{14.48}$$

$$= \frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\alpha^2\frac{2xx' - (\cosh(\beta\hbar\omega))(x^2 + x'^2)}{2\sinh(\beta\hbar\omega)}\right] \tag{14.49}$$

Therefore

$$\rho(q, q') = 2\sinh(\beta\hbar\omega/2)\frac{\alpha}{\sqrt{\pi}}\frac{1}{\sqrt{2\sinh(\beta\hbar\omega)}} \exp\left[\alpha^2\frac{2xx' - (\cosh(\beta\hbar\omega))(x^2 + x'^2)}{2\sinh(\beta\hbar\omega)}\right] \tag{14.50}$$

and using

$$\sinh 2x = 2\sinh x \cosh x \tag{14.51}$$

we obtain

$$\begin{aligned}
\rho(q,q') &= 2\sinh(\beta\hbar\omega/2)\frac{\alpha}{\sqrt{\pi}}\frac{1}{\sqrt{4\sinh(\beta\hbar\omega/2)\cosh(\beta\hbar\omega/2)}} \\
&\quad \exp\left[\alpha^2\frac{2xx'-(\cosh(\beta\hbar\omega))(x^2+x'^2)}{2\sinh(\beta\hbar\omega)}\right] \qquad (14.52)\\
&= \frac{\alpha}{\sqrt{\pi}}\sqrt{\tanh(\beta\hbar\omega/2)}\exp\left[\alpha^2\frac{2xx'-(\cosh(\beta\hbar\omega))(x^2+x'^2)}{2\sinh(\beta\hbar\omega)}\right] \qquad (14.53)\\
&= \frac{\alpha}{\sqrt{\pi}}\sqrt{\tanh(\beta\hbar\omega/2)}\exp\left[-\alpha^2\frac{(\cosh(\beta\hbar\omega))(x^2+x'^2)-2xx'}{2\sinh(\beta\hbar\omega)}\right] \qquad (14.54)
\end{aligned}$$

But

$$(x^2+x'^2)a-2bxx' = (x+x')^2(a-b)/2+(x-x')^2(a+b)/2 \qquad (14.55)$$

and therefore

$$\cosh(\beta\hbar\omega)(x^2+x'^2)-2xx' = (x+x')^2(\cosh(\beta\hbar\omega)-1)/2+(x-x')^2(\cosh(\beta\hbar\omega)+1)/2 \qquad (14.56)$$

Also, since

$$\begin{aligned}
\cosh^2\frac{x}{2} &= \frac{\cosh x+1}{2} \qquad (14.57)\\
\sinh^2\frac{x}{2} &= \frac{\cosh x-1}{2} \qquad (14.58)
\end{aligned}$$

we have that

$$\cosh(\beta\hbar\omega)(x^2+x'^2)-2xx' = (x+x')^2\sinh^2(\beta\hbar\omega/2)+(x-x')^2\cosh^2(\beta\hbar\omega/2) \qquad (14.59)$$

Hence, combining terms we have

$$\rho(q,q') = \frac{\alpha}{\sqrt{\pi}}\sqrt{\tanh(\beta\hbar\omega/2)}\exp\left[-\alpha^2\frac{(\cosh(\beta\hbar\omega))(x^2+x'^2)-2xx'}{2\sinh(\beta\hbar\omega)}\right] \tag{14.60}$$

$$= \frac{\alpha}{\sqrt{\pi}}\sqrt{\tanh(\beta\hbar\omega/2)}\exp\left[-\alpha^2\frac{(x+x')^2\sinh^2(\beta\hbar\omega/2)+(x-x')^2\cosh^2(\beta\hbar\omega/2)}{2\sinh(\beta\hbar\omega)}\right] \tag{14.61}$$

$$= \frac{\alpha}{\sqrt{\pi}}\sqrt{\tanh(\beta\hbar\omega/2)}\exp\left[-\alpha^2\frac{(x+x')^2\sinh^2(\beta\hbar\omega/2)+(x-x')^2\cosh^2(\beta\hbar\omega/2)}{4\cosh(\beta\hbar\omega/2)\sinh(\beta\hbar\omega/2)}\right] \tag{14.62}$$

$$= \frac{\alpha}{\sqrt{\pi}}\sqrt{\tanh(\beta\hbar\omega/2)}\exp\left[-\alpha^2\frac{(x+x')^2\tanh(\beta\hbar\omega/2)+(x-x')^2\coth(\beta\hbar\omega/2)}{4}\right] \tag{14.63}$$

$$= \sqrt{\frac{m\omega}{\hbar\pi}\tanh(\beta\hbar\omega/2)}\exp\left[-\frac{m\omega}{4\hbar}\left\{(x+x')^2\tanh(\beta\hbar\omega/2)+(x-x')^2\coth(\beta\hbar\omega/2)\right\}\right] \tag{14.64}$$

Puting $\beta = 1/kT$ we finally have

$$\rho(x,x') = \sqrt{\frac{m\omega\tanh(\frac{\hbar\omega}{2kT})}{\pi\hbar}}\exp[-\frac{m\omega}{4\hbar}((x-x')^2\coth(\frac{\hbar\omega}{2kT})+(x+x')^2\tanh(\frac{\hbar\omega}{2kT})] \tag{14.65}$$

Corresponding Wigner Distribution

We now calculate the corresponding Wigner distribution. We have

$$W(x,p) = \frac{1}{\pi\hbar}\int dy \rho(x-y,x+y)e^{2ipy/\hbar} \tag{14.66}$$

$$= \frac{1}{\pi\hbar}\sqrt{\frac{m\omega\tanh(\frac{\hbar\omega}{2kT})}{\pi\hbar}}\int \exp[-\frac{m\omega}{4\hbar}((2y')^2\coth(\frac{\hbar\omega}{2kT}) + (2x)^2\tanh(\frac{\hbar\omega}{2kT})]e^{2ipy/\hbar} \tag{14.67}$$

$$= \frac{1}{\pi\hbar}\sqrt{\frac{m\omega\tanh(\frac{\hbar\omega}{2kT})}{\pi\hbar}}\exp[-\frac{m\omega}{4\hbar}(2x)^2\tanh(\frac{\hbar\omega}{2kT})] \tag{14.68}$$

$$\int \exp[-\frac{m\omega}{4\hbar}((2y')^2\coth(\frac{\hbar\omega}{2kT})]e^{2ipy/\hbar} \tag{14.69}$$

$$= \frac{1}{\pi\hbar}\sqrt{\frac{m\omega\tanh(\frac{\hbar\omega}{2kT})}{\pi\hbar}}\sqrt{\frac{\pi}{\frac{m\omega}{4\hbar}2^2\coth(\frac{\hbar\omega}{2kT})}}\exp[-\frac{m\omega}{4\hbar}(2x)^2\tanh(\frac{\hbar\omega}{2kT})] \tag{14.70}$$

$$\exp\left[-\frac{4p^2/\hbar^2}{4\frac{m\omega}{4\hbar}(2)^2\coth(\frac{\hbar\omega}{2kT})}\right] \tag{14.71}$$

$$= \frac{1}{\pi\hbar}\tanh(\frac{\hbar\omega}{2kT})\exp\left[-\frac{m\omega}{\hbar}x^2\tanh(\frac{\hbar\omega}{2kT}) - \frac{p^2}{m\omega\hbar\coth(\frac{\hbar\omega}{2kT})}\right] \tag{14.72}$$

$$= \frac{1}{\pi\hbar}\tanh(\frac{\hbar\omega}{2kT})\exp\left[-\left\{\frac{m\omega}{\hbar}x^2 + \frac{p^2}{m\omega\hbar}\right\}\tanh(\frac{\hbar\omega}{2kT})\right] \tag{14.73}$$

$$\tag{14.74}$$

which gives that

$$W(x,p) = \frac{1}{\pi\hbar}\tanh(\frac{\hbar\omega}{2kT})\exp\left[-\left\{\frac{m\omega}{\hbar}x^2 + \frac{p^2}{m\omega\hbar}\right\}\tanh(\frac{\hbar\omega}{2kT})\right] \tag{14.75}$$

Chapter 15

Quantum Joint Distribution Function of Total Force at One Time for the Pure Case

We now do the case where we have N oscillators and where the total force is

$$\mathbf{F}(t) = \sum_{i=1}^{N} \mathbf{f}_i(t) \tag{15.1}$$

We further assume that the N body wave function is given by the product of individual wave functions, $\psi(q)$

$$\psi_N(q_1, q_2 ... q_N) = \prod_{i=1}^{N} \psi(q_i) \tag{15.2}$$

The characteristic function operator is

$$\mathbf{M}_F(\theta; t) \; = \; e^{i\theta \mathbf{F}(t)} \; = e^{i\theta \sum_{i=1}^{N} \mathbf{f}_i(t)} = \Pi_i M_{f_i}(\theta) \tag{15.3}$$

From the last chapter we have that

$$M_f(\theta;t) = e^{-\frac{m\omega}{4\hbar}\theta^2\omega^2\coth\frac{\hbar\omega}{2kT}} \tag{15.4}$$

and hence we have

$$\mathbf{M}_F(\theta;t) \ = \Pi_i e^{-\theta^2\frac{m_i\omega_i^3}{4}\coth\frac{\hbar\omega_i^3}{2kT}} \ = e^{-\theta^2\sum_i\frac{m_i\omega_i^3}{4}\coth\frac{\hbar\omega_i^3}{2kT}} \tag{15.5}$$

This is the characteristic function of a Gaussian distribution with zero mean and standard deviation given by

$$\sigma^2 = \sum_i \frac{m_i\omega_i^3}{2}\coth\frac{\hbar\omega_i^3}{2kT}. \tag{15.6}$$

Hence the distribution is

$$P(F) = \frac{1}{\sqrt{2\pi\sum_i\frac{m_i\omega_i^3}{2}\coth\frac{\hbar\omega_i^3}{2kT}}}\exp\left[-\frac{F^2}{\sum_i\frac{m_i\omega_i^3}{2}\coth\frac{\hbar\omega_i^3}{2kT}}\right] \tag{15.7}$$

Classical limits

We now consider some limiting cases for Eq. (15.7). Using Eq. (15.6)

$$\lim_{T\to\infty}\coth\frac{h\omega_i}{2kT} \sim \frac{2kT}{h\omega_i} \tag{15.8}$$

we have that

$$\sigma^2 \sim kT\sum m_i\omega_i^2 \tag{15.9}$$

and

$$P(F) \sim \frac{1}{\sqrt{\pi kT\sum m_i\omega_i^2}}e^{-\frac{F^2}{kT\sum m_i\omega_i^2}} \tag{15.10}$$

These limiting cases are identical to the classical cases as given by Eq. (7.10).

Chapter 16

Quantum Characteristic Function and Distribution for $\mathbf{f}(t) = a(t)\mathbf{q} + b(t)\mathbf{p}$ at Two Different Times

We now find the joint distribution of the total force at two different times. For two times we write

$$\mathbf{F}(t_1) = \sum_{i=1}^{N} \mathbf{f}_i(t_1) \quad ; \quad \mathbf{F}(t_2) = \sum_{i=1}^{N} \mathbf{f}_i(t_2) \tag{16.1}$$

and therefore

$$\mathbf{M}(\alpha, \beta; t_1, t_2) = e^{i\alpha \sum_{i=1}^{N} \mathbf{f}_i(t_1) + i\beta \sum_{i=1}^{N} \mathbf{f}_i(t_2)} \tag{16.2}$$

$$= e^{\sum_{i=1}^{N} \{i\alpha \mathbf{f}(t_1) + i\beta \mathbf{f}(t_2)\}} \tag{16.3}$$

We consider first the simplification of

$$\mathbf{M}_{f_1,f_2}(\alpha, \beta; t_1, t_2) = e^{i\alpha \mathbf{f}(t_1) + i\beta \mathbf{f}(t_2)} \tag{16.4}$$

Using

$$i\alpha\mathbf{f}(t_1)+i\beta\mathbf{f}(t_2)=i\alpha\left[a(t_1)\mathbf{q}+b(t_1)\mathbf{p}\right]+i\beta\left[a(t_2)\mathbf{q}+b(t_2)\mathbf{p}\right] \tag{16.5}$$

$$=i\left[\alpha a(t_1)+\beta a(t_2)\right]\mathbf{q}+i\left[\alpha b(t_1)+\beta b(t_2)\right]\mathbf{p} \tag{16.6}$$

we obtain

$$\mathbf{M}_{f_1,f_2}(\alpha,\beta;t_1,t_2)=e^{i\alpha\mathbf{f}(t_1)+i\beta\mathbf{f}(t_2)} \tag{16.7}$$

$$=e^{i[\alpha a(t_1)+\beta a(t_2)]\mathbf{q}+i[\alpha b(t_1)+\beta b(t_2)]\mathbf{p}} \tag{16.8}$$

$$=e^{i[\alpha a(t_1)+\beta a(t_2)][\alpha b(t_1)+\beta b(t_2)]\hbar/2}e^{i[\alpha a(t_1)+\beta a(t_2)]\mathbf{q}}e^{i[\alpha b(t_1)+\beta b(t_2)]\mathbf{p}} \tag{16.9}$$

Hence

$$M_{f_1,f_2}(\alpha,\beta;t_1,t_2)=\langle\mathbf{M}_{f_1,f_2}(\alpha,\beta;t_1,t_2)\rangle \tag{16.10}$$

$$=\int\psi^*(q)e^{i\alpha\mathbf{f}(t_1)+i\beta\mathbf{f}(t_2)}\psi(q)dq \tag{16.11}$$

$$=\int\psi^*(q)e^{i[\alpha a(t_1)+\beta a(t_2)][\alpha b(t_1)+\beta b(t_2)]\hbar/2}e^{i[\alpha a(t_1)+\beta a(t_2)]\mathbf{q}}e^{i[\alpha b(t_1)+\beta b(t_2)]\mathbf{p}}\psi(q)dq \tag{16.12}$$

$$=\int\psi^*(q)e^{i[\alpha a(t_1)+\beta a(t_2)][\alpha b(t_1)+\beta b(t_2)]\hbar/2}e^{i[\alpha a(t_1)+\beta a(t_2)]\mathbf{q}}\psi(q+\left[\alpha b(t_1)+\beta b(t_2)\right]\hbar)dq \tag{16.13}$$

$$=\int\psi^*(q-\left[\alpha b(t_1)+\beta b(t_2)\right]\hbar/2)e^{i[\alpha a(t_1)+\beta a(t_2)]q}\psi(q+\left[\alpha b(t_1)+\beta b(t_2)\right]\hbar/2)dq \tag{16.14}$$

One can find the distribution for f at two different times by way of

$$P(f_1,f_2;t_1,t_2)\;=\;\frac{1}{4\pi^2}\iint M_{f_1,f_2}(\alpha,\beta)\,e^{-i\alpha f_1-i\beta f_2}\,d\alpha d\beta \tag{16.15}$$

Substituting Eq. (16.14) into Eq. (16.15) we have that

$$P(f_1, f_2; t_1, t_2) = \frac{1}{4\pi^2} \iiint \psi^*(q - [\alpha b(t_1) + \beta b(t_2)]\,\hbar/2) e^{i[\alpha a(t_1) + \beta a(t_2)]q} \tag{16.16}$$

$$\psi(q + [\alpha b(t_1) + \beta b(t_2)]\,\hbar/2) e^{-i\alpha f_1 - i\beta f_2}\, d\alpha d\beta dq \tag{16.17}$$

To evaluate this we first make a change of variables for the α, β variables

$$\lambda = \alpha a(t_1) + \beta a(t_2) \tag{16.18}$$

$$\theta = \alpha b(t_1) + \beta b(t_2) \tag{16.19}$$

The inverse transformation is

$$\alpha = \frac{\lambda b(t_2) - \theta a(t_2)}{a(t_1)b(t_2) - a(t_2)b(t_1)} \tag{16.20}$$

$$\beta = \frac{\theta a(t_1) - \lambda b(t_1)}{a(t_1)b(t_2) - a(t_2)b(t_1)} \tag{16.21}$$

and hence

$$P(f_1, f_2; t_1, t_2) = \frac{1}{4\pi^2} \frac{1}{a(t_1)b(t_2) - a(t_2)b(t_1)} \tag{16.22}$$

$$\iiint \psi^*(q - \theta\hbar/2)\psi(q + \theta\hbar/2) \tag{16.23}$$

$$\exp\left[i\lambda q - i\frac{\lambda b(t_2) - \theta a(t_2)}{a(t_1)b(t_2) - a(t_2)b(t_1)} f_1 - i\frac{\theta a(t_1) - \lambda b(t_1)}{a(t_1)b(t_2) - a(t_2)b(t_1)} f_2\right] d\theta d\lambda dq \tag{16.24}$$

$$= \iiint \psi^*(q - \theta\hbar/2)\psi(q + \theta\hbar/2) \tag{16.25}$$

$$\exp i\theta \left[\frac{a(t_2)f_1 - a(t_1)f_2}{a(t_1)b(t_2) - a(t_2)b(t_1)}\right] \delta\left[q - \frac{b(t_2)f_1 - b(t_1)f_2}{a(t_1)b(t_2) - a(t_2)b(t_1)}\right] \tag{16.26}$$

We now express, $P(f_1, f_2; t_1, t_2)$ in terms of the Wigner distribution

$$= \frac{1}{2\pi} \frac{1}{a(t_1)b(t_2) - a(t_2)b(t_1)} \iint W(q, \frac{-a(t_2)f_1 + a(t_1)f_2}{a(t_1)b(t_2) - a(t_2)b(t_1)}) \tag{16.27}$$

$$\exp\left[i\lambda q - i\frac{\lambda b(t_2)}{a(t_1)b(t_2) - a(t_2)b(t_1)} f_1 - i\frac{-\lambda b(t_1)}{a(t_1)b(t_2) - a(t_2)b(t_1)} f_2\right] dq d\lambda \tag{16.28}$$

The integral over λ is a delta function and we obtain that

$$P(f_1, f_2; t_1, t_2) = \frac{1}{a(t_1)b(t_2) - a(t_2)b(t_1)} W\left(\frac{b(t_2)f_1 - b(t_1)f_2}{a(t_1)b(t_2) - a(t_2)b(t_1)}, \frac{-a(t_2)f_1 + a(t_1)f_2}{a(t_1)b(t_2) - a(t_2)b(t_1)}\right) \tag{16.29}$$

Chapter 17

Quantum Joint Distribution Single Force at Different Times for the pure case

We now calculate the joint quantum distribution of force for two different times. The force at one time is

$$\mathbf{F}(t) = m\omega^2(\mathbf{q}\cos\omega t + \mathbf{p}\frac{\sin\omega t}{m\omega}) \tag{17.1}$$

and the joint characteristic function for two forces at different times is

$$\mathbf{M}(\alpha,\beta) = e^{i\alpha\mathbf{F}(t_1)+i\beta\mathbf{F}(t_2)} \tag{17.2}$$

$$= \exp\left[im\omega^2(\alpha\cos\omega t_1 + \beta\cos\omega t_2)\mathbf{q} + i\omega(\alpha\sin\omega t_1 + \beta\sin\omega t_2)\mathbf{p}\right] \tag{17.3}$$

Using the fact that if

$$[A,[A,B]] = [B,[A,B]] = 0 \tag{17.4}$$

then

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} = e^B e^A e^{\frac{1}{2}[A,B]} \tag{17.5}$$

and setting

$$A = im\omega^2(\alpha \cos \omega t_1 + \beta \cos \omega t_2)\mathbf{q} \tag{17.6}$$

$$B = i\omega(\alpha \sin \omega t_1 + \beta \sin \omega t_2)\mathbf{p} \tag{17.7}$$

we obtain that

$$[A, B] = -m\omega^3(\alpha \cos \omega t_1 + \beta \cos \omega t_2)(\alpha \sin \omega t_1 + \beta \sin \omega t_2)[q, p]$$

Therefore

$$\mathbf{M}(\alpha, \beta) = e^{im\omega^2(\alpha \cos \omega t_1 + \beta \cos \omega t_2)\mathbf{q}} e^{i\omega(\alpha \sin \omega t_1 + \beta \sin \omega t_2)\mathbf{p}} \tag{17.8}$$

$$e^{\frac{i\hbar m\omega^3}{2}(\alpha \cos \omega t_1 + \beta \cos \omega t_2)(\alpha \sin \omega t_1 + \beta \sin \omega t_2)} \tag{17.9}$$

where we have used the fact

$$e^{i\omega(\alpha \sin \omega t_1 + \beta \sin \omega t_2)\mathbf{p}}\psi(x) = \psi(x - \hbar\omega(\alpha \sin \omega t_1 + \beta \sin \omega t_2)) \tag{17.10}$$

The expected value for a pure case with wave function $\psi(x)$ is hence

$$M(\alpha,\beta) =< \mathbf{M}(\alpha,\beta) >= \int \psi^*(x) M(\alpha,\beta)\psi(x)dx \tag{17.11}$$

$$= e^{\frac{i\hbar m\omega^3}{2}(\alpha\cos\omega t_1+\beta\cos\omega t_2)(\alpha\sin\omega t_1+\beta\sin\omega t_2)}$$

$$\int \psi^*(x) e^{im\omega^2(\alpha\cos\omega t_1+\beta\cos\omega t_2)x}\psi(x+\hbar\omega(\alpha\sin\omega t_1+\beta\sin\omega t_2))dx \tag{17.12}$$

$$= e^{\frac{i\hbar m\omega^3}{2}(\alpha\cos\omega t_1+\beta\cos\omega t_2)(\alpha\sin\omega t_1+\beta\sin\omega t_2)} \int \psi^*(x-\frac{1}{2}\hbar\omega(\alpha\sin\omega t_1+\beta\sin\omega t_2)) \tag{17.13}$$

$$e^{im\omega^2(\alpha\cos\omega t_1+\beta\cos\omega t_2)(x-\frac{1}{2}\hbar\omega(\alpha\sin\omega t_1+\beta\sin\omega t_2))}\psi(x+\frac{1}{2}\hbar\omega(\alpha\sin\omega t_1+\beta\sin\omega t_2))dx$$

$$= \int \psi^*(x-\frac{1}{2}\hbar\omega(\alpha\sin\omega t_1+\beta\sin\omega t_2))e^{im\omega^2(\alpha\cos\omega t_1+\beta\cos\omega t_2)x} \tag{17.14}$$

$$\psi(x+\frac{1}{2}\hbar\omega(\alpha\sin\omega t_1+\beta\sin\omega t_2))dx \tag{17.15}$$

The probability distribution is calculated by way of

$$P(f_1,f_2) = \iint M(\alpha,\beta)e^{-i\alpha f_1 - i\beta f_2}d\alpha d\beta \tag{17.16}$$

To simplify the characteristic function, we make the following transformation,

$$\beta' = \alpha\sin\omega t_1 + \beta\sin\omega t_2 \tag{17.17}$$

$$\alpha' = \alpha\cos\omega t_1 + \beta\cos\omega t_2 \tag{17.18}$$

where the inverse transformation is

$$\alpha = \frac{\beta' \cos \omega t_2 - \alpha' \sin \omega t_2}{\sin \omega (t_1 - t_2)} \tag{17.19}$$

$$\beta = \frac{\beta' \cos \omega t_1 - \alpha' \sin \omega t_1}{\sin \omega (t_2 - t_1)} \tag{17.20}$$

Now

$$M(\alpha', \beta') = \int \psi^*(x - \frac{1}{2}\hbar\omega\beta')\psi(x + \frac{1}{2}\hbar\omega\beta')e^{im\omega^2\alpha' x}dx \tag{17.21}$$

and therefore the distribution function can be rewritten as an integration over α' and β'

$$P(f_1, f_2) = \frac{1}{\sin \omega(t_2 - t_1)} \int M(\alpha', \beta') \exp \tag{17.22}$$

$$\left[-i \frac{\beta' \cos \omega t_2 - \alpha' \sin \omega t_2}{\sin \omega(t_1 - t_2)} f_1 - i \frac{\beta' \cos \omega t_1 - \alpha' \sin \omega t_1}{\sin \omega(t_2 - t_1)} f_2 \right] d\alpha' d\beta' \tag{17.23}$$

$$= \frac{2\pi}{\sin \omega(t_2 - t_1)} \int \psi^*(x - \frac{1}{2}\hbar\omega\beta')\psi(x + \frac{1}{2}\hbar\omega\beta')\delta(m\omega^2 x - \frac{f_1 \sin \omega t_2 - f_2 \sin \omega t_1}{\sin \omega(t_2 - t_1)}) \tag{17.24}$$

$$\exp \left[i \frac{\cos \omega t_2 f_1 - \cos \omega t_1 f_2}{\sin \omega(t_2 - t_1)} \beta' \right] dx d\beta' \tag{17.25}$$

$$= \frac{2\pi}{\sin \omega(t_2 - t_1)} \tag{17.26}$$

$$\int \psi^*(\frac{f_1 \sin \omega t_2 - f_2 \sin \omega t_1}{m\omega^2 \sin \omega(t_2 - t_1)} - \frac{1}{2}\hbar\omega\beta')\psi(\frac{f_1 \sin \omega t_2 - f_2 \sin \omega t_1}{m\omega^2 \sin \omega(t_2 - t_1)} + \frac{1}{2}\hbar\omega\beta') \tag{17.27}$$

$$\exp \left[i \frac{\cos \omega t_2 f_1 - \cos \omega t_1 f_2}{\sin \omega(t_2 - t_1)} \beta' \right] d\beta' \tag{17.28}$$

By comparing this result with quantum Wigner function, Eq.(12.17), we have

$$P(f_1, f_2) = \frac{2\pi}{\sin \omega(t_2 - t_1)} W(\frac{f_1 \sin \omega t_2 - f_2 \sin \omega t_1}{m\omega^2 \sin \omega(t_2 - t_1)}, \frac{f_1 \cos \omega t_2 - f_2 \cos \omega t_1}{\sin \omega(t_2 - t_1)}) \tag{17.29}$$

Marginals and moments

We now verify that the marginals are satisfied. The distribution should satisfy

$$\int W(f_1, f_2) df_2 = P(f_1) \tag{17.30}$$

where $P(f_1)$ is given by Eq. (13.11). Using Eq.(12.17) we have

$$W(f_1, f_2) = \frac{2\pi}{\sin\omega(t_2 - t_1)} \int \psi^*(\frac{f_1 \sin\omega t_2 - f_2 \sin\omega t_1}{m\omega^2 \sin\omega(t_2 - t_1)} - \frac{1}{2}\hbar\omega\beta) \tag{17.31}$$

$$\psi(\frac{f_1 \sin\omega t_2 - f_2 \sin\omega t_1}{m\omega^2 \sin\omega(t_2 - t_1)} + \frac{1}{2}\hbar\omega\beta) e^{i\frac{f_1 \cos\omega t_2 - f_2 \cos\omega t_1}{\sin\omega(t_2 - t_1)}\beta} d\beta \tag{17.32}$$

No consider

$$P(f_1) = \int W(f_1, f_2) df_2 \tag{17.33}$$

$$= \frac{2\pi}{\sin\omega(t_2 - t_1)} \int \psi^*(\frac{f_1 \sin\omega t_2 - f_2 \sin\omega t_1}{m\omega^2 \sin\omega(t_2 - t_1)} - \frac{1}{2}\hbar\omega\beta) \tag{17.34}$$

$$\psi(\frac{f_1 \sin\omega t_2 - f_2 \sin\omega t_1}{m\omega^2 \sin\omega(t_2 - t_1)} + \frac{1}{2}\hbar\omega\beta) e^{i\frac{f_1 \cos\omega t_2 - f_2 \cos\omega t_1}{\sin\omega(t_2 - t_1)}\beta} d\beta df_2 \tag{17.35}$$

To simplify this, let

$$\frac{f_1 \sin\omega t_2 - f_2 \sin\omega t_1}{m\omega^2 \sin\omega(t_2 - t_1)} = q \tag{17.36}$$

$$\frac{\beta}{\sin\omega t_1} = \theta \tag{17.37}$$

and where the inverse transformation is

$$f_2 = \frac{f_1 \sin \omega t_2 - q m \omega^2 \sin \omega (t_2 - t_1)}{\sin \omega t_1} \tag{17.38}$$

$$\beta = \theta \sin \omega t_1 \tag{17.39}$$

$$d\beta df_2 = m\omega^2 \sin \omega (t_2 - t_1) dq d\theta \tag{17.40}$$

We have that

$$\int W(f_1, f_2) df_2 = 2\pi m \omega^2 \int \psi^*(q - \frac{\theta}{2}\omega\hbar \sin \omega t_1)\psi(q - \frac{\theta}{2}\omega\hbar \sin \omega t_1) \tag{17.41}$$

$$e^{i\frac{f_1 \cos \omega t_2 - \frac{f_1 \sin \omega t_2 - q m \omega^2 \sin \omega (t_2 - t_1)}{\sin \omega t_1} \cos \omega t_1}{\sin \omega (t_2 - t_1)} \theta \sin \omega t_1} dq d\theta \tag{17.42}$$

$$= 2\pi m \omega^2 \int \psi^*(q - \frac{\theta}{2}\omega\hbar \sin \omega t_1)\psi(q - \frac{\theta}{2}\omega\hbar \sin \omega t_1) \tag{17.43}$$

$$e^{i[-f_1 + q \cos \omega t_1]\theta} dq d\theta \tag{17.44}$$

$$= \frac{1}{\omega \sin \omega t_1} \int W(q, \frac{f - m\omega^2 \cos \omega t_1 q}{\omega \sin \omega t_1}) dq \tag{17.45}$$

This is same result as Eq.(13.20)

Autocorrelation function.

We now calculate the autocorrelation function of force for two different times,

$$\langle f_1 f_2 \rangle = \int f_1 f_2 W(f_1, f_2) df_2 df_1 = \frac{2\pi}{\sin \omega (t_2 - t_1)} \int f_1 f_2 \psi^*(\frac{f_1 \sin \omega t_2 - f_2 \sin \omega t_1}{m\omega^2 \sin \omega (t_2 - t_1)} - \frac{1}{2}\hbar\omega\beta) \tag{17.46}$$

$$\psi(\frac{f_1 \sin \omega t_2 - f_2 \sin \omega t_1}{m\omega^2 \sin \omega (t_2 - t_1)} + \frac{1}{2}\hbar\omega\beta) e^{i\frac{f_1 \cos \omega t_2 - f_2 \cos \omega t_1}{\sin \omega (t_2 - t_1)}\beta} d\beta df_1 df_2 \tag{17.47}$$

making the following transformation

$$\frac{f_1 \sin \omega t_2 - f_2 \sin \omega t_1}{m\omega^2 \sin \omega(t_2 - t_1)} = q \tag{17.48}$$

$$\frac{f_1 \cos \omega t_2 - f_2 \cos \omega t_1}{\sin \omega(t_2 - t_1)} = p \tag{17.49}$$

$$f_1 = qm\omega^2 \cos \omega t_1 - p \sin \omega t_1 \tag{17.50}$$

$$f_2 = qm\omega^2 \cos \omega t_2 - p \sin \omega t_2 \tag{17.51}$$

$$\langle f_1 f_2 \rangle = \int (qm\omega^2 \cos \omega t_1 - p \sin \omega t_1)(qm\omega^2 \cos \omega t_2 - p \sin \omega t_2) \tag{17.52}$$

$$\psi^*(q - \frac{1}{2}\hbar\omega\beta)\psi(q + \frac{1}{2}\hbar\omega\beta)e^{ip\beta} d\beta dq dp \tag{17.53}$$

$$= \int [q^2 m^2 \omega^4 \cos \omega t_1 \cos \omega t_2 - qpm\omega^2 \sin \omega(t_1 + t_2) + p^2 \sin \omega t_1 \cos \omega t_2] \tag{17.54}$$

$$\psi^*(q - \frac{1}{2}\hbar\omega\beta)\psi(q + \frac{1}{2}\hbar\omega\beta)e^{ip\beta} d\beta dq dp \tag{17.55}$$

$$=< q^2 > m^2\omega^4 \cos \omega t_1 \cos \omega t_2 + < p^2 > \sin \omega t_1 \sin \omega t_2 - < qp > m\omega^2 \sin \omega(t_1 + t_2) \tag{17.56}$$

and hence

$$\langle f_1 f_2 \rangle =< p^2 > \cos \omega(t_1 - t_2) \tag{17.57}$$

where we assume oscillators are in thermal equilibrium, hence

$$< q^2 > m^2\omega^4 =< p^2 > \tag{17.58}$$

Chapter 18

Quantum Characteristic Function of a Single Oscillator in Terms of the Density Matrix for two Different Times: an Alternate Derivation

We now give an alternate derivation of the quantum characteristic function and distribution for two different times as derived in the previous chapter. We want to evaluate

$$M(\alpha, \beta) = < e^{i\alpha F(t_1) + i\beta F(t_2)} > \tag{18.1}$$

with

$$F(t) = m\omega^2 (\mathbf{q} \cos \omega t + \mathbf{p} \frac{\sin \omega t}{m\omega}) \tag{18.2}$$

now

$$[F(t_2), F(t_1)] = i\omega \sin \omega(t_1 - t_2)\hbar \tag{18.3}$$

and for such a case

$$e^{i\alpha F(t_1)+i\beta F(t_2)} = e^{i\beta F(t_2)/2} e^{i\alpha F(t_1)} e^{i\beta F(t_2)/2} \tag{18.4}$$

The method we use is described in **[22].** One express everything in terms of the eigenvalue and eigenfunctions of the operator

$$F(t_2) = m\omega^2(\mathbf{q}\cos\omega t_2 + \mathbf{p}\frac{\sin\omega t_2}{m\omega}) \tag{18.5}$$

First consider the eigenvalue problem for $\mathbf{f}(t) = a(t)\mathbf{q} + b(t)\mathbf{p}$

$$\mathbf{f}(t) u_\lambda(q) = \lambda u_\lambda(q) \tag{18.6}$$

or

$$\left[a(t)\mathbf{q} + b(t)\mathbf{p}\right] u_\lambda(q) = \lambda u_\lambda(q) \tag{18.7}$$

Putting in

$$\mathbf{p} = -i\hbar\frac{d}{dq} \tag{18.8}$$

we have

$$\frac{d}{dq}u_\lambda(q) = \frac{i(\lambda - a(t_2)\mathbf{q})}{\hbar b(t_2)} u_\lambda(q) \tag{18.9}$$

The normalized solution is

$$u_\lambda(q) = \frac{1}{\sqrt{2\pi\hbar b(t_2)}} e^{\frac{i}{\hbar b(t_2)}[\lambda q - a(t_2)q^2/2]} \tag{18.10}$$

For our case

$$a = m\omega^2 \cos \omega t \tag{18.11}$$

$$b = \omega \sin \omega t \tag{18.12}$$

and we have that

$$\frac{i}{\hbar b(t_2)}[\lambda q - a(t_2)q^2/2] = \frac{i}{\hbar\omega \sin \omega t_2}[\lambda q - m\omega^2 \cos \omega t_2 q^2/2] \tag{18.13}$$

$$= \frac{i}{\hbar}[\frac{\lambda q}{\omega \sin \omega t_2} - \frac{m\omega q^2}{2 \tan \omega t_2}] \tag{18.14}$$

and therefore

$$u_\lambda(q) = \frac{1}{\sqrt{2\pi\hbar\omega \sin \omega t_2}} \exp\left[\frac{i}{\hbar}\left(\frac{\lambda q}{\omega \sin \omega t_2} - \frac{m\omega q^2}{2 \tan \omega t_2}\right)\right] \tag{18.15}$$

Now take the wave function and expanded in the following way

$$\psi(q) = \int \eta(\lambda) u_\lambda(q) d\lambda \tag{18.16}$$

For $u_\lambda(q)$ we will take it at t_2

$$u_\lambda(q) = \frac{1}{\sqrt{2\pi\hbar b(t_2)}} e^{\frac{i}{\hbar b(t)}[\lambda q - a(t_2)q^2/2]} \tag{18.17}$$

$$u_\lambda(q) = \frac{1}{\sqrt{2\pi\hbar b(t_2)}} e^{\frac{i}{\hbar b(t_2)}[\lambda q - a(t_2)q^2/2]} \tag{18.18}$$

$$= \frac{1}{\sqrt{2\pi\hbar\omega \sin \omega t_2}} \exp\left[\frac{i}{\hbar}\left(\frac{\lambda q}{\omega \sin \omega t_2} - \frac{m\omega q^2}{2 \tan \omega t_2}\right)\right] \tag{18.19}$$

Now consider

$$M(\alpha,\beta) =< e^{i\beta F(t_2)/2} e^{i\alpha F(t_1)} e^{i\beta F(t_2)/2} > \tag{18.20}$$

$$= \iint \psi^*(q) e^{i\beta F(t_2)/2} e^{i\alpha F(t_1)} e^{i\beta F(t_2)/2} \psi(q) dq \tag{18.21}$$

$$= \iint \eta^*(\lambda') u^*_{\lambda'}(q) e^{i\beta F(t_2)/2} e^{i\alpha F(t_1)} e^{i\beta F(t_2)/2} \eta(\lambda) u_\lambda(q) d\lambda d\lambda' dq \tag{18.22}$$

$$= \iiint \eta^*(\lambda')\eta(\lambda) u^*_{\lambda'}(q) e^{i\beta(\lambda+\lambda')/2} e^{i\alpha F(t_1)} u_\lambda(q) d\lambda d\lambda' dq \tag{18.23}$$

Since $u_\lambda(q)$ is the eigenfunctions of $F(t_2)$ with eigenvalue λ, we have

$$e^{i\beta F(t_2)/2} u_\lambda(q) = e^{i\beta\lambda/2} u_\lambda(q) \tag{18.24}$$

$$u^*_{\lambda'}(q) e^{i\beta F(t_2)/2} = e^{i\beta\lambda'/2} u_{\lambda'}(q) \tag{18.25}$$

Now consider

$$e^{i\alpha F(t_1)} u_\lambda(q) = e^{i\alpha[a(t_1)\mathbf{q}+b(t_1)\mathbf{p}]} u_\lambda(q) \tag{18.26}$$

$$= e^{i\alpha a(t_1)(\mathbf{q}+\alpha b(t_1)h/2)} e^{i\alpha b(t_1)\mathbf{p}} u_\lambda(q) \tag{18.27}$$

$$= e^{i\alpha a(t_1)(\mathbf{q}+\alpha b(t_1)h/2)} u_\lambda(q+\alpha b(t_1)h) \tag{18.28}$$

and therefore

$$M(\alpha,\beta) = \iiint \eta^*(\lambda')\eta(\lambda) u^*_{\lambda'}(q) e^{i\beta(\lambda+\lambda')/2} e^{i\alpha a(t_1)(\mathbf{q}+\alpha b(t_1)\hbar/2)} u_\lambda(q+\alpha b(t_1)\hbar) d\lambda d\lambda' dq \tag{18.29}$$

$$= \iiint \eta^*(\lambda')\eta(\lambda) u^*_{\lambda'}(q-\alpha b(t_1)\hbar/2) e^{i\beta(\lambda+\lambda')/2} e^{i\alpha a(t_1)q} u_\lambda(q+\alpha b(t_1)\hbar/2) d\lambda d\lambda' dq \tag{18.30}$$

Now consider the integration over q. We now substitute $u_\lambda(q)$ from Eq. (18.19) to obtain

$$\int u^*_{\lambda'}(q-\alpha b(t_1)\hbar/2)e^{i\alpha a(t_1)q}u_\lambda(q+\alpha b(t_1)\hbar/2)dq \tag{18.31}$$

$$= e^{i\alpha a(t_1)\alpha b(t_1)\hbar/2}\int u^*_{\lambda'}(q)e^{i\alpha a(t_1)q}u_\lambda(q+\alpha b(t_1)\hbar)dq \tag{18.32}$$

$$= \frac{e^{i\alpha^2 a(t_1)b(t_1)\hbar/2}}{2\pi\hbar b(t_2)}\int e^{-\frac{i}{\hbar b(t_2)}[\lambda' q-a(t_2)q^2/2]}e^{i\alpha a(t_1)q}e^{\frac{i}{\hbar b(t_2)}[\lambda(q+\alpha b(t_1)\hbar)-a(t_2)(q+\alpha b(t_1)\hbar)^2/2]}dq \tag{18.33}$$

$$= \frac{e^{i\alpha^2 a(t_1)b(t_1)\hbar/2}}{2\pi\hbar b(t_2)}e^{\frac{i}{\hbar b(t_2)}[\lambda\alpha b(t_1)\hbar-a(t_2)(\alpha b(t_1)\hbar)^2/2]}\int e^{\frac{i}{\hbar b(t_2)}[\lambda-\lambda'+\alpha\hbar(a(t_1)b(t_2)-a(t_2)b(t_1))]q}dq \tag{18.34}$$

$$= \frac{e^{i\alpha^2[a(t_1)b(t_1)-\frac{a(t_2)b^2(t_1)}{b(t_2)}]\hbar/2+\frac{i\lambda\alpha b(t_1)}{b(t_2)}}}{2\pi\hbar b(t_2)}\int e^{\frac{i}{\hbar b(t_2)}[\lambda-\lambda'+\alpha\hbar(a(t_1)b(t_2)-a(t_2)b(t_1))]q}dq \tag{18.35}$$

Using Eq. (1.3) and integrating over $x=\frac{q}{\hbar b(t_2)}$, we obtain

$$\frac{1}{2\pi}e^{\frac{i\hbar}{2}\alpha^2 m\omega^3\frac{\sin\omega t_1}{\sin\omega t_2}\sin\omega(t_2-t_1)+i\lambda\alpha\frac{\sin\omega t_1}{\sin\omega t_2}}\int e^{ix(\lambda-\lambda'^3\sin\omega(t_1-t_2))}dx \tag{18.36}$$

$$= e^{\frac{i\hbar}{2}\alpha^2 m\omega^3\frac{\sin\omega t_1}{\sin\omega t_2}\sin\omega(t_2-t_1)+i\lambda\alpha\frac{\sin\omega t_1}{\sin\omega t_2}}\delta(\lambda-\lambda'^3\sin\omega(t_1-t_2)) \tag{18.37}$$

Therefore

$$< M(\alpha,\beta) >= \int\int \eta^*(\lambda')\eta(\lambda)e^{i\beta(\lambda+\lambda')/2}e^{\frac{i\hbar}{2}\alpha m\omega^3\frac{\sin\omega t_1}{\sin\omega t_2}\sin\omega(t_2-t_1)+i\lambda\alpha\frac{\sin\omega t_1}{\sin\omega t_2}} \tag{18.38}$$

$$\delta(\lambda-\lambda'^3\sin\omega(t_1-t_2))d\lambda d\lambda' \tag{18.39}$$

$$= \int \eta^*(\lambda+\alpha\hbar m\omega^3\sin\omega(t_1-t_2))\eta(\lambda) \tag{18.40}$$

$$e^{i\beta(2\lambda+\alpha\hbar m\omega^3\sin\omega(t_1-t_2))/2+\frac{i\hbar}{2}\alpha m\omega^3\frac{\sin\omega t_1}{\sin\omega t_2}\sin\omega(t_2-t_1)+i\lambda\alpha\frac{\sin\omega t_1}{\sin\omega t_2}}d\lambda \tag{18.41}$$

$$= \int \eta^*(\lambda+\alpha\hbar m\omega^3\sin\omega(t_1-t_2))\eta(\lambda) \tag{18.42}$$

$$e^{i\lambda(\beta+\alpha\frac{\sin\omega t_1}{\sin\omega t_2})+\frac{i\alpha\hbar}{2}m\omega^3\sin\omega(t_1-t_2)(\beta+\alpha\frac{\sin\omega t_1}{\sin\omega t_2})}d\lambda \tag{18.43}$$

$$= \int \eta^*(\lambda+\alpha\hbar m\omega^3\sin\omega(t_1-t_2))\eta(\lambda)e^{i[\lambda+\frac{i\alpha\hbar}{2}m\omega^3\sin\omega(t_1-t_2)](\beta+\alpha\frac{\sin\omega t_1}{\sin\omega t_2})}d\lambda \tag{18.44}$$

$$= \int \eta^*(\lambda+\frac{1}{2}\alpha\hbar m\omega^3\sin\omega(t_1-t_2))\eta(\lambda-\frac{1}{2}\alpha\hbar m\omega^3\sin\omega(t_1-t_2))e^{i\lambda(\beta+\alpha\frac{\sin\omega t_1}{\sin\omega t_2})}d\lambda \tag{18.45}$$

Now we consider the density matrix ρ in the λ representation

$$\rho\left(\lambda,\lambda'\right) = \left\langle\lambda|e^{-\beta H}|\lambda'\right\rangle \tag{18.46}$$

The reverse transformation is

$$\psi(x)e^{\frac{imx^2}{2h\tan\omega t_2}} = \int \eta(\lambda)e^{\frac{i\lambda x}{\hbar\omega\sin\omega t_2}}d\lambda \tag{18.47}$$

$$\eta(\lambda) = \frac{1}{2\pi\hbar\omega\sin\omega t_2}\int \psi(x)e^{\frac{i}{\hbar}(\frac{mx^2}{2\tan\omega t_2}-\frac{\lambda x}{\hbar\omega\sin\omega t_2})}dx \tag{18.48}$$

$$\eta^*(\lambda)\eta(\lambda') = \frac{1}{4\pi^2\hbar^2\omega^2\sin^2\omega t_2}\int\int \psi^*(x)\psi(x'^{-\frac{i}{\hbar}(\frac{mx^2}{2\tan\omega t_2}-\frac{\lambda x}{\hbar\omega\sin\omega t_2})+\frac{i}{\hbar}(\frac{mx'^2}{2\tan\omega t_2}-\frac{\lambda' x'}{\hbar\omega\sin\omega t_2})}dxdx' \tag{18.49}$$

$$= \frac{1}{4\pi^2\hbar^2\omega^2\sin^2\omega t_2}\int\int \psi^*(x)\psi(x')e^{-\frac{i}{\hbar}[\frac{m}{2\tan\omega t_2}(x^2-x'^2)-\frac{\lambda x}{\hbar\omega\sin\omega t_2}+\frac{\lambda' x'}{\hbar\omega\sin\omega t_2}]}dxdx' \tag{18.50}$$

Substitute this into Eq. (13.19)

$$\eta^*(\lambda + \frac{1}{2}\alpha\hbar m\omega^3 \sin\omega(t_1 - t_2))\eta(\lambda - \frac{1}{2}\alpha\hbar m\omega^3 \sin\omega(t_1 - t_2))$$

$$= \frac{1}{4\pi^2\hbar^2\omega^2 \sin^2 \omega t_2}\iiint \psi^*(x)\psi(x') \tag{18.51}$$

$$e^{-\frac{im}{2\hbar \tan\omega t_2}(x^2 - x'^2) + \frac{i}{\hbar\omega \sin\omega t_2}[\lambda(x-x') + \frac{1}{2}\alpha\hbar m\omega^3 \sin\omega(t_1 - t_2))(x+x')]} dxdx' \tag{18.52}$$

and therefore

$$< M(\alpha,\beta) >= \frac{1}{4\pi^2\hbar^2\omega^2 \sin^2 \omega t_2}\iiint \psi^*(x)\psi(x') \tag{18.53}$$

$$e^{-\frac{im}{2\hbar \tan\omega t_2}(x^2 - x'^2) + \frac{i}{\hbar\omega \sin\omega t_2}[\lambda(x-x') + \frac{1}{2}\alpha\hbar m\omega^3 \sin\omega(t_1 - t_2))(x+x')]} e^{i\lambda(\beta + \alpha\frac{\sin\omega t_1}{\sin\omega t_2})} dxdx'd\lambda \tag{18.54}$$

$$= \frac{1}{2\pi\hbar\omega \sin\omega t_2}\int \psi^*(x)\psi(x'^{\frac{1}{2}\alpha\hbar m\omega^3 \sin\omega(t_1 - t_2))(x+x')}\delta(x - x' + (\beta\sin\omega t_2 + \alpha\sin\omega t_1))dxdx' \tag{18.55}$$

$$= \frac{1}{2\pi\hbar\omega \sin\omega t_2}\int \psi^*(x)\psi(x + (\beta\sin\omega t_2 + \alpha\sin\omega t_1))e^{\frac{1}{2}\alpha\hbar m\omega^3 \sin\omega(t_1 - t_2))[2x + (\beta\sin\omega t_2 + \alpha\sin\omega t_1)]}dx \tag{18.56}$$

This is the same as Eq(17.15)

Chapter 19

Quantum Characteristic Function for Multiple Oscillators

We now consider the quantum distribution for N oscillators where the total force is

$$F(t) = \sum_{j=1}^{N} m_j \omega_j^2 \left(q_j \cos \omega_j t + p_j \frac{\sin \omega_j t}{m_j \omega_j} \right) \tag{19.1}$$

Then, the characteristic function for two different time is

$$M(\alpha, \beta) = e^{i\alpha F(t_1) + i\beta F(t_2)} \tag{19.2}$$

Since the oscillators are independent, p_j and $q_k$will commute when $j \neq k$. Therefore the total characteristic function will be product of the individual characteristic functions.

The individual characteristics function which we have calculated before, Eq. (19.2), is a diagonal matrix, the diagonal elements are

$$M_j(\alpha, \beta) = e^{-\frac{n_j m_j \hbar \omega_j^3}{4}(\alpha^2 + \beta^2 + 2\alpha\beta \cos \omega_j (t_2 - t_1))} e^{i 2 \omega_j \sqrt{\frac{n_j m_j \hbar \omega_j}{2}}(\alpha \cos \omega_j t_1 + \beta \cos \omega_j t_2)} \tag{19.3}$$

where n_j ranges from 0 to N. Therefore the total characteristic function is

$$M(\alpha, \beta) = \Pi_j M_j(\alpha, \beta) \tag{19.4}$$

$$e^{-\sum_j \frac{n_j m_j \hbar \omega_j^3}{4}(\alpha^2+\beta^2+2\alpha\beta\cos\omega_j(t_2-t_1))} e^{i\sum_j 2\omega_j\sqrt{\frac{n_j m_j \hbar \omega_j}{2}}(\alpha\cos\omega_j t_1+\beta\cos\omega_j t_2)} \tag{19.5}$$

To eliminate the cross term $\alpha\beta$, we make the following transformation

$$\alpha \to \frac{1}{\sqrt{2}}(\alpha' + \beta') \tag{19.6}$$

$$\beta \to \frac{1}{\sqrt{2}}(\alpha' - \beta') \tag{19.7}$$

and hence

$$M(\alpha', \beta') = \tag{19.8}$$

$$\exp[-\sum_j \{\frac{n_j m_j \omega_j^3 \hbar}{4}[(1+\cos\omega_j(t_2-t_1))\alpha'^2 + (1-\cos\omega_j(t_2-t_1))\beta'^2] \tag{19.9}$$

$$+ i\omega_j\sqrt{n_j m_j \omega_j \hbar}[\alpha'(\cos\omega_j t_1 + \cos\omega_j t_2) + \beta'(\cos\omega_j t_1 - \cos\omega_j t_2)]\}] \tag{19.10}$$

Calculating the joint distribution,

$$P(F_1, F_2) = \frac{1}{4\pi^2}\int\int M(\alpha', \beta') e^{-\frac{i\alpha'}{\sqrt{2}}(F_1+F_2)-\frac{i\beta'}{\sqrt{2}}(F_1-F_2)} d\alpha' d\beta' \tag{19.11}$$

Here α' and β' is already separated integration and $1 + \cos\omega_j(t_2 - t_1) > 0$, therefore it can be integrated,

$$P(F_1,F_2)=\frac{1}{\pi}\frac{\exp\left[-\frac{\{\sum_j[n_j\omega_j\sqrt{n_jm_j\omega_j\hbar}(\cos\omega_jt_1+\cos\omega_jt_2)]-\frac{1}{\sqrt{2}}(F_1+F_2)\}^2}{\sum_j n_jm_j\omega_j^3\hbar(1+\cos\omega_j(t_2-t_1))}\right]}{\sqrt{\sum_j n_jm_j\omega_j^3\hbar(1+\cos\omega_j(t_2-t_1))}} \tag{19.12}$$

$$\frac{\exp\left[-\frac{\{\sum_{j'}[\omega_{j'}\sqrt{n_{j'}m_{j'}\omega_{j'}\hbar}(\cos\omega_{j'}t_1-\cos\omega_{j'}t_2)]-\frac{1}{\sqrt{2}}(F_1-F_2)\}^2}{\sum_{j'} n_{j'}m_{j'}\omega_{j'}^3\hbar(1-\cos\omega_{j'}(t_2-t_1))}\right]}{\sqrt{\sum_{j'} n_{j'}m_{j'}\omega_{j'}^3\hbar(1-\cos\omega_{j'}(t_2-t_1))}} \tag{19.13}$$

$$\sum_j n_jm_j\omega_j^3\hbar=\sum_{j'} n_{j'}m_{j'}\omega_{j'}^3\hbar=N \tag{19.14}$$

$$\sum_j n_jm_j\omega_j^3\hbar\cos\omega_jt=\sum_{j'} n_{j'}m_{j'}\omega_{j'}^3\hbar\cos\omega_{j'}t=C(t) \tag{19.15}$$

$$P(F_1,F_2)=\frac{1}{\pi}\frac{\exp\{-\frac{[C(t_1)+C(t_2)-\frac{1}{2}(F_1+F_2)]^2(N-C(t_2-t_1)+[C(t_1)-C(t_2)-\frac{1}{2}(F_1-F_2)]^2(N+C(t_2-t_1))}{N^2-C^2(t_2-t_1)}\}}{\sqrt{N^2-C^2(t_2-t_1)}} \tag{19.16}$$

$$=\frac{\exp\{-\frac{2N[C^2(t_1)+C^2(t_2)+\frac{1}{4}(F_1^2+F_2^2)+C(t_1)F_1+C(t_2)F_2]-2C(t_2-t_1)[2C(t_1)C(t_2)-F_1F_2-C(t_1)F_2-C(t_2)F_1]}{N^2-C^2(t_2-t_1)}}{\pi\sqrt{N^2-C^2(t_2-t_1)}}\} \tag{19.17}$$

This is 2-dimensional normal distribution with correlation

$$\rho=\frac{C(t_2-t_1)}{N}=\frac{\sum_j n_jm_j\omega_j^3\hbar\cos\omega_j(t_2-t_1)}{\sum_j n_jm_j\omega_j^3\hbar}$$

Chapter 20

Quantum Joint Distribution Function of Force at Different Times Using Annihilation and Creation Operators

In this chapter we will use creation and annihilation operators instead of position and momentum operators to obtain the joint distributions. The annihilation and creation operators are

$$a_i^\dagger = \sqrt{\frac{\hbar}{2m\omega}}\,[q - ip] \tag{20.1}$$

$$a_i = \sqrt{\frac{\hbar}{2m\omega}}\,[q + ip] \tag{20.2}$$

and inversely

$$\mathbf{q}_i = \sqrt{\frac{\hbar}{2m\omega}}(a_i^\dagger + a_i) \tag{20.3}$$

$$\hat{p}_i = i\sqrt{\frac{m\hbar\omega}{2}}(a_i^\dagger - a_i) \tag{20.4}$$

The Hamiltonian of a single oscillators is

$$H = \hbar\omega_i(a_i^\dagger a_i + \frac{1}{2}) \tag{20.5}$$

and the quantum canonical ensemble density-matrix (non-normalized) at temperature T is given by

$$\rho = e^{-\frac{H}{kT}} \tag{20.6}$$

Furthermore the expectation value of operator A is given by

$$< A >= \frac{\mathrm{Tr}(\rho A)}{\mathrm{Tr}(\rho)} \tag{20.7}$$

where Tr is the trace operator and ρ is density-matrix. The characteristic function, Eq. (19.3), expressed in terms of annihilation and creation operators becomes

$$M(\alpha, \beta) = e^{(v_j a_i^\dagger - v_i^* a_i)} \tag{20.8}$$

where

$$v_i = \omega_i\sqrt{\frac{m_i\hbar\omega_i}{2}}(i\alpha\cos\omega_i t_1 + i\beta\cos\omega_i t_2 - \alpha\sin\omega_i t_1 - \beta\sin\omega_i t_2) \tag{20.9}$$

The eigenfunctions $|\alpha >$ of the annihilation operator are the coherent states and have the following properties

$$a|\alpha> = \alpha|\alpha> \tag{20.10}$$

$$<\alpha|\alpha> = 1 \tag{20.11}$$

$$<\alpha|a^\dagger| = \alpha^* <\alpha| \tag{20.12}$$

$$<\alpha|\beta> = e^{-|\alpha-\beta|^2} \tag{20.13}$$

$$\frac{1}{\pi}\int d^2\alpha|\alpha><\alpha| = 1 \tag{20.14}$$

The normalized coherent state can be expanded in term of number states $|n>$ by way of

$$|\alpha>= e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n> \tag{20.15}$$

The trace of an arbitrary operator A can be calculated using coherent state by integrating over the entire complex plan

$$\mathrm{Tr}(A) = \frac{1}{\pi}\int d^2\alpha <\alpha|A|\alpha> \tag{20.16}$$

Also, the trace of the density-matrix is

$$\mathrm{Tr}(\rho) = \frac{1}{\pi}\int d^2\alpha <\alpha|e^{-\frac{1}{kT}\hbar\omega_i(a_i^\dagger a_i+\frac{1}{2})}|\alpha> \tag{20.17}$$

Now using the fact that [22]

$$e^{-\frac{1}{kT}\hbar\omega_i a^\dagger a} = N\{e^{(e^{-\frac{1}{kT}\hbar\omega_i}-1)a^\dagger a}\} \tag{20.18}$$

where the notation $N\{\}$ means that the operators inside $\{\}$ are normal ordered. We then have

$$\mathrm{Tr}(\rho) = \frac{1}{\pi} e^{-\frac{1}{2kT}\hbar\omega_i} \int d^2\alpha < \alpha | N\{e^{(e^{-\frac{1}{kT}\hbar\omega_i}-1)a^\dagger a}\} | \alpha > \tag{20.19}$$

$$= \frac{1}{\pi} e^{-\frac{1}{2kT}\hbar\omega_i} \int d^2\alpha e^{(e^{-\frac{1}{kT}\hbar\omega_i}-1)\alpha^* \alpha} \tag{20.20}$$

$$= \frac{e^{-\frac{\hbar\omega_i}{2kT}}}{1 - e^{-\frac{\hbar\omega_i}{kT}}} \tag{20.21}$$

Now we calculate the expectation value of the characteristic function operator. We have,

$$< M(\alpha, \beta) > = \frac{1}{Tr(\rho)} \int P_i(m_i, \omega_i) \mathrm{Tr}(\rho M(\alpha, \beta)) dm_i d\omega_i \tag{20.22}$$

$$= \frac{1}{Tr(\rho)} \int P_i(m_i, \omega_i) \mathrm{Tr}[e^{-\frac{1}{kT}\hbar\omega_i(a_i^\dagger a_i + \frac{1}{2})} e^{(v_j a_i^\dagger - v_i^* a_i)}]/Tr(\rho) dm_i d\omega_i \tag{20.23}$$

Using

$$e^{A+B} = e^{-\frac{1}{2}[A,B]} e^A e^B \tag{20.24}$$

which is the case when

$$[A, [A, B]] = [B, [A, B]] = 0 \tag{20.25}$$

then

$$e^{(v_j a_i^\dagger - v_i^* a_i)} = e^{\frac{1}{2} v_i^* v_i} e^{-v_i^* a_i} e^{v_i a_i^\dagger} \tag{20.26}$$

Eq.(20.23) can be simplified as follows

$$< M(\alpha,\beta) > = \frac{1}{Tr(\rho)} \int P_i(m_i,\omega_i) e^{\frac{1}{2}v_i^* v_i - \frac{1}{2kT}\hbar\omega_i} Tr(e^{v_i a_i^\dagger} e^{-\frac{1}{kT}\hbar\omega_i a_i^\dagger a_i} e^{-v_i^* a_i}) dm_i d\omega_i \tag{20.27}$$

$$= \frac{1}{Tr(\rho)} \int P_i(m_i,\omega_i) \frac{1}{\pi} e^{\frac{1}{2}v_i^* v_i - \frac{1}{2kT}\hbar\omega_i} \tag{20.28}$$

$$\int d^2\alpha < \alpha | e^{v_i a_i^\dagger} e^{-\frac{1}{kT}\hbar\omega_i a_i^\dagger a_i} e^{-v_i^* a_i} | \alpha > dm_i d\omega_i \tag{20.29}$$

$$= \frac{1}{Tr(\rho)} \int P_i(m_i,\omega_i) \frac{1}{\pi} e^{\frac{1}{2}v_i^* v_i - \frac{1}{2kT}\hbar\omega_i} \tag{20.30}$$

$$\int d^2\alpha < \alpha | e^{v_i a_i^\dagger} N\{e^{(e^{-\frac{1}{kT}\hbar\omega_i} - 1) a^\dagger a}\} e^{-v_i^* a_i} | \alpha > dm_i d\omega_i \tag{20.31}$$

$$= \frac{1}{Tr(\rho)} \int P_i(m_i,\omega_i) \frac{1}{\pi} e^{\frac{1}{2}v_i^* v_i - \frac{1}{2kT}\hbar\omega_i} \int d^2\alpha e^{v_i \alpha_i^*} e^{(e^{-\frac{1}{kT}\hbar\omega_i} - 1)\alpha^* \alpha} e^{-v_i^* \alpha_i} dm_i d\omega_i \tag{20.32}$$

Substituting Eq.(20.21) for eq(20.32) we have

$$< M(\alpha,\beta) >= \int P_i(m_i,\omega_i) e^{-\frac{\hbar m_i \omega_i^3}{4} \coth(\frac{\hbar\omega_i}{2kT})[\alpha^2+\beta^2+2\alpha\beta\cos\omega_i(t_1-t_2)]} dm_i d\omega_i \tag{20.33}$$

The distribution corresponding to this characteristic function is 2-D normal distribution

$$P(x,y) = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-r^2}} e^{-\frac{1}{2(1-r^2)}\left[\frac{(x-a)^2}{\sigma_x^2} + \frac{(y-b)^2}{\sigma_y^2} - 2r\frac{(x-a)(y-b)}{\sigma_x\sigma_y}\right]} \tag{20.34}$$

This result is similar to classical harmonic oscillator, Eq.(8.31) The corresponding parameter of σ^2 and r are

$$\sigma^2 = \sum_{i=1}^{N} \frac{\hbar m_i \omega_i^3}{2} \coth\frac{\hbar\omega_i}{2kT} \tag{20.35}$$

$$r = \frac{\sum_{i=1}^{N} \frac{\hbar m_i \omega_i^3}{2} \coth\frac{\hbar\omega_i}{2kT} \cos\omega_i(t_1-t_2)}{\sum_{i=1}^{N} \frac{\hbar m_i \omega_i^3}{2} \coth\frac{\hbar\omega_i}{2kT}} \tag{20.36}$$

The autocorrelation function between the two forces is

$$< F_1F_2 > = \int r\sigma^2 \prod_{i=1}^{N} P_i(m_i, \omega_i) dm_i d\omega_i \tag{20.37}$$

$$= \int P_i(m_i, \omega_i) \sum_{i=1}^{N} \frac{\hbar m_i \omega_i^3}{2} \coth \frac{\hbar \omega_i}{2kT} \cos \omega_i (t_1 - t_2) dm_i d\omega_i \tag{20.38}$$

In the case where all oscillators have identical distribution functions the result is similar to classical case as well

$$< F_1F_2 > = \int D(m, \omega) \frac{\hbar m \omega^3}{2} \coth \frac{\hbar \omega}{2kT} \cos \omega (t_1 - t_2) dm d\omega \tag{20.39}$$

$$= N \int P(m, \omega) \frac{\hbar m \omega^3}{2} \coth \frac{\hbar \omega}{2kT} \cos \omega (t_1 - t_2) dm d\omega \tag{20.40}$$

where $D(m, \omega)$ and $P(m, \omega)$ has the same definition as Eq. (8.44) and Eq. (8.46).

The first Markovian condition requires that eq(20.40) is delta function, thus

$$P(m, \omega) \frac{\hbar m \omega^3}{2} \coth \frac{\hbar \omega}{2kT} = C' \tag{20.41}$$

$$P(m, \omega) = \frac{2C'}{\hbar m \omega^3} \tanh \frac{\hbar \omega}{2kT} \tag{20.42}$$

where C' is a constant. However, this constant is different from classical case due to different normalizing condition

$$\int P(m, \omega) dm d\omega = \int \frac{2C'}{\hbar m \omega^3} \tanh \frac{\hbar \omega}{2kT} dm d\omega = 1 \tag{20.43}$$

If we compare this with classical case, Eq.(8.48), where $P(m, \omega) = \frac{C}{m\omega^2}$, we see that the choice of $P(m, \omega)$ for a quantum Markovian system depends on the temperature.

For the case where $T \to 0$

$$\lim_{T\to 0} \tanh \frac{\hbar\omega}{2kT} = 1 \tag{20.44}$$

$$P(m,\omega) = \frac{2C'}{\hbar m\omega^3} \tag{20.45}$$

$$\int \frac{2C'}{\hbar m\omega^3} dm d\omega = 1 \tag{20.46}$$

At a very high temperature when, $2kT \gg \hbar\omega_{max}$, where we assume there is a cut off in the probability distribution $P(m,\omega)$ at a maximum ω_{max} we have that

$$\lim_{2kT\gg\hbar\omega_{max}} \tanh \frac{\hbar\omega}{2kT} = \frac{\hbar\omega}{2kT} \tag{20.47}$$

$$P(m,\omega) = \frac{C'}{m\omega^2} \tag{20.48}$$

This result is exactly same as Eq. (8.47). We can also obtain the same condition by using the classical limit where $\hbar \to 0$. On the other hand, if we can use the probability distribution of classical case in quantum autocorrelation function

$$< F_1F_2 >= N \int \frac{C\hbar\omega}{2} \coth \frac{\hbar\omega}{2kT} \cos\omega(t_1 - t_2) dm d\omega \tag{20.49}$$

We can see the spectrum of quantum random force F is

$$S_{\text{quantum}}(\omega)_F = \frac{CN\hbar\omega}{2} \coth \frac{\hbar\omega}{2kT} \tag{20.50}$$

while the classical spectrum is constant

$$S_{\text{classical}}(\omega)_F = CNkT \tag{20.51}$$

For a more general result we can assume the initial wave function of is an ensemble of wave functions $\psi_1(q)$, $\psi_2(q)$ ... $\psi_z(q)$, where q is a N-dimensional vector of all positions of individual oscillators. We can define the characteristic function for Z different initial conditions as

$$M(\alpha,\beta) = \sum_{k=1}^{Z} \int \psi_k^*(q) e^{i\alpha F(t_1)+i\beta F(t_2)} \psi_k(q) dq \prod_{i=1}^{N} P_i(m_i,\omega_i) dm_i d\omega_i \tag{20.52}$$

Since all oscillators are independent, the wave function of the system is product of individual wave functions

$$\psi_k(q) = \prod_{j=1}^{N} \psi_{k,i}(q_i) \tag{20.53}$$

$$[i\alpha f_i(t_1) + i\beta f_i(t_2), i\alpha f_j(t_1) + i\beta f_j(t_2)] = 0 : i \neq j \tag{20.54}$$

The characteristic function is now

$$M(\alpha,\beta) = \sum_{k=1}^{Z} \prod_{i=1}^{N} \int \psi_{k,i}^*(q_i) e^{i\alpha f_i(t_1)+i\beta f_i(t_2)} \psi_{k,i}(q_i) P_i(m_i,\omega_i) dq_i dm_i d\omega_i \tag{20.55}$$

We redefine the inner integral as

$$M(\alpha,\beta) = \sum_{k=1}^{Z} \prod_{i=1}^{N} \int M_{k,i}(\alpha,\beta) P_i(m_i,\omega_i) dm_i d\omega_i \tag{20.56}$$

where

$$M_{k,i}(\alpha,\beta) = \int \psi_{k,i}^*(q_i) e^{i(t_1)+i\beta f_i(t_2)} \psi_{k,i}(q_i) dq_i \tag{20.57}$$

We use Eq. (8.8) and Eq. (8.9) to obtain that

$$i\alpha f_i(t_1) + i\beta f_i(t_2) = i m_i \omega_i^2 [\alpha \cos\omega_i t_1 + \beta \cos\omega_i t_2] \hat{q}_i(0) + i\omega_i [\alpha \sin\omega_i t_1 + \beta \sin\omega_i t_2] \hat{p}_i(0) \tag{20.58}$$

The position and momentum operator satisfy

$$[\hat{q}_i(0), \hat{p}_i(0)] = i\hbar \tag{20.59}$$

and using the relation $e^{A+B} = e^{\frac{1}{2}[A,B]}e^A e^B$ we have

$$e^{i\alpha(t_1)+i\beta f_i(t_2)} = e^{\frac{i\hbar m_i \omega_i^3}{2}[\alpha\cos\omega_i t_1+\beta\cos\omega_i t_2][\alpha\sin\omega_i t_1+\beta\sin\omega_i t_2]} \tag{20.60}$$

$$e^{im_i\omega_i^2[\alpha\cos\omega_i t_1+\beta\cos\omega_i t_2]\hat{q}_i(0)} e^{i\omega_i[\alpha\sin\omega_i t_1+\beta\sin\omega_i t_2]\hat{p}_i(0)} \tag{20.61}$$

Since $e^{ix\mathbf{p}}$ is displacement operator,

$$e^{ix\mathbf{p}}\psi(q) = \psi(q + x\hbar) \tag{20.62}$$

and $\hat{q}_i(0)$ is q_i in position representation, we have that

$$M_{k,i}(\alpha, \beta) = e^{\frac{i\hbar m_i \omega_i^3}{2}[\alpha\cos\omega_i t_1+\beta\cos\omega_i t_2][\alpha\sin\omega_i t_1+\beta\sin\omega_i t_2]} \tag{20.63}$$

$$\int \psi_{k,i}^*(q_i) e^{im_i\omega_i^2[\alpha\cos\omega_i t_1+\beta\cos\omega_i t_2]q_i} \psi_{k,i}(q_i + \omega_i[\alpha\sin\omega_i t_1 + \beta\sin\omega_i t_2]\hbar)dq_i \tag{20.64}$$

By replacing q_i with $q_i - \omega_i[\alpha\sin\omega_i t_1 + \beta\sin\omega_i t_2]\frac{\hbar}{2}$, we obtain that

$$M_{k,i}(\alpha, \beta) = \int \psi_{k,i}^*(q_i - \omega_i[\alpha\sin\omega_i t_1 + \beta\sin\omega_i t_2]\frac{\hbar}{2}) e^{im_i\omega_i^2[\alpha\cos\omega_i t_1+\beta\cos\omega_i t_2]q_i} \tag{20.65}$$

$$\psi_{k,i}(q_i + \omega_i[\alpha\sin\omega_i t_1 + \beta\sin\omega_i t_2]\frac{\hbar}{2})dq_i \tag{20.66}$$

The probability distribution function is then

$$P_{k,i}(f_1, f_2) = \frac{1}{4\pi^2}\int M_{k,i}(\alpha, \beta) e^{-i\alpha f_1 - i\beta f_2} d\alpha d\beta \tag{20.67}$$

and by a change of variables

$$\lambda = \alpha m_i \omega_i^2 \cos \omega_i t_1 + \beta m_i \omega_i^2 \cos \omega_i t_2 \tag{20.68}$$

$$\theta = \alpha \omega_i \sin \omega_i t_1 + \beta \omega_i \sin \omega_i t_1 \tag{20.69}$$

We obtain

$$P_{k,i}(f_1, f_2) = \frac{1}{4\pi^2} \frac{1}{m_i \omega_i^3 |\sin \omega_i (t_2 - t_1)|} \int \psi^*_{k,i}(q_i - \theta \frac{\hbar}{2}) \psi_{k,i}(q_i + \theta \frac{\hbar}{2}) \tag{20.70}$$

$$\exp[i\lambda q - i \frac{\lambda \omega_i \sin \omega_i t_2 - \theta m_i \omega_i^2 \cos \omega_i t_2}{m_i \omega_i^3 \sin \omega_i (t_2 - t_1)} f_1 - \frac{-\lambda \omega_i \sin \omega_i t_1 + \theta m_i \omega_i^2 \cos \omega_i t_1}{m_i \omega_i^3 \sin \omega_i (t_2 - t_1)} f_2] d\lambda d\theta dq_i \tag{20.71}$$

Comparison with the Wigner function

The Wigner distribution is defined by

$$W(q,p) = \frac{1}{\pi \hbar} \int \psi^*(q+y) \psi(q-y) e^{2ipy/\hbar} \tag{20.72}$$

Setting

$$p = \frac{-\cos \omega_i t_2 f_1 + \cos \omega_i t_1 f_2}{\omega_i \sin \omega_i (t_2 - t_1)} \tag{20.73}$$

we have

$$P_{k,i}(f_1, f_2) = \frac{1}{2\pi m_i \omega_i^3 |\sin \omega_i (t_2 - t_1)|} \int W_{k,i}(q_i, \frac{-\cos \omega_i t_2 f_1 + \cos \omega_i t_1 f_2}{\omega_i \sin \omega_i (t_2 - t_1)}) \tag{20.74}$$

$$\exp i\lambda [q_i - \frac{\sin \omega_i t_2}{m_i \omega_i^2 \sin \omega_i (t_2 - t_1)} f_1 + \frac{\sin \omega_i t_1}{m_i \omega_i^2 \sin \omega_i (t_2 - t_1)} f_2] dq_i d\lambda \tag{20.75}$$

$$= \frac{1}{m_i \omega_i^3 |\sin \omega_i (t_2 - t_1)|} W_{k,i}(\frac{\sin \omega_i t_2 f_1 - \sin \omega_i t_1 f_2}{m_i \omega_i^2 \sin \omega_i (t_2 - t_1)}, \frac{-\cos \omega_i t_2 f_1 + \cos \omega_i t_1 f_2}{\omega_i \sin \omega_i (t_2 - t_1)}) \tag{20.76}$$

We now take

$$\rho(x,x') = \sqrt{\frac{m\omega\tanh(\frac{\hbar\omega}{2kT})}{\pi\hbar}}\exp[-\frac{m\omega}{4\hbar}((x-x')^2\coth(\frac{\hbar\omega}{2kT}) + (x+x')^2\tanh(\frac{\hbar\omega}{2kT})] \quad (20.77)$$

and furthermore we have that the corresponding Wigner distribution is

$$W(x,p) = \frac{1}{\pi\hbar}\int dy\rho(x-y,x+y)e^{2ipy/\hbar} \quad (20.78)$$

$$= \frac{1}{\pi\hbar}\tanh(\frac{\hbar\omega}{2kT})\exp[-(\frac{p^2}{m\hbar\omega} + \frac{m\omega^2x^2}{\hbar\omega})\coth(\frac{\hbar\omega}{2kT})] \quad (20.79)$$

Substituting Eq. () into Eq. (20.76)

$$P_i(f_1,f_2) = \frac{1}{m_i\omega_i^3|\sin\omega_i(t_2-t_1)|}\frac{1}{\pi\hbar}\tanh(\frac{\hbar\omega_i}{2kT})\exp[-(\frac{p_i^2}{m_i\hbar\omega_i} + \frac{m_i\omega_i x^2}{\hbar})\coth(\frac{\hbar\omega_i}{2kT})] \quad (20.80)$$

$$= \frac{1}{\pi\hbar m_i\omega_i^3\coth(\frac{\hbar\omega_i}{2kT})|\sin\omega_i(t_2-t_1)|}\exp[-\frac{\coth(\frac{\hbar\omega_i}{2kT})}{m_i\omega_i^3\sin^2\omega_i(t_2-t_1)} \quad (20.81)$$

$$(f_1^2+f_2^2-2f_1f_2\cos\omega_i(t_2-t_1))]$$

Compare this with standard two dimensional Gaussian distribution, the corresponding parameters are

$$\sigma^2 = \frac{\hbar m_i\omega_i^3}{2}\coth(\frac{\hbar\omega_i}{2kT}) \quad (20.82)$$

$$r = \cos\omega_i(t_2-t_1) \quad (20.83)$$

This result is same as Eq. (8.34) with only one oscillator.

Chapter 21

Time-Frequency Wigner Evolution of the Quantum Langevin Equation

This chapter is based on our paper on the time-frequency Wigner evolution of the quantum Langevin equation[6]. Our aim is to study the time-frequency evolution of the quantum Langevin equation and in particular to obtain the power spectrum of momentum analogous to the result obtained by Wang and Uhlenbeck [23] for the classical Langevin equation (for a history see [24]). We will obtain the time dependent spectrum, that is, both the transient and steady state solution. One of the fundamental issues in this regard is how to define a time dependent spectrum and this will be discussed in the next section. In the rest of the introduction we briefly discuss the classical Langevin equation and the result of Wang and Uhlenbeck. We emphasize that the Wang and Uhlenbeck result only holds for time going to infinity if the system was started at a finite time, or, alternatively, if the current time is finite and the system was started at minus infinity. That is, an infinite amount of time has to pass. We emphasize this point because our intent is to consider finite time, that is we find the stochastic properties of the full solution, the transient and steady state part.

The classical Langevin equation is

$$m\frac{d^2x(t)}{dt^2}+\gamma\frac{dx(t)}{dt}+V'(x)=\xi(t) \tag{21.1}$$

where $x(t)$ is the position of the particle, γ is the friction constant, m is the mass of the particle and $V(x)$ is the potential. In Eq. (21.1) $\xi(t)$ is the random fluctuating force and in the classical case the random force is taken to be white noise,

$$E[\xi(t))]=0 \tag{21.2}$$

$$\langle\xi(t)\xi(t')\rangle=2D\delta(t'-t) \tag{21.3}$$

Of course in equilibrium $D=\gamma kT$ where k is the Boltzman constant and T the temperature. From a physics point of view the fact that indeed $D=\gamma kT$ is of paramount importance and the relation is generally obtained by applying the fluctuation dissipation theorem. The viewpoint we take here is to consider Eq. (21.1) as a stochastic differential equation and momentarily not couple D to the other parameters. That is, we start a particle from a fixed position/velocity that is subsequently influenced by the stationary heat bath that itself is kept stationary. The Langevin equation for momentum is

$$\dot{p}(t)+\beta p(t)=\xi(t) \tag{21.4}$$

where now we have taken the case of zero external potential and where

$$\beta=\frac{\gamma}{m} \tag{21.5}$$

Eq. (21.4) is now in the generic notation of Wang and Uhlenbeck. The power spectrum is defined by

$$S(\omega) = \int R_p(\tau) e^{-i\tau\omega} d\tau \tag{21.6}$$

where

$$R_p(\tau) = \langle p(t)p(t+\tau) \rangle \tag{21.7}$$

In Eq. (21.7) there is the tacit assumption that indeed $\langle p(t)p(t+\tau) \rangle$ is independent of time but that is not the case. As previously noted, it is the case for infinite time. Wang and Uhlenbeck showed that in that case the power spectrum is

$$S(\omega) = \frac{2D}{\beta^2 + \omega^2} \tag{21.8}$$

The importance of this result is manyfold but most importantly it shows that the power spectrum falls off relatively slowly and hence large velocity fluctuations are relatively more possible than for example if the power spectrum was an exponential decay one. For white noise Galleani and Cohen obtained the full solution and showed how it evolves into this solution for infinite time [25, 26, 27, 28]. Our aim here is to get the quantum transient and its evolution towards equilibrium. Since we are interested in the evolution of the power spectrum we have to consider the concept of a time-varying spectrum and this is done in the next section.

The response of systems to random inputs has a long history in engineering [29, 30]. Generally speaking the standard methods do not handle nonstationary noise and we have devised a method that allows one to do that by way of the time-frequency representations, such as the Wigner distribution. We also point out that in general much of the physics literature applies the fluctuation-disspiation theorem and couples the noise source to the friction source. However in the engineering literature and in the viewpoint presented here one looks at the governing equation as being driven by the external noise source.

Time dependent spectrum

For many natural and man made time series (signals) the distribution of frequencies varies with time. Among the most common are such signals as pressure waves, electromagnetic pulses, biologicals, among many others [15, 14]. There have been many approaches developed and the field is generally called time-frequency analysis and while most of the methods developed deal with deterministic signals they can be generalized to random signals. One of the approaches is to define a quasi-distribution, or representation that indicates how the frequencies are changing in time. One such representation is the Wigner distribution which applies to deterministic signals and the Wigner *spectrum* which applies to random functions. The Wigner distribution in physics is usually defined for position and momentum. Here we are considering it as a time-varying spectrum, that is, a function of time and frequency. This development was started in the 1940's and has become the main method to study time-varying spectra in engineering. To understand how one arrives at the Wigner spectrum one first defines the Wigner distribution, $W_X(t,\omega)$, of a deterministic time function $X(t)$ by [20, 31]

$$W_X(t,\omega) = \frac{1}{2\pi}\int X^*(t-\tau/2)X(t+\tau/2)e^{-i\tau\omega}d\tau \tag{21.9}$$

Then to handle random functions one now defines Wigner-Ville spectrum $\overline{W}_X(t,\omega)$ by taking the ensemble average of the Wigner distribution of $X(t)$ [15]

$$\overline{W}_X(t,\omega) = \frac{1}{2\pi}\int \langle X^*(t-\tau/2)X(t+\tau/2)\rangle\, e^{-i\tau\omega}d\tau \tag{21.10}$$

In Eq. (21.10) $\langle\rangle$ is the ensemble averaging operator. The advantage of the Wigner spectrum, in contrast to the standard power spectrum is that the Wigner spectrum can describe a time-varying stochastic process. Also, one defines

$$R(t,\tau) = \langle X^*(t-\tau/2)X(t+\tau/2)\rangle \tag{21.11}$$

and hence

$$\overline{W}_X(t,\omega) = \frac{1}{2\pi}\int R(t,\tau)e^{-i\tau\omega}d\tau \tag{21.12}$$

$R(t,\tau)$ may be thought of as a time dependent autocorrelation function. We also mention that there are many other ways to approach the issue [15, 14, 32, 33, 34, 35, 36] of time dependent spectrum and that among the earliest papers was that of Eberly and Wódkiewicz [37], where they defined the "physical spectrum of light" which is very similar to spectrograms as defined in engineering.

The time-frequency Wigner spectrum of quantum noise

In the quantum case one has [38, 39, 40, 18, 41, 4]

$$m\frac{d^2\mathbf{x}(t)}{dt^2} + m\beta\frac{d\mathbf{x}(t)}{dt} + V'(\mathbf{x}) = \xi(t) \tag{21.13}$$

where $\mathbf{x}$ is the position operator and $\xi(t)$ is the noise operator that satisfies

$$\langle[\xi(t),\xi(t')]_+\rangle = \frac{2\gamma\hbar}{\pi}\int_0^\infty \omega\coth\frac{\hbar\omega}{2kT}\cos\omega(t-t')d\omega \tag{21.14}$$

$$= \frac{\gamma\hbar}{\pi}\int_{-\infty}^{\infty} \omega e^{i\omega(t-t')}\coth\frac{\hbar\omega}{2kT}d\omega \tag{21.15}$$

We will consider Eq. (21.13) as a classical type equations, sometimes called the *quasiclassical* Langevin equation, where we replace the operators by ordinary variables and take for the autocorrelation function

$$R(\tau) = \frac{1}{2}\left\langle [\xi(t), \xi(t+\tau)]_+ \right\rangle \tag{21.16}$$

$$= \frac{\gamma\hbar}{2\pi}\int_{-\infty}^{\infty} \omega e^{i\omega\tau} \coth\frac{\hbar\omega}{2kT} d\omega \tag{21.17}$$

Using Eq. (21.6) for the definition of power spectrum one has

$$S(\omega) = \gamma\hbar\omega \coth\frac{\hbar\omega}{2kT} \tag{21.18}$$

To use some of the techniques previously developed for arbitrary colored noise we now artificially rewrite these equations in the following form. We define

$$Z = \frac{\hbar}{2kT} \tag{21.19}$$

and write

$$\dot{p}(t) + \beta p(t) = \xi(t) \tag{21.20}$$

$$R_\xi(\tau) = 2DZ\int_{-\infty}^{\infty} \omega e^{i\omega\tau} \coth Z\omega d\omega \tag{21.21}$$

where the power spectrum of the noise is now

$$S_\xi(\omega) = 2DZ\omega \coth Z\omega \tag{21.22}$$

We introduced D to make it look like the classical Langevin equation and we can now view Eq. (21.20) as a stochastic differential equation where the driving force is a colored noise that depends on two parameters D and Z. This will show the structure of the solution in a simpler way and furthermore special cases can be studied easier. Specifically, the white noise case is obtained when $Z \to 0$, since

$$\lim_{Z\to 0} R_\xi(\tau) = 2D\delta(\tau) \tag{21.23}$$

Now consider the general issue of the Wigner spectrum when the autocorrelation function is a function of the difference in time [28]

$$\langle X^*(t')X(t)\rangle = K(t-t') \tag{21.24}$$

The Wigner spectrum of such a process is then

$$\overline{W}_X(t,\omega) = \frac{1}{2\pi}\int \langle X^*(t-\tau/2)X(t+\tau/2)\rangle\, e^{-i\tau\omega} d\tau \tag{21.25}$$

$$= \frac{1}{2\pi}\int K(t+\tau/2-(t-\tau/2))e^{-i\tau\omega} d\tau \tag{21.26}$$

which gives

$$\overline{W}_X(t,\omega) = \frac{1}{2\pi}\int K(\tau)e^{-i\tau\omega} d\tau \tag{21.27}$$

As expected, it is independent of time and equal to the power spectrum except for the 2π factor which just comes the way the Wigner spectrum is defined. For the specific case of quantum noise we have that the Wigner spectrum of quantum noise is

$$\overline{W}_\xi(t,\omega) = \frac{DZ}{\pi}\omega \coth Z\omega \tag{21.28}$$

However as we will see the output of the Langevin equation does depend on time. For future use we note that when indeed we have the Wigner spectrum of the form given by Eq. (21.28), then the power spectrum and Wigner spectrum are related by

$$S(\omega) = 2\pi \overline{W}_X(t,\omega) \text{ (for the stationary situation)} \tag{21.29}$$

Time Evolution of the Wigner spectrum

We want to obtain the Wigner spectrum of the momentum process

$$\overline{W}_p(t,\omega) = \frac{1}{2\pi} \int \langle p^*(t-\tau/2)p(t+\tau/2)\rangle \, e^{-i\tau\omega} d\tau \tag{21.30}$$

where the momentum process is the stochastic solution of Eq. (21.20). We now describe two separate approaches to the calculation of $\overline{W}_p(t,\omega)$.

Direct approach. In the direct approach there are four steps. One symbolically "solves" Eq. (21.20) for $p(t)$ and forms $p^*(t-\tau/2)p(t+\tau/2)$. One then calculates the ensemble average $\langle\, p^*(t-\tau/2)p(t+\tau/2)\ \rangle$ and then calculates the Wigner spectrum by way of Eq. (21.30). We have found that this approach is generally quite difficult to carry out, particularly for time dependent problems.

Differential equation approach . This approach was developed by Galleani and Cohen and involves writing a differential equation for the Wigner spectrum directly and solving it [25, 26, 27, 28]. This gives the solution without calculating the intermediate steps involved in the direct approach.

The idea is to convert a differential equation of the form

$$a_n \frac{d^n x(t)}{dt^n} + a_{n-1}\frac{d^{n-1}x(t)}{dt^{n-1}} \cdots + a_1 \frac{dx(t)}{dt} + a_0 x(t) = f(t) \tag{21.31}$$

into the phase space differential equation a differential equations for the Wigner distribution of $x(t)$. The method to do that is to write the differential equation in polynomial form

$$P(D)x(t) = f(t) \tag{21.32}$$

where D and $P(D)$ are respectively

$$D = \frac{d}{dt} \tag{21.33}$$

$$P(D) = a_n D^n + a_{n-1} D^{n-1} ... + a_1 D + a_0 \tag{21.34}$$

We also define the operators

$$A = \frac{1}{2}\frac{\partial}{\partial t} - i\omega \quad ; \quad B = \frac{1}{2}\frac{\partial}{\partial t} + i\omega \tag{21.35}$$

The differential equation for the Wigner distribution $W_x(t,\omega)$, of $x(t)$,

$$W_x(t,\omega) = \frac{1}{2\pi}\int x^*(t-\tau/2)x(t+\tau/2)e^{-i\tau\omega}d\tau \tag{21.36}$$

is then given by [25, 26, 27, 28]

$$P^*(A)P(B)W_x(t,\omega) = W_f(t,\omega) \tag{21.37}$$

If one considers random functions one takes the ensemble average of both sides of Eq.(21.37). Applying Eq. (21.37) to Eq. (21.4) with one straightforwardly obtains

$$\left[\frac{1}{4}\frac{\partial^2}{\partial t^2} + \beta\frac{\partial}{\partial t} + \beta^2 + \omega^2\right]\overline{W}_p(t,\omega) = \frac{DZ}{\pi}\omega\coth Z\omega \tag{21.38}$$

To the best authors' knowledge, Eq.(21.38) for the time-dependent Wigner spectrum of momentum for the Langevin equation driven by quantum noise is given here for the first time. Eq.(21.38) when the driving force is white noise was solved by Galleani and Cohen. The solution with quantum noise is obtained relativity easy because the left hand side contains no derivatives with respect to ω,

$$\overline{W}_p(t,\omega) = \frac{W_\xi}{\beta^2+\omega^2}\left[1-e^{-\frac{2\gamma}{m}t}\cos 2\omega t\right] \tag{21.39}$$

$$= \frac{1}{\beta^2+\omega^2}\frac{DZ}{\pi}\omega\coth Z\omega\left[1-e^{-\frac{2\gamma}{m}t}\cos 2\omega t\right] \tag{21.40}$$

We see that Eq. (21.40) can now be thought of as the generalization of the Wang and Uhlenbeck result in two ways. First, it gives a time dependent spectrum of momentum and secondly it applies to quantum noise. We now consider some limiting values. First we consider the steady state solution, that is, for time going to infinity

$$\overline{W}_p(\infty,\omega) = \lim_{t\to\infty}\overline{W}_p(t,\omega) = \frac{DZ}{\pi}\frac{\omega}{\beta^2+\omega^2}\coth Z\omega \tag{21.41}$$

Explicitly, the power spectrum is then,

$$S(\omega) = 2DZ\frac{\omega}{\beta^2+\omega^2}\coth Z\omega \tag{21.42}$$

The white noise limit is obtained by considering

$$\lim_{Z\to 0}\overline{W}_p(\infty,\omega) = \frac{2D}{\beta^2+\omega^2}\frac{1}{2\pi}\text{(Wang-Uhlenbeck)}$$

Quantum Wiener Process ($\gamma = 0$).The case without friction is of some interest and in the classical case it is called the Wiener process. In this case we have

$$\dot{p}(t) = \xi(t) \tag{21.43}$$

and in analogy with the classical case we call this the quantum Wiener process. The differential equation for the Wigner spectrum is

$$\frac{1}{4}\frac{\partial^2\overline{W}_p(t,\omega)}{\partial t^2}+\omega^2\overline{W}_p(t,\omega)=\frac{DZ}{\pi}\omega\coth Z\omega \tag{21.44}$$

and the solution is

$$\begin{aligned} W_p(t,\omega) &= \frac{DZ}{\pi}\omega\coth Z\omega(1-\cos 2\omega t) && (21.45)\\ &= \frac{2DZ}{\pi}\omega\coth Z\omega\sin^2\omega t && (21.46)\end{aligned}$$

Discussion and future research.

In the above we have considered the evolution of the spectrum of momentum for the Langevin equation when the driving noise is quantum noise. We have done so by defining the Wigner spectrum for momentum and finding and solving the differential equation governing it. By taking the long time limit we obtained the stationary solution and further by taking Planck's constant going to zero we obtained the result of Wang and Uhlenbeck.

We point out that there are many ways to solve the harmonic oscillator by transforming the equations of motion into different domains. One can then write a joint distribution for these new variables. This can be a fruitful approach but one of main issue in this regard is that while a joint classical probability distribution can consistently be transformed from one domain to another, a similar procedure is not available for joint quantum representations [13, 42, 11, 43, 44]. That is, if a classical problem is solved for two different sets of variables and their joint distribution is written for each of the variables then the transformation from one joint distribution to another is straightforward. However that is not the case of quais-probability distributions and this would certainly be an interesting problem to study [13].

There is also the question of handling noise in different representations and fundamental issues arise in both the quantum and classical case. A step toward this problem is discussed in [13, 11, 44].

We now mention some extensions that are currently being pursued. Of particular interest is the fact that the Wigner distribution spectrum has what are called cross terms which are “artifacts” and sometimes obscure the evolution [15, 35]. Suppose a signal is

$$x(t) \;=\; x_1(t) \;+ x_2(t) \tag{21.47}$$

Substituting this into the definition, we have

$$W(t,\omega) \;=\; W_{11}(t,\omega) + W_{22}(t,\omega) + W_{12}(t,\omega) + W_{21}(t,\omega) \tag{21.48}$$

where

$$W_{12}(t,\omega) \;=\; \frac{1}{2\pi}\int x_1{}^{*}(t-\tau/2)\, x_2(t+\tau/2)\, e^{-j\tau\omega}\, d\tau \tag{21.49}$$

and similarly for W_{12}. We note that since $W_{12} \;= W_{21}^{*}$

$$W(t,\omega) \;=\; W_{11}(t,\omega) + W_{22}(t,\omega) + 2\,\mathrm{Re}\;\;\{W_{12}(t,\omega)\} \tag{21.50}$$

That is, the Wigner distribution of the sum of two signals is not the sum of the Wigner distribution of each signal but has the additional term 2 Re $\{W_{12}(t,\omega)\}$. This term is often called the interference term or the cross term and sometimes are referred to as artifacts. The extent to which distributions enhance or reduce the cross terms has been studied and has led to new distributions[15, 35, 33, 34]. We point out that ensemble averaging can have a strong effect on the cross terms because they oscillate greatly. One way to study this issue for our particular case is to calculate other representations. There have been may representations that have been studied and proposed besides the Wigner distribution [43, 15, 44, 12, 35, 34]. and their properties studied. All distributions can be studied by way of the kernel method which characterizes a particular distribution. In particular, all distributions, the general class, may be obtained from [43]

$$C(t,\omega) \;=\; \frac{1}{4\pi^2}\iiint s^*(u-\tau/2)\,s(u+\tau/2)\,\phi(\theta,\tau)\,e^{-j\theta t-j\tau\omega+j\theta u}\,du\,d\tau\,d\theta \tag{21.51}$$

where $\phi(\theta,\tau)$ is the kernel and characterizes the distribution and its properties. For example the Wigner distribution and Choi Williams are obtained by taking $\phi(\theta,\tau)$ equal to 1,exp$[-\theta\tau/\sigma]$, respectively. One can express the general class, $C(t,\omega)$, in terms of the Wigner distribution

$$C(t,\omega) \;=\; \iint g_{12}(t'-t,\omega'-\omega)\,W(t',\omega')\,dt'\,d\omega' \tag{21.52}$$

with

$$g(t,\omega) \;=\; \frac{1}{4\pi^2}\iint \phi(\theta,\tau)\,e^{j\theta t+j\tau\omega}\,d\theta\,d\tau \tag{21.53}$$

and hence $C(t,\omega)$ can be calculated directly from the Wigner solution. Of particular interest is the Choi-Williams distribution[33] or the whole class of distributions that are called reduced interference distributions [15, 35, 33, 34]. Another interesting quantity that is being studied is the instantaneous random frequency. One of the advantages of the Wigner spectrum approach is that the random instantaneous frequency can be readily calculated since it is the first conditional moment of frequency for a given time [45]. Also, we are currently calculating the Wigner spectrum of position for the standard Langevin equation and also for the case of Brownian motion of a harmonic oscillator driven by quantum noise.

Chapter 22

Concluding Remarks

We have derived a noise model for the classical and quantum case. The advantage of this model is that one can calculate all relevant statistical quantities exactly and explicitly. In both the quantum and classical case our general approach has been to use the characteristic function. In the quantum case we have had to use the Weyl correspondence rule to define the quantum characteristic function and this is necessary because the position and creation operators do not commute. For the quantum case the expressions can often be put in terms of the Wigner distribution. As to future work in this regard we point out that there are other correspondence rules besides the Weyl correspondence. Furthermore each correspondence rule corresponds to a particular distribution. It would be interesting to repeat the calculations using these other correspondence rules and distributions. Alternatively one can use the transformation method that allows one to transform distribution functions. Also, we have considered the evolution of the spectrum of momentum for the Langevin equation when the driving noise is quantum noise. We have done so by defining the Wigner spectrum for momentum and finding and solving the differential equation governing it. By taking the long time limit we obtained the stationary solution and further by taking Planck's constant going to zero we obtained the result of Wang and Uhlenbeck.

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