

# CHAPTER III

## CLASSICAL AND QUANTUM

### BROWNIAN MOTION

#### (FUNCTIONAL INTEGRAL APPROACH)

#### 3.1 HISTORY OF THE FOUNDATION OF BROWNIAN MOTION

In the year 1905 Einstein [11] discovered new fundamental laws outside the field of relativity. At the time when Einstein came to Bern, he was intensely occupied with the problem of light and motion but he saw that the final goal could be attained only by attacking the problem from various angles. One of the paths to the goal, he realized, was to investigate the relations between light and heat, and between heat and motion.

It had been known for some time that heat is connected with the irregular motion of molecules. The higher temperature, the more violent is this motion. The statistical behavior of particles in such irregular motion had been investigated chiefly by the Scottish physicist James Clerk Maxwell (1831-79) and the Austrian Ludwig Boltzmann (1844-1906). At the time of Maxwell and Boltzmann, however, the molecular constitution of matter was still a hypothesis, since there was as yet no very direct proof of the existence of the molecule, which could be doubted. Einstein strongly felt the necessity of investigating this matter more thoroughly and obtain more direct proof of molecular motion.

It had been known that small but microscopically visible particles, when suspended in a fluid with approximately the same density, exhibit a constant, apparently irregular zigzag motion. It had been discovered by Scottish botanist Robert Brown for pollen dust suspended in water, and for this reason it is known as "Brownian motion" and the microscopically visible particle suspended in water is called "Brownian particle". He also observed that very fine particles of minerals undergo similar incessant motion as if they were living object. The Brownian motion is not caused by any external influence jarring the vessel or by currents of water in the vessel, and the agitation increases in intensity when the temperature of the water is raised. For this reason it had been conjectured that the motion is connected with the heat motion of the molecules. According

to this view, the kinetic energy of the water molecules is constant collision with the microscopic particle produces irregular forces in random direction, which gives rise to the observed motions. The idea of combining such a motion –Brownian motion- with molecular motion became fairly widespread in the latter half of the nineteenth century when atomism had not yet been fully recognized as reality.

In 1902 Einstein had restated Boltzmann's theory of random motion in a simplified form. He now treated the Brownian motion with this method and arrived at a surprisingly simple result. In this way Einstein [6] was able to derive the mean square value of the displacement of the particle which could be immediately observed by the experiment. This famous formula [7] is of the form

$$\overline{x^2} = \frac{2k_B T}{f} \cdot t \quad (3.1)$$

where  $f$  is the friction coefficient,  $T$  the absolute temperature and  $t$  the time. This formula stated that the average displacement of the particles in any direction increased as the square root of the time. The influence of the surrounding medium is characterized by  $f$  as well as by  $T$ .

The actual observations were later made by the French physicist Jean Perrin, who completely verified Einstein's theory. He gave the following set of counts of the displacement of a grain of radius  $2.1 \times 10^{-5}$  cm. at 30 sec. intervals. Out of a number  $N$  of such observations the number of observed value of displacement between  $x_1$  and  $x_2$  should be

$$\frac{N}{\pi^{1/2}} \int_{x_1}^{x_2} \exp(-x^2/4Dt) \frac{dx}{(4Dt)^{1/2}} \quad (3.2)$$

where  $D$  is the diffusion coefficient.

Eq. (3.2) comes from the fact that the probability density of finding the particle at point  $x$  and time  $t$  when it starts from  $x = 0$  at time  $t = 0$  of a free particle, which was originally derived by Einstein [6], is of the form

$$F(x, t) = \frac{1 \cdot \exp(-x^2/4Dt)}{(4\pi Dt)^{1/2}} \quad (3.3)$$

He derived this equation by finding for  $F$  a partial differential equation, which in this case is the diffusion equation:

$$\frac{\partial F}{\partial t} = D \frac{\partial^2 F}{\partial x^2} \quad \text{with the initial condition } F(x,0) = \delta(x) \quad (3.4)$$

This initial condition is clear from the definition of  $F(x,t)$  because for  $t = 0$ , there is certainly that  $x = 0$ . Einstein simply derived the relation between the diffusion coefficient  $D$  and the friction coefficient  $f$  by using the osmotic pressure idea [6]. Perrin showed that (see Table 3.1) eq. (3.2) agreed with the experimental observed value.

Range $x \times 10^4$ cm	1st set		2nd set		Total	
	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.
0 - 3.4	82	91	86	84	168	175
3.4 - 6.8	66	70	65	63	131	132
6.8 - 10.2	46	39	31	36	77	75
10.2 - 17.0	27	23	23	21	50	44

Table 3.1 : Observations and calculations if the distribution of the displacements of a Brownian particle

The phenomenon of Brownian motion has subsequently always been included among the best "direct" proof of the existence of the molecule. At any rate, Einstein's theory had a great impact at that time, finally convincing people of the theory of heat as molecular motion, and so paved the way to modern physics of the twentieth century. It also greatly influences pure mathematics, that is, the theory of stochastic processes.

There many interesting papers written by Einstein and others people who develop this field. For the reader who is interested in this theory, you should read papers and books on references [6] – [10] especially the book in ref. [6] that contains five papers written between 1905 and 1908 by Albert Einstein. The theory of Brownian motion was further developed by P. Langevin, M. Smoluchowski, G.E. Uhlenbeck, L.S. Ornstein, and many others. The classical theory was excellently reviewed by Wang and Uhlenbeck [8] which we will mainly use this work to review the theory in the next section.

### 3.2 GAUSSIAN RANDOM PROCESS, METHOD OF RICE, AND FOKKER - PLANCK EQUATION

After the work of Einstein, many people tried to develop the method in order to solve the problem more systematically and also more generally than the old one. The very

famous method is starting from the so-called "Langevin equation" [1] and then, by using this equation, finding some interested (ensemble) average quantities at a given time  $t$  such as the mean square value of the displacement. However, this method is not general enough. In some cases, if one wants to find the average value of some strange quantities, say the general function of random variables, it may be that one can't directly use the Langevin equation to find them. By this reason, it is more advantageous, at the beginning of the problem, to find the probability distributions because the average value of any function of random variables can be calculated if one wants to know it. Moreover, the probability distribution gives us the pictorial information about the specific quantity such as the location of Brownian particle at a given time interval.

Now, we will review two well-known methods i.e., method of Rice and Fokker-Planck which provide the ways to obtain the probability distributions. These methods are not dealing with the general random processes but are dealing with the so-called "Gaussian random processes" [8], [10]. However, it is sufficient [8] to deal with Gaussian random processes for the Brownian motion problem. Before describing what Gaussian random process is, we should first review some important concepts and quantities. Consider the random process  $y(t)$  which roughly (for precise definition, see ref. [12], [13] or other books in the field of stochastic processes) means that the variable  $y$  does not depend on a completely definite way on the independent variable  $t$  as in causal process, instead one gets in different observations different function  $y(t)$ , so that only certain probability distributions are directly observable. The random process  $y(t)$  is completely described by the following set of probability distributions:

$W_1(y, t) dy =$  probability of finding  $y$  in the range  $(y, y + dy)$  at time  $t$ .

$W_2(y_1, t_1; y_2, t_2) dy_1 dy_2 =$  joint probability of finding  $y$  in the range  $(y_1, y_1 + dy_1)$  at time  $t_1$  and in the range  $(y_2, y_2 + dy_2)$  at time  $t_2$ .

$W_3(y_1, t_1; y_2, t_2; y_3, t_3) dy_1 dy_2 dy_3 =$  joint probability of finding a triple of values of  $y$  in the ranges  $dy_1, dy_2, dy_3$  at time  $t_1, t_2, t_3$ .

And so on

(3.5)

The set of functions in eq. (3.5) must fulfill the following obvious conditions:

(a)  $W_n \geq 0$

(b)  $W_n(y_1 t_1; y_2 t_2 \dots y_n t_n)$  is symmetric function in the set of variables  $y_1 t_1 \dots y_n t_n$ .

This is clear since  $W_n$  is a joint probability.

(c)  $W_k(y_1 t_1; \dots y_k t_k) = \int \dots \int dy_{k+1} \dots dy_n W_n(y_1 t_1; \dots y_n t_n)$

since each function  $W_n$  must imply all the previous  $W_k$  with  $k < n$ .

In most application (especially for the Brownian motion problem) we can make a simplification because the processes are "stationary" [1], [6] in time. This means that the underlying mechanism which causes the fluctuations does not change in a course of time. A shift of the  $t$ -axis will then not influence the functions  $W_n$ . In other word, there is no preferred origin in time for the statistical description of  $y$  i.e., the same ensemble ensues when all member functions of the ensemble are shifted by arbitrary amounts in time. In this case, it is clear that the ensemble average of  $y$  must be independent of time and the set of functions in eq. (3.5) becomes:

$W_1(y)dy$  = probability of finding  $y$  between  $y$  and  $y + dy$  (it is independent of time)

$W_2(y_1 y_2 t) dy_1 dy_2$  = joint probability of finding a pair of value of  $y$  in the range  $dy_1$  and  $dy_2$  which are a time interval  $t$  apart from each other ( $t$  is therefore =  $t_2 - t_1$ )

And so on (3.7)

There is another assumption called "ergodic assumption" which is usually assumed in the Brownian motion problem. This assumption means that the function  $y(t)$  for each system of the ensemble will, in the course of sufficiently long time, pass through all the values accessible to it. By this assumption, it is clear that the time average of  $y$  in each system of the ensemble is the same. By these reasons, for "Stationary ergodic ensemble", one can cut the record in many pieces of time length  $T$  (where  $T$  is long compared to all period occurring in the process) from "one" record  $y(t)$  taken over a sufficiently long time and these pieces should then constitute as good a representative ensemble of the statistical behavior of  $y$  as the original ensemble. Hence, for stationary ergodic ensemble, the time average should be equivalent to the ensemble average (this

can be proved mathematically, see ref. [1]) and one can, therefore, use either one of them without distinguishing them as in general processes.

The "Gaussian random process" is characterized by the fact that all basic distribution functions eq. (3.5) are Gaussian distributions, and one could take this fact as the defining property of the process. Consider the stationary random function  $y(t)$  over a long time  $T$  and suppose that  $y(t)$  is repeated periodically with the period  $T$ . One can then develop  $y(t)$  in a Fourier series:

$$y(t) = \sum_{n=1}^{\infty} a_n \cos 2\pi f_n t + b_n \sin 2\pi f_n t; \quad ; f_n = n/T \quad (3.8)$$

There is no constant term  $a_0$  since we will assume that the average value of  $y$  is zero. The coefficient  $a_n$  and  $b_n$  are random variables, and we will assume that they are all independent of each other and Gaussianly distributed with average value zero, so that one has for the probability that  $a_n$  and  $b_n$  are in certain ranges  $da_n, db_n$  the expression:

$$W(a_1 a_2 \dots; b_1 b_2 \dots) = \prod_n \frac{1}{\sigma_n \sqrt{2\pi}} \exp\left[-(a_n^2 + b_n^2)/2\sigma_n^2\right] \quad (3.9)$$

where  $\sigma_n^2 = \langle a_n^2 \rangle = \langle b_n^2 \rangle \equiv G(f_n)/T$ .  $G(f)$  which is defined here by this relation is called the "spectral density". In order to determine the probability distribution of  $y$ , we will use the theorem about Gaussian distribution:

Suppose the variable  $x_1, x_2, \dots, x_n$  are distributed according to:

$$W(x_1, \dots, x_n) = \prod_{i=1}^n \frac{1}{\sigma_i (2\pi)^{1/2}} \exp(-x_i^2/2\sigma_i^2) \quad (3.10)$$

Let  $z_1, z_2, \dots, z_s$  ( $s \leq n$ ) be  $s$  linear combination of the  $x_i$ :

$$z_k = \sum_{i=1}^n a_{ki} x_i \quad ; k = 1, 2, \dots, s \quad (3.11)$$

where  $a_{ki}$  are constants. One can prove [8] that  $z_k$  will be distributed according to the  $s$ -dimensional Gaussian distribution:

$$W(z_1, \dots, z_s) = \frac{1}{(2\pi)^{s/2} B^{1/2}} \exp\left[-\frac{1}{2B} \sum_{k,l=1}^s B_{kl} z_k z_l\right] \quad (3.12)$$

Here  $B_{kl}$  is the cofactor of the element  $b_{kl}$  in the matrix  $b_{kl}$  where

$$b_{kl} = \sum_{i=1}^n a_{ki} a_{li} \sigma_i^2 = \langle z_k z_l \rangle \quad (3.13)$$

and  $B$  is the determinant of the matrix  $b_{kl}$ . As a special case, taken for instance,  $s = 2$ . One then gets the two-dimensional Gaussian distribution, which according to eq. (3.12) can be written in the form:

$$W(z_1, z_2) = \frac{1}{2\pi\rho\tau(1-\rho^2)^{1/2}} \exp\left[-\frac{1}{2(1-\rho^2)}\left\{\frac{z_1^2}{\sigma^2} + \frac{z_2^2}{\tau^2} - \frac{2\rho}{\sigma\tau} z_1 z_2\right\}\right] \quad (3.14)$$

where  $\sigma^2 = \langle z_1^2 \rangle$ ,  $\tau^2 = \langle z_2^2 \rangle$  and  $\langle z_1 z_2 \rangle = \sigma\rho\tau$ .  $\rho$  here is called the "correlation coefficient"

By using this theorem, if one compare eq. (3.9) with eq. (3.10) and eq. (3.8) with eq. (3.11), the joint probability distribution of finding  $y_1 = y(t_1)$  and  $y_2 = y(t_2)$  can be obtained by using the eq. (3.14) as

$$W(y_1, y_2) = \frac{1}{2\pi\rho\tau(1-\rho^2)^{1/2}} \exp\left[-\frac{1}{2(1-\rho^2)}\left\{\frac{y_1^2}{\sigma^2} + \frac{y_2^2}{\tau^2} - \frac{2\rho}{\sigma\tau} y_1 y_2\right\}\right] \quad (3.15)$$

Here  $\sigma^2 = \langle y_1^2 \rangle$ ,  $\tau^2 = \langle y_2^2 \rangle$  and  $\langle y_1 y_2 \rangle = \sigma\rho\tau$ .  $\rho$  again is called the correlation coefficient.

From eq. (3.8) and the definition of spectral density (below eq. (3.9)), we can express many forms of expectation value in terms of this spectral density. For example,

$$\left. \begin{aligned} \langle y^2 \rangle &= \int_0^\infty G(f) df \\ \langle y_1 y_2 \rangle &= \int_0^\infty G(f) \cos 2\pi f \tau df \quad ; \quad \tau = t_2 - t_1 \\ \langle \dot{y}^2 \rangle &= 4\pi^2 \int_0^\infty f^2 G(f) df \end{aligned} \right\} \quad (3.16)$$

Notice that  $\langle y^2 \rangle$ ,  $\langle \dot{y}^2 \rangle$  are independent of time and  $\langle y_1 y_2 \rangle$  which is called the "correlation function" (since it determines the correlation behavior of random variables at different time) depends only on the time interval  $\tau = t_2 - t_1$  as they should be since the process is stationary. In this method, one can see that not only  $W_2(y_1 t_1; y_2 t_2)$  can be found

but the joint distribution function  $W_n(y_1 t_1 \dots y_n t_n)$  which will be the n-dimensional Gaussian distribution depends only on  $t_2 - t_1, t_2 - t_2, \dots, t_n - t_{n-1}$  and the distribution function concerning the differentiation of  $y$  such as  $W_4(y\dot{y}_1, y\dot{y}_2, \tau)$  where  $\tau = t_2 - t_1$  can be found too since the expectation value in eq. (3.13) is always computed by the use of eq. (3.8). Moreover, all expectation value of the form  $\langle y_1'' \dot{y}_1''' y_2^k \dot{y}_2^l \rangle$  can also be determined in terms of the spectral density by the use of eq. (3.8) (e.g.,  $\langle \dot{y}^2 \rangle$  in eq. (3.16)).

The method for determining the probability distribution that we have shown above is called the "Method of Rice" which actually works within the domain of Gaussian random process. By above discussions, the problem seems to be completely solved by this method if one only knows the spectral density or the correlation function. In the actual problems of Brownian motion this spectral density can be found from the so-called Langevin equation which will be discussed in the next section. It should be emphasized, however, that for many applications it is an advantage that one can leave open the questions of the actual shape of the spectrum.

Now, we will review the next method which is called the "method of Fokker-Planck [8], [15] ". Before reviewing it, it is first necessary to describe roughly about the "Markoff processes [8], [12], [13]". A Markoff process is defined by the equation:

$$P_n(y_1 t_1, y_2 t_2 \dots y_{n-1} t_{n-1} | y_n t_n) = P_2(y_{n-1} t_{n-1} | y_n t_n) \quad (3.17)$$

where  $P_n(y_1 t_1, y_2 t_2 \dots y_{n-1} t_{n-1} | y_n t_n)$  is the conditional probability density of finding  $y_n$  at time  $t_n$  when giving  $y_1, y_2, \dots, y_{n-1}$  at time  $t_1, t_2, \dots, t_{n-1}$  respectively. This equation means that the event at time  $t_n$  depends on the only one of previous event at time  $t_{n-1}$ . By this definition, it is implied intuitively that the Markoff processes is completely described by  $W_2$ . This fact can be proved easily by first considering the obvious equation (from now on we shall restrict ourselves to stationary processes):

$$W_2(y_1, y_2) = W_1(y_1) P_2(y_1 | y_2, t) \quad (3.18)$$

From eqs. (3.17) and eq. (3.18), it is easy to prove that all the  $W_n$  for  $n > 2$  can be found when only  $W_2$  is known. For example, for  $n = 3$

$$W_3(y_1 t_1; y_2 t_2; y_3 t_3) = \frac{W_2(y_1 t_1; y_2 t_2) W_2(y_2 t_2; y_3 t_3)}{W_1(y_2 t_2)} \quad (3.19)$$



where  $W_1(y_2, t_2)$  can be found from  $W_2$  by using eq. (3.6) property (C),  $W_1(y_2, t_2) = \int W_2(y_1, t_1; y_2, t_2) dy_1$ . Eq. (3.19) shows clearly that the Markoff process is completely described by  $W_2$ . Moreover, in Brownian motion problem, the Markoff process is also completely described by  $P_2$  since one always has the expression (because the conditional effect on the probability should be absent in the course of very long time),

$$W_2(y_2) = \lim_{t \rightarrow \infty} P_2(y_1 | y_2, t) \quad (3.20)$$

and when combining with eq. (3.18),  $W_2$  can be found. The basic equation for the theory which follows from the definition of a Markoff process is called the "Smoluchowski equation". It shows that  $P_2$  must fulfill :

$$P_2(y_1 | y_2, t) = \int P_2(y_1 | y, t_0) P_2(y | y_2, t - t_0) dy \quad (3.21)$$

For all values of  $t_0$  between zero and  $t$

In general, the process may not be a Markoff process so it can not be completely described by  $W_2$ . However, in the physical applications it occurs very often that when a process is not Markoff process one can still consider it as a kind of "projection" of a more complicated Markoff process. Besides  $y$ , one then considers another dependent variable  $z$  (which may be, for instance,  $dy/dt$  or it may be a coordinate of another system), and it may be that for two variables  $y, z$  combined, the process is then Markoff process, so that:

$$P_2(y_1, z_1 | y_2, z_2, t) = \iint P_2(y_1, z_1 | yz, t_0) P_2(yz | y_2, z_2, t - t_0) dydz \quad (3.22)$$

By this reason, it is sometime, in physical applications, reasonable to assume the process a Markoff process and as a consequence, we have the Smoluchowski equation. Fortunately, there is a theorem which was first pointed out by J.L. Doob [14] about a Markoff process. It shows that the Gaussian process will be Markoffian only when the correlation function  $\rho(t) \propto \exp(-\beta t)$ , so according to eq. (3.16) the spectral density  $G(f) \propto 1/(\beta^2 + (2\pi f)^2)$  where  $\beta$  is constant. This theorem can be generalized to n-dimensional Gaussian process. it will be Markoffian only when the correlation matrix [8]  $R(t) \propto e^{Qt}$  where  $Q$  is a constant matrix. Now, we will derive the Fokker-Planck equation [8] by first assuming that the process is a Markoff process. Hence, we have the Smoluchowski equation (from now on we shall omit subscript 2 on  $P_2$  for the convenience),

$$P(x|y, t + \Delta t) = \int P(x|z, t)P(z|y, \Delta t)dz \quad (3.23)$$

Let  $R(y)$  is an arbitrary function which goes to zero for  $|y| \rightarrow \infty$  sufficiently fast. Consider,

$$\int R(y) \frac{\partial}{\partial t} P(x|y, t) dy = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int R(y) [P(x|y, t + \Delta t) - P(x|y, t)] dy \quad (3.24)$$

Inserting eq. (3.23) into eq. (3.24), we obtain

$$\int R(y) \frac{\partial P}{\partial t} dy = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int dy R(y) \int dz P(x|z, t) P(z|y, \Delta t) - \int dz R(z) P(x|z, t) \right] \quad (3.25)$$

In the double integration, interchange the order of integration and develop  $R(y)$  in a Taylor series. The problem arises now !, if the series are not terminated, then the final result is very cumbersome and seems to be useless for practical calculation. This problem can be removed by making some reasonable physical assumptions. Consider the moments of the change in space coordinate in a small time  $\Delta t$  They are given by:

$$a_n(z, \Delta t) = \int (y - z)^n P(z|y, \Delta t) dy \quad (3.26)$$

We shall "assume" that for  $\Delta t \rightarrow 0$ , only the first and second moments become proportional to  $\Delta t$  (since the Brownian particle should move by a very small amount distance within a small time  $\Delta t$ ) so that

$$\left. \begin{aligned} A(z) &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} a_1(z, \Delta t) \\ B(z) &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} a_2(z, \Delta t) \\ \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} a_n(z, \Delta t) &= 0 \quad \forall n \geq 3 \end{aligned} \right\} \quad (3.27)$$

By this assumption, one can stop the Taylor series of  $R(y)$  at term  $(z - y)^2$  and one gets

$$\int dy R(y) \left[ \frac{\partial P}{\partial t} + \frac{\partial}{\partial y} (AP) - \frac{1}{2} \frac{\partial^2}{\partial y^2} (BP) \right] = 0 \quad (3.28)$$

Since this must hold for any function  $R(y)$ , the expression in the square brackets must be zero, which gives the general Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial y} [A(y)P] + \frac{1}{2} \frac{\partial^2}{\partial y^2} [B(y)P] \text{ with the initial condition } P(x|y,0) = \delta(y-x) \quad (3.29)$$

This method is elegant in the sense that it makes the original problem of finding the probability distribution to be the problem of solving the partial differential equation for the conditional probability and, actually, if one can solve it, the (Brownian motion) problem will be completely solved since this process is already Markoff process (which have been assumed at the beginning of the derivation) which means that the process is completely described by  $P_z$ . However, it is impossible, at this point, to solved this equation since we don't know the form of  $A(z)$  and  $B(z)$ , because to know them, one must have already known  $P(z|y, \Delta t)$ , see eq. (3.26). Notice that this method does not seems to be referred to Gaussian random processes at all but, instead, uses the assumption eq. (3.27). We will discuss the connection between this assumption and Gaussian random process the connection between this assumption and Gaussian random process in the next section.

From the method of Rice and Fokker-Planck, one can see that, in the method of Rice, the problem is completely solved if one knows the spectral density or correlation function and, in method of Fokker-Planck, the problem is completely solved if one knows  $A(z)$  and  $B(z)$ . All of these quantities can be obtained by the so-called Langevin equation which will be described in the next section.

### 3.3 LANGEVIN EQUATION AND CLASSICAL BROWNIAN MOTION

In previous section, we have reviewed the general mathematical method using to determine the probability distribution without using in specific problem. In this section, we will use these methods to study the specific physical phenomena which is already mentioned in section 3.1 as "Brownian motion". The Brownian motion can serve as a prototype problem whose analysis provides considerable insight into the mechanisms responsible for the existence of fluctuation and "dissipation of energy". The problem is also of great practical interest because such fluctuations constitute a background of "noise" which imposes limitations on the possible accuracy of delicate physical measurements.

For the sake of simplicity we shall treat the problem of Brownian motion in one dimension. We consider thus a Brownian particle of mass  $m$  whose (center-of-mass) coordinate at time  $t$  designated by  $x(t)$  and whose corresponding velocity is  $v = dx/dt$ . This particle immersed in a liquid at the absolute temperature  $T$ . It would be a hopelessly complex task to describe in details the interaction of the (center-of-mass) coordinate  $x$  with all the many degrees of freedom other than  $x$ . But these other degrees of freedom can be regarded as constituting a heat reservoir at some temperature  $T$ , and their interaction with  $x$  can be lumped into some net force  $F(t)$  effectively in determining the time dependent of  $x$ .

Focusing attention on the (center-of-mass) coordinate  $x$ . Newton's second law of motion can then be written in the form

$$m \frac{dv}{dt} = F(t) + K(t) \quad (3.29)$$

where  $K(t)$  is the external force such as gravity. Basically,  $F(t)$  must depend on the positions of a great many atoms which are in constant motion. Thus  $F(t)$  is some rapidly fluctuating function of the time  $t$  and varies in a highly irregular fashion. The rate at which  $F(t)$  varies can be characterized by some "correlation time"  $\tau^*$  which measure roughly the mean time between two successive maxima (minima) of the fluctuating function  $F(t)$ . This time  $\tau^*$  is quite small on a macroscopic scale i.e., about  $10^{-13}$  second if  $F(t)$  describes interaction with molecules of a typical liquid. When looking at eq. (3.29), one can not do anything with it since the complication of  $F(t)$ . So, what one should do is to play with the average procedure. First, integrate eq. (3.29) over some time interval  $\tau$  which is small on a macroscopic scale, but large in the sense that  $\tau \gg \tau^*$ . Then one gets.

$$m[v(t + \tau) - v(t)] = K(t)\tau + \int_t^{t+\tau} F(t') dt' \quad (3.30)$$

where we have assumed that the external force  $K(t)$  is varying slowly enough that it changes by a negligible amount during a time  $\tau$ . Taking an ensemble average of eq. (3.30) and thinking that  $F(t)$  changes sign many times in the time  $\tau$  so that the average value of it vanishes, one get

$$m \frac{d\bar{v}}{dt} = K(t) \quad (3.31)$$

Suppose that  $K(t) = 0$ , one can see that  $\bar{v}$  will not tend to zero as it should be when the particle reaches to the equilibrium. The reason is that we were too careless in treating the effect of  $F(t)$  in eq. (3.30). So,  $F(t)$  it self should contain a slowly varying part  $\bar{F}$  tending to restore the particle to equilibrium. Hence, we can write,

$$F(t) = \bar{F}(t) + \xi(t) \quad (3.32)$$

where  $\xi(t)$  is the rapidly fluctuating part of  $F$  whose average value vanishes. The slowly varying part must be some function of  $\bar{v}$  which is such that  $\bar{F}(\bar{v}) = 0$  in equilibrium when  $\bar{v} = 0$ . If  $\bar{v}$  is not too large,  $\bar{F}(\bar{v})$  can be expanded in a power series in  $\bar{v}$  whose first non vanishing term must be linear in  $\bar{v}$ . Thus  $\bar{F}$  must have the general form

$$\bar{F} = -\alpha\bar{v} \quad (3.33)$$

Where  $\alpha$  is some positive constant which is called "friction constant" and where minus sign indicates explicitly that the force  $\bar{F}$  acts in such a direction that it tends to reduce  $\bar{v}$  to zero as time increases. From eq. (3.32), it is reasonable that the velocity should be analogously composed of slowly and rapidly fluctuating part,

$$v(t) = \bar{v}(t) + v'(t) \quad (3.34)$$

where  $\bar{v}(t)$  and  $v'(t)$  denote the slowly varying part and the rapidly fluctuating part of  $v(t)$  whose average value vanishes respectively.

Inserting eqs. (3.32), (3.33) and (3.34) into eq. (3.29), we obtain

$$m \frac{dv}{dt} + \alpha v = K(t) + \xi(t) \quad (3.35)$$

where we have put  $\alpha\bar{v} \approx \alpha v$  with the negligible error. This comes from the fact that the rapidly fluctuation contribution  $\alpha v'$  can be neglected comparing to the predominant fluctuating term  $\xi(t)$  since the mass  $m$  is appreciable, see eq. (3.29). Equation (3.34) is called "Lagevin equation [1]". It differs from the original eq. (3.29) by explicitly decomposing the force  $F(t)$  into a slowly varying part  $-\alpha v$  representing a dynamical friction experienced by the particle and into a rapidly fluctuating part  $\xi(t)$  which is the

characteristic of Brownian motion. In the theory of Brownian motion, it is always postulated and not derived that the fluctuating part  $\xi(t)$  must satisfy [8], [7]:

$$\left. \begin{aligned} \langle \xi(t_1)\xi(t_2)\dots\xi(t_{2n-1}) \rangle &= 0, \\ \langle \xi(t_1)\xi(t_2)\dots\xi(t_{2n}) \rangle &= \sum_{\text{all pair}} \langle \xi(t_i)\xi(t_j) \rangle \cdot \langle \xi(t_k)\xi(t_l) \rangle \dots \end{aligned} \right\} \quad (3.36)$$

where the sum has to be taken over all the different ways in which one can divide the  $2n$  time points  $t_1, \dots, t_{2n}$  into  $n$  pairs.

The important point of this postulate eq. (3.36) is that it is "equivalent [8]" to the definition of Gaussian random process i.e., when writing  $\xi(t)$  in the Fourier series, its coefficients must be Gaussianly distributed, see eq. (3.8) and eq. (3.9). Moreover, one can easily show that eq. (3.27) which is first used as the assumption in order to derive Fokker-Planck equation can be derived by this postulate. By these reasons, one can conclude that under the domain of "Gaussian random process", we haven our discussions, two approaches to find the probability distribution of the problem. First, method of Rice and, second, the Fokker-Planck equation. For simplicity, if we treat  $\xi(t)$  as a "pure random process" i.e., the correlation occurs within only an infinitesimal time interval, then the correlation function of  $\xi(t)$  can be written in the form

$$\langle \xi(t_1)\xi(t_2) \rangle = 2KT\alpha\delta(t_1 - t_2) = 2Dm^2\delta(t_1 - t_2) \quad ; D = \frac{KT\alpha}{m^2} \quad (3.37)$$

Inserting eq. (3.37) into eq. (3.16), we get the spectral density of the reservoir corresponding the pure random process in the form

$$G_\xi = 2 \int_{-\infty}^{\infty} \langle \xi_1 \xi_2 \rangle \cos 2\pi f \tau d\tau = 4Dm^2 \quad (3.38)$$

It is called a "white spectrum" which is the constant for all  $f$ . Since  $\xi(t)$  is a Gaussian random process, it is clear that  $v(t)$  will also be a Gaussian random process. By using eqs. (3.38) and (3.35), the Gaussian random process  $v(t)$  has a spectral density in the form

$$G_v(f) = \frac{G_\xi / m^2}{\gamma^2 + (2\pi f)^2} = \frac{4D}{\gamma^2 + (2\pi f)^2}; \gamma = \alpha/m \quad (3.39)$$

By using eqs. (3.39), (3.16) and (3.14), one obtains

$$W_2(v_1, v_2, t) = \frac{\gamma}{2\pi D(1-\rho^2)^{1/2}} \exp\left[\frac{-\gamma}{2D(1-\rho^2)}\{v_1^2 + v_2^2 - 2\rho v_1 v_2\}\right] \quad (3.40)$$

where  $\rho = \exp(-\gamma t)$

Notice that  $G_v(f) \propto 1/\gamma^2 + (2\pi f)^2$ . Hence, the process  $v(t)$  is Markoff process due to the theorem of Doob. So, we also use Fokker-planck method for this process. From eq. (3.35), integrating both sides with respect to  $t$  from  $t$  to  $t + \Delta t$  and with eq. (3.37), it is easy to prove that  $A(v) = -\gamma v$  and  $B(v) = 2D$ . When inserting these quantities into eq. (3.28), we obtain the Fokker-Planck equation in the form,

$$\frac{\partial P}{\partial t} = \gamma \frac{\partial(vP)}{\partial v} + D \frac{\partial^2 P}{\partial v^2} \quad \text{with initial condition } P(v_0|v, t=0) = \delta(v - v_0) \quad (3.41)$$

where we suppose that at  $t = 0, v = v_0$ . The fundamental solution of this equation with this initial condition is

$$P(v_0|v, t) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left[-(v - \bar{v})^2/2\sigma^2\right] \quad (3.42)$$

where  $\bar{v} = v_0 \exp(-\gamma t)$  and  $\sigma^2 = \langle (v - \bar{v})^2 \rangle = (D/\gamma)[1 - \exp(-2\gamma t)]$

By using eq. (3.20), one can show from eq. (3.42) that

$$W_1(v) = \lim_{t \rightarrow \infty} P(v_0|v, t) = \left(\frac{\gamma}{2\pi D}\right)^{1/2} \exp\left(\frac{-\gamma v^2}{2D}\right) \quad (3.43)$$

Notice that this result is the Maxwell-Boltzmann distribution as it should be since the Brownian particle should reach to equilibrium for sufficiently long time. Moreover, when substituting eq. (3.42) and eq. (3.34) into eq. (3.18), we also get the same result of  $W_2(v_1, v_2, t)$  as in eq. (3.40) which was derived by the method of Rice. As one can see in this section, the Langevin eq. (3.35) with the postulate eq. (3.36) and also the assumption eq. (3.37) when using together with method of Rice or Fokker-Planck equation constitutes the "real basis foundation of (classical) Brownian motion"

There are others interested problems in Brownian motion. One of them is the problem about the relation between dissipation which is described in term of friction and fluctuation due to the random force. One can think that the friction constant  $\alpha$  must in some ways be expressible in term of the random force itself since the frictional restoring force is also caused by the interaction described by this random force. Of course, from eq. (3.30), by assuming that the correlation time  $\tau^*$  (which is of the order of mean period

of fluctuation of the random force and is also the relaxation time for the environment to come to internal equilibrium when disturbed by a sudden small change of Brownian particle) is much smaller than any macroscopically small time interval, one can prove that [1],

$$\gamma = \frac{1}{mKT} \int_0^{\infty} \langle \xi(0)\xi(t) \rangle dt \quad ; \gamma = \alpha/m \quad (3.44)$$

This equation which is sometime called "fluctuation-dissipation theorem" provides us with an explicit expression for the friction constant  $\alpha$  in term of correlation function of  $\xi(t)$ . Note that this equation is quite consistent, however not necessary, with the case of pure random process i.e., the correlation function is in the form of eq. (3.37) which corresponds to the white spectrum eq. (3.38). In real nature, such a pure random process can only be thought of as an approximation or the limiting case of some processes. Hence, instead of eq. (3.37), the correlation function should be in a more complicated form and also the spectrum should not be white i.e., it is not constant for all  $f$ . By these reasons, since eq. (3.44) is quite consistent with pure random process, it should change the form for the general processes in real nature. Since eq. (3.44) was derived by the use of the Langevin eq. (3.35), the Langevin equation, in general, should also change its form.

In other word, the assumption that the slowly varying part of random force is proportional to the slowly varying part of the velocity, which is the average of velocity, is quite reasonable when the process is pure. By this reason, the friction in general, instead of describing by friction constant, will be "retarded" and the Langevin equation should be generalized to [10], [15], [16]

$$m\ddot{x}(t) + m \int_{-\infty}^t \gamma(t-t') \dot{x}(t') dt' + V'(x) = \xi(t) \quad (3.45)$$

This equation describe the motion of Brownian particle in contact with the heat reservoir which is a source of "coloured noise". In this case, we define the so-called "frequency dependent damping coefficient" by [10]

$$\tilde{\gamma}(\omega) = \int_0^{\infty} \gamma(t) e^{i\omega t} dt \quad (3.46)$$

and one can prove the fluctuation-dissipation theorem [10],

$$\tilde{\gamma}(\omega) = \frac{1}{mKT} \int_0^{\infty} \langle \xi(0)\xi(t) \rangle e^{i\omega t} dt \quad (3.47)$$



Moreover, from eq. (3.45) (if the external force is zero) we can easily derive the relation between the spectral density of velocity and of reservoir as,

$$G_v(\omega) = \frac{G_\xi(\omega) m^2}{|i\omega + \tilde{\gamma}(\omega)|^2} \quad (3.48)$$

By this equation, if one model the spectrum of reservoir  $G_\xi(\omega)$  (it is equivalent to the model of the correlation function  $\langle \xi(0)\xi(t) \rangle$ ), one can find the spectrum of the velocity  $G_v(\omega)$  from which the correlation function  $\langle v(0)v(t) \rangle$  is obtained by the Wiener-Khintchine theorem [1], [10]. Moreover, it is easy to show from eq. (3.47) that the spectral density will be related with the real part of  $\tilde{\gamma}(\omega)$  by,

$$G_\xi(\omega) = 4mKT \operatorname{Re}\{\tilde{\gamma}(\omega)\} \quad (3.49)$$

Here we define the spectral density from eq(3.16) i.e.,  $G(f) = G(\omega) = 2 \int_{-\infty}^{\infty} \langle \xi_1 \xi_2 \rangle \cos(\omega t) dt$

Notice that if the retarded friction is not retard i.e.,  $\gamma(t-t') = \gamma\delta(t-t')$  then eq. (3.45) reduces to the old Langevin eq. (3.35),  $\tilde{\gamma}(\omega) = \gamma$ , eq. (3.47) reduces to eq. (3.44) and also tells us that  $\langle \xi_1 \xi_2 \rangle$  must obey eq. (3.37) which is the case of pure random process corresponding to white spectrum, eq. (3.48) reduces to eq. (3.39), and eq. (3.49) reduces to eq. (3.38).

### 3.4 LIMITATION OF CLASSICAL BROWNIAN MOTION AND SYSTEM-PLUS-RESERVOIR MODEL.

From previous section, the Brownian motion problem seems to be completely solved based on Langevin equation with Fokker-Planck equation or method of Rice. However, in order to obtain the Langevin equation, there are two main assumptions. First, the mass of Brownian particle must be sufficiently large in such a way that we can neglect the rapidly fluctuating part of velocity when comparing to the rapidly fluctuating part of force, second, the correlation time  $\tau^*$ . Which is the relaxation time for the environment to come to internal equilibrium must be much smaller than any microscopically small time intervals. This correlation time  $\tau^*$  will be larger when the temperature is lower. As we have known, the quantum behavior will occur to the microscopically particle which has very small mass such as electron and also occurs at sufficiently low temperature. By these reasons, we can not write down the Langevin equation of the form like eq. (3.35) or eq.

(3.45) for quantum particle (suppose that, at first approximation, ignore the uncertainty principle between coordinate and momentum) and although we can write it, the quantization procedure can not be progressed. This comes from the fact that the standard procedure of quantization relies upon the existence of Lagrangian or Hamiltonian function for the system which we can not find it since an equation of motion of the form eq. (3.35) or eq. (3.45) can't be obtained from the application of Hamilton's principle to any Lagrangian which has no explicit time dependence. Now, the question arises: how can one formulate the problem of quantum Brownian motion which is the Brownian motion under the situation where quantum behavior occurs?

By the above discussions, we cannot do any quantization procedure when dealing with the random force since the Hamiltonian or Lagrangian function can not be found. By this reason, one way we can do is to "model" the mechanism of dissipation explicitly without dealing with any random quantities, and from this model the Hamiltonian or Lagrangian function can be found so the quantization procedure will be progressed. Now the question arises again: how can one find the expectation value of any observable of the Brownian particle such as the momentum of Brownian particle from this model? The answer is simple, they can be found from the density matrix (which in fact is the reduced density matrix which will be discussed in section 3.6) as presented in Chapter II. This model we mentioned above is called the phenomenological "system-plus-reservoir" model. This model regards the system and its environment as together founding closed universe which and be described by a Lagrangian or Hamiltonian. In this picture the phenomenon of dissipation is simply the transfer of energy from the single degree of freedom characterizing the "system" to the very complex set of degrees of freedom describing the "environment". It is implicitly assumed that the energy, once transferred, will be effectively disappeared into the environment and will not recover within any time of physical interest.

The simplest model one can envisage is a model where the environment consists of a set of harmonic oscillators coupling "linearly" via the coordinate  $x$  of the Brownian particle. Caldeira and Leggett [17] pointed out that the environment consisting of harmonic oscillator is rather general and often provides a suitable description of a realistic

environment at sufficiently low temperature. The restriction of a realistic environment at sufficiently low temperature. The restriction of linearity i.e., "any one degree of freedom of the environment is sufficiently weakly perturbed" that it is permitted to put up a system-reservoir coupling which is linear in the reservoir coordinate and is physically reasonable when the system is macroscopic. Note that this does not necessarily imply that the dissipative influence on the system is "weak" as well, since the number of environment degree of freedom coupled to the system is very large.

The most general form of the Hamiltonian for the universe complying with these requirements is [16]

$$H = H_S + H_R + H_I \quad (3.50)$$

where

$$H_S = \frac{P^2}{2M} + V(x) \quad (3.51)$$

is the Hamiltonian of the isolated system i.e., the Brownian particle of mass  $M$  in potential  $V(x)$  (it may depend explicitly on time),

$$H_R = \sum_{\alpha=1}^N \left( \frac{1}{2} \frac{P_{\alpha}^2}{m_{\alpha}} + \frac{1}{2} m_{\alpha} \omega_{\alpha}^2 q_{\alpha}^2 \right) \quad (3.52)$$

describes the reservoir consisting of  $N$  harmonic oscillators which is usually large in number, and

$$H_I = - \sum_{\alpha=1}^N F_{\alpha}(x) q_{\alpha} + \Delta V(x) \quad (3.53)$$

is the interaction term. For the latter purpose, we added a counter-term  $\Delta V(x)$  which may depend on the parameters  $m_{\alpha}, \omega_{\alpha}$  of the environment, and on  $F_{\alpha}(x)$ , but not on the dynamical variable  $q_{\alpha}$ . If we assume for the moment that  $\Delta V(x)$  is zero, the minimum value of the potential energy of the universe which can be attained for given  $x$  is when  $q_{\alpha} = F_{\alpha}(x)/m_{\alpha}\omega_{\alpha}^2$  for all  $\alpha$ . To ensure that the system can not lower its potential energy below the original uncoupled value by moving off the  $x$  axis in the many-dimensional space where axis are  $x$  and  $q_{\alpha}$ 's, one can choose  $\Delta V(x)$  as

$$\Delta V(x) = - \sum_{\alpha} F_{\alpha}^2(x)/2m_{\alpha}\omega_{\alpha}^2 \quad (3.54)$$

This form of  $\Delta V(x)$  in eq. (3.54) compensates the coupling-induced renormalization of the potential and it is introduced here as a matter of convenience which

is reasonable if one wishes to consider solely the effect of dissipation. Naturally, such a term can always be split off from  $V(\mathbf{x})$  in eq. (3.51).

If we require that the interaction be separable and dissipation be "strictly linear" [17],  $F_\alpha(\mathbf{x})$  can be written in the form,

$$F_\alpha(\mathbf{x}) = c_\alpha x \quad (3.55)$$

Where  $c_\alpha$  is constant for all  $\alpha$

From eqs. (3.51) – (3.55), the Hamiltonian eq. (3.50) takes the specific form,

$$H = \frac{P^2}{2M} + V(x) + \frac{1}{2} \sum_{\alpha=1}^N \left\{ \frac{p_\alpha^2}{m_\alpha} + m_\alpha \omega_\alpha^2 \left( q_\alpha - \frac{c_\alpha x}{m_\alpha \omega_\alpha^2} \right)^2 \right\} \quad (3.56)$$

This Hamiltonian has been used to model dissipation for about thirty years. In the more recent literature, the model described by eq. (3.56) is usually called the "Caldeira-Leggett model".

### 3.5 PHENOMENOLOGICAL CALDEIRA-LEGGETT MODELLING [16]

In previous section, it is clear from the model that the Brownian particle should be transferred its energy to the environment. By this behavior, one may ask a question that: can one write the equation of motion of the Brownian particle in the form like eq. (3.45)? To answer this question, one should first find the equation of motion of the universe and then eliminate the coordinate of the environment later. We obtain for the model by eq. (3.56) the equation of motion

$$M\ddot{x}(t) + \frac{\partial V(x(t))}{\partial x(t)} - \sum_{\alpha=1}^N c_\alpha \left( q_\alpha(t) - \frac{c_\alpha x(t)}{m_\alpha \omega_\alpha^2} \right) = 0, \quad (3.57)$$

$$m_\alpha \ddot{q}_\alpha(t) + m_\alpha \omega_\alpha^2 q_\alpha(t) - c_\alpha x(t) = 0$$

From this equation, after eliminating the environmental coordinates  $q_\alpha$ , the equation of motion for  $x(t)$  can be written as

$$M\ddot{x}(t) + M \int_{-\infty}^t \gamma(t-t') \dot{x}(t') dt' + V'(x) = \xi(t) \quad (3.58)$$

where

$$\xi(t) = -\sum_{\alpha=1}^N c_{\alpha} \left[ \left( q_{\alpha}(0) + \frac{c_{\alpha}}{m_{\alpha} \omega_{\alpha}^2} x(0) \right) \cos(\omega_{\alpha} t) + \frac{\dot{q}_{\alpha}(0)}{\omega_{\alpha}} \sin(\omega_{\alpha} t) \right] \quad (3.59)$$

and

$$\gamma(t) = \frac{1}{M} \sum_{\alpha=1}^N \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}^2} \cos(\omega_{\alpha} t) \quad (3.60)$$

Substituting eq. (3.60) for  $\gamma(t)$  in eq. (3.46), the frequency-dependent damping coefficient  $\tilde{\gamma}(\omega)$  is in the form

$$\tilde{\gamma}(\omega) = \frac{i\omega}{m} \sum_{\alpha=1}^N \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}^2} \cdot \frac{1}{(\omega^2 - \omega_{\alpha}^2)} \quad (3.61)$$

At this point, it is convenient to introduce the "spectral function" of the environmental coupling,  $J(\omega)$ , by

$$J(\omega) = \frac{\pi}{2} \sum_{\alpha=1}^N \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}} \delta(\omega - \omega_{\alpha}) \quad (3.62)$$

Since we wish the environment to constitute a proper heat bath causing dissipation, we now consider  $J(\omega)$  as continuous. Then the sum in eq. (3.61) is replaced by the integral

$$\tilde{\gamma}(\omega) = -\frac{i\omega}{M} \cdot \frac{2}{\pi} \int_0^{\infty} d\omega' \frac{J(\omega')}{\omega'} \cdot \frac{1}{\omega'^2 - \omega^2 - i0^+} \quad (3.63)$$

By this manipulation, the function  $\tilde{\gamma}(\omega)$  acquires a real part

$$\text{Re}\{\tilde{\gamma}(\omega)\} = \frac{1}{M} \cdot \frac{J(\omega)}{\omega} \quad (3.64)$$

From eqs.(3.49) and (3.64), the spectral function  $J(\omega)$  will be related with the spectral density  $G_{\xi}(\omega)$  (if we treat  $\xi(t)$  in eq. (3.59) as a random force ) by

$$G_{\xi}(\omega) = 4KT \frac{J(\omega)}{\omega} \quad (3.65)$$

For frequency-dependent damping, it is sometimes convenient to determine  $\tilde{\gamma}(\omega)$  through analytic continuation of the Laplace transform  $\hat{\gamma}(z)$  of the  $\gamma(t)$ ,

$$\tilde{\gamma}(\omega) = \hat{\gamma}(z = -i\omega) \quad (3.66)$$

From eq. (3.63) and eq. (3.66), one can show that

$$\hat{\gamma}(z) = \frac{z}{M} \cdot \frac{2}{\pi} \int_0^{\infty} d\omega' \frac{J(\omega')}{\omega'} \cdot \frac{1}{\omega'^2 + z^2} \quad (3.67)$$

Moreover, from eq. (3.64) and eq. (3.46), it is easy to show that

$$J(\omega) = M\omega \int_0^{\infty} \gamma(t) \cos(\omega t) dt \quad (3.68)$$

It is worth to note from the above equations that the model described by the Hamiltonian (3.56) is fixed completely by the mass  $M$ , the potential  $V(x)$ , and the spectral function  $J(\omega)$ .

### 3.6 REDUCED DENSITY MATRIX AND REDUCED PARTITION FUNCTION [16]

From the Caldeira-Leggett model, the quantization procedure in quantum mechanics can be done since the Hamiltonian or Lagrangian has already been known. So, from chapter II, it is clear that one can find the density matrix of the universe based on this model Hamiltonian. From the model Hamiltonian eq. (3.56), the corresponding Euclidean Lagrangian contains contributions from the system (S), the reservoir (R), and their interaction (I) can be written in the form  $L^E = L_S^E + L_R^E + L_I^E$  where

$$\left. \begin{aligned} L_S^E &= \frac{1}{2} M \dot{x}^2 + V(x) \\ L_R^E &= \frac{1}{2} \sum_{\alpha=1}^N m_{\alpha} (\dot{q}_{\alpha}^2 + \omega_{\alpha}^2 q_{\alpha}^2) \\ L_I^E &= \sum_{\alpha=1}^N \left( -c_{\alpha} q_{\alpha} x + \frac{1}{2} \frac{c_{\alpha}^2 x^2}{m_{\alpha} \omega_{\alpha}^2} \right) \end{aligned} \right\} \quad (3.69)$$

As in chapter II, the Euclidean action is defined by

$$S^E[x, \bar{q}] = S_S^E[x] + S_R^E[\bar{q}] + S_I^E[x, \bar{q}], \quad S_S^E[x] = \int_0^U L_S^E d\tau, \quad S_R^E[\bar{q}] = \int_0^U L_R^E d\tau, \quad S_I^E[x, \bar{q}] = \int_0^U L_I^E d\tau \quad (3.70)$$

where  $\bar{q} = (q_1, q_2, \dots, q_N)$

As in eq. (2.31), the (normalized) density matrix of the universe can be written as a path integral in the usual form,

$$K(x'', \bar{q}'', x', \bar{q}') = Z^{-1} \int_{x(0)=x'}^{x(U)=x''} Dx(\tau) \int_{\bar{q}(0)=\bar{q}'}^{\bar{q}(U)=\bar{q}''} D^N q(\tau) \exp(-S^E[x, \bar{q}]/\hbar) \quad (3.71)$$

where  $D^N q(\tau) = Dq_1(\tau)Dq_2(\tau)\dots Dq_N(\tau)$  and  $Z$  is a partition function of the universe normalizes the density operator  $\hat{K}$  ( $K(x'', \bar{q}'', x', \bar{q}') = \langle x'', \bar{q}'' | \hat{K} | x', \bar{q}' \rangle$ ), so that  $\text{Tr} \hat{K} = 1$ .

Since the real interest of the problem is not the whole universe but just the behavior of the Brownian particle (system) only, we should focus our interest on a reduced description in which the reservoir coordinates are eliminated. In statistical sense i.e., the average value of any observable can be computed via the trace process, it is reasonable to define the "reduced density operator" by partial trace of the density operator  $\hat{K}$  of the universe with respect to reservoir states,  $\hat{\rho} = \text{Tr}_R \hat{K}$ . When expressing in coordinate representation, the "reduced density matrix" ( $\rho(x'', x') = \langle x'' | \hat{\rho} | x' \rangle$ ) is of the form,

$$\rho(x'', x') = \int_{-\infty}^{\infty} d^N q' k(x'', \bar{q}'; x', \bar{q}') \quad (3.72)$$

where  $d^N q' = dq'_1 dq'_2 \dots dq'_N$

From eq. (3.71) and the definition of Euclidean action (3.70), eq. (3.72) can be written in the form,

$$\rho(x'', x') = Z_d^{-1} \int_{x(0)=x'}^{x(U)=x''} Dx(\tau) \exp(-S_S^E[x]/\hbar) F^E[x]; Z_d = \frac{Z}{Z_R} \quad (3.73)$$

where

$$F^E[x] = Z_R^{-1} \oint D^N q(\tau) \exp(-S_{R,I}^E[x, \bar{q}]/\hbar) \quad (3.74)$$

with

$$S_{R,I}^E[x, \bar{q}] = S_R^E[\bar{q}] + S_I^E[x, \bar{q}] \quad (3.75)$$

where  $\oint D^N q(\tau) = \int_{-\infty}^{\infty} d^N q' \int_{\bar{q}(0)=\bar{q}'}^{\bar{q}(U)=\bar{q}'}$  denotes the sum over all close paths or periodic paths with period  $U = \beta\hbar$  taking by the coordinate  $\bar{q}(\tau)$ .

$F^E[x]$  in eq. (3.74) is called the "influence functional" because it describes the environmental influences on the system. This comes from the fact that it contains the sum

over all close paths of every environmental coordinates and leaves only the system coordinate  $x$  as the domain of the functional. The factor  $Z_R^{-1}$  is introduced here in order to normalize  $F^E[x]$ , so that  $F^E[x]=1$  when the coupling is switched off. Hence, it is clear that  $Z_R$  must be the partition function of the system of  $N$  independent harmonic oscillators of the form [2],

$$Z_R = \prod_{\alpha=1}^N \frac{1}{2 \sinh(\omega_\alpha U/2)} \quad (3.76)$$

$Z_d^{-1}$  in eq. [3.73] is introduced in order to normalize the density operator  $\hat{\rho}$ , so that  $\text{Tr}\hat{\rho}=1$ . Since  $\rho(x'',x')$  is called the reduced density matrix,  $Z_d^{-1}$  is correspondingly called as the "reduced partition function" i.e., the partition function which contains the reduced description of the system from the entire universe. Note that it connects with the partition function of the universe  $Z$  by the relation  $Z_d = Z/Z_R$  which is reduced to the partition function of the original isolated system when the coupling is switched off. From eq. (3.73), it is clear that the reduced partition function  $Z_d^{-1}$  can be written in the form,

$$Z_d = \oint Dx(\tau) \exp(-S_S^E[x]/\hbar) / F^E[x] \quad (3.77)$$

where  $\oint Dx(\tau) = \int_{-\infty}^{\infty} dx' \int_{x(0)=x'}^{x(U)=x'} Dx(\tau)$  denotes the sum over all close path taken by the coordinate  $x(\tau)$ .

Now, from the model Hamiltonian eq. (3.56) or equivalently the Lagrangian eq. (3.69), it makes the calculation of the influence functional eq. (3.74) to be exact since everything is Gaussian in the path integration. From eq. (3.69), eq. (3.70), and eq. (3.75), eq. (3.74) can be written in the form,

$$\begin{aligned} F^E[x] &= Z_R^{-1} \oint D^N q(\tau) \exp \left\{ -\frac{1}{\hbar} \left[ \sum_{\alpha=1}^N \int_0^U \left( \frac{m_\alpha}{2} (\dot{q}_\alpha^2 + \omega_\alpha^2 q_\alpha^2) - c_\alpha q_\alpha x + \frac{1}{2} \frac{c_\alpha^2 x^2}{m_\alpha \omega_\alpha^2} \right) d\tau \right] \right\} \\ &= Z_R^{-1} \prod_{\alpha=1}^N \exp \left( -\frac{1}{2\hbar} \int_0^U \frac{c_\alpha^2 x^2}{m_\alpha \omega_\alpha^2} d\tau \right) \cdot \oint Dq_n(\tau) \exp \left\{ -\frac{1}{\hbar} \int_0^U \left( \frac{m_\alpha}{2} (\dot{q}_\alpha^2 + \omega_\alpha^2 q_\alpha^2) - c_\alpha q_\alpha x \right) d\tau \right\} \end{aligned} \quad (3.78)$$



Notice that the path integration over the environmental coordinate  $q_a(\tau)$  in eq. (3.78) is in the standard form of forced harmonic oscillator [2], [3]. The evaluation of this path integration is straight forward, and one can show that (see Appendix A)

$$\begin{aligned} & \oint Dq_a(\tau) \exp \left\{ -\frac{1}{\hbar} \int_0^U \left( \frac{m_a}{2} (\dot{q}_a^2 + \omega_a^2 q_a^2) - c_a q_a x \right) d\tau \right\} \\ &= \frac{1}{2 \sinh(\omega_a U/2)} \exp \left\{ \frac{c_a^2}{4m_a \omega_a \hbar} \int_0^U \int_0^U \frac{\cosh(\omega_a [|\tau - \tau'| - U/2])}{\sinh(\omega_a U/2)} x(\tau) x(\tau') d\tau' d\tau \right\}. \end{aligned} \quad (3.79)$$

Inserting eq. (3.79) into eq. (3.78), we get

$$F^E[x] = \exp \left\{ -\frac{1}{\hbar} \sum_{\alpha=1}^N \left[ \frac{c_a^2}{4m_a \omega_a} \int_0^U \int_0^U \frac{\cosh(\omega_a [|\tau - \tau'| - U/2])}{\sinh(\omega_a U/2)} x(\tau) x(\tau') d\tau' d\tau + \int_0^U \frac{c_a^2 x^2}{2m_a \omega_a^2} d\tau \right] \right\}. \quad (3.80)$$

To change eq. (3.80) into the "nonlocal" form, we have to use the simple identity,  $x(\tau)x(\tau') = \frac{1}{2} (x^2(\tau) + x^2(\tau') - [x(\tau) - x(\tau')]^2)$ . When inserting this identity into eq. (3.80) and using the definition of the spectral function (3.62) and the equation  $\int_0^U \int_0^U \frac{\cosh(\omega_a [|\tau - \tau'| - U/2])}{\sinh(\omega_a U/2)} x^2(\tau) d\tau' d\tau = \frac{2}{\omega_a} \int_0^U x^2(\tau) d\tau$ , we obtain

$$F^E[x] = \exp \left\{ -\frac{1}{2\hbar} \int_0^U \int_0^U K(|\tau - \tau'|) [x(\tau) - x(\tau')]^2 d\tau' d\tau \right\} \quad (3.81)$$

where

$$K(\tau) = \frac{1}{2\pi} \int_0^\infty J(\omega) \frac{\cosh(\omega[\tau - U/2])}{\sinh(\omega U/2)} d\omega \quad (3.82)$$

is called the "damping Kernel" (in chapter IV is called the "normal damping Kernel" in order to make it different from the "anomalous damping Kernel").

Notice that eq. (3.81) is "entirely" nonlocal since the local contribution to  $K(\tau)$  just cancels the potential renormalization term (second term in the exponent of eq. (3.80) which is originated from  $\Delta V(x)$  in eq. (3.54). When inserting eq. (3.81) into eqs. (3.73)

and (3.77), we obtain the reduced density matrix and reduced partition function of the forms,

$$\rho(x'', x') = Z_d^{-1} \int_{x(0)=x'}^{x(U)=x''} Dx(\tau) \exp(-S_{\text{eff}}^{\text{E}}[x]/\hbar) \quad (3.83)$$

and

$$Z_d = \oint Dx(\tau) \exp(-S_{\text{eff}}^{\text{E}}[x]/\hbar) \quad (3.84)$$

where the "effective action"  $S_{\text{eff}}^{\text{E}}[x]$  is given by the expression

$$S_{\text{eff}}^{\text{E}}[x] = \int_0^U \left( \frac{1}{2} M \dot{x}^2 + V(x) \right) d\tau + \frac{1}{2} \int_0^U \int_0^U K(|\tau - \tau'|) [x(\tau) - x(\tau')]^2 d\tau d\tau' \quad (3.85)$$

Another (formally equivalent) form of the effective action, which has been used in many papers such as ref. [17], [18], can be derived if we agree to continue the path  $x(\tau)$  outside the range  $0 \leq \tau \leq U = \beta\hbar$  by the prescription  $x(\tau + U) = x(\tau)$ . Then we can transform the expression eq. (3.85) into [5], [7]

$$S_{\text{eff}}^{\text{E}}[x] = \int_0^U \left( \frac{1}{2} M \dot{x}^2 + V(x) \right) d\tau + \frac{1}{2} \int_0^U d\tau \int_{-\infty}^{\infty} d\tau' K_0(\tau - \tau') [x(\tau) - x(\tau')]^2 \quad (3.86)$$

where

$$K_0(\tau) = \frac{1}{2\pi} \int_0^{\infty} J(\omega) \exp(-\omega|\tau|) d\omega \quad (3.87)$$

Eq. (3.85) and eq. (3.86) tell us that the environment affects the system in such a way that the system has the nonlocal behavior and the environmental effect on it is contained in the damping kernel. From eq. (3.82) or eq. (3.87), it is clear the behavior of damping Kernel depends on the form of spectral function as it should be since the spectral function contains the behavior of the coupling. There are many forms of spectral function which are widely used in Brownian motion problem such as the spectral function in the case of "Ohmic damping". For Ohmic damping, the damping coefficient is frequency-independent,

$$\tilde{\gamma}(\omega) = \gamma \quad (3.88)$$

where  $\gamma$  is a constant real number. From eq. (3.64), this Ohmic damping may be described by the model eq. (3.56) with the spectral function

$$J(\omega) = \eta\omega \quad \text{for all frequency } \omega, \quad (3.89)$$

where  $\eta = M\gamma$  is the viscosity coefficient.

The Ohmic damping is sometimes called "Markoffian damping" since from eq. (3.65) and eq. (3.89) the spectral density of the environment  $G_\xi(\omega) = \text{constant}$  so the spectral density of the velocity of Brownian particle  $G_v(\omega) \propto 1/\gamma^2 + \omega^2$  which, due to the theorem of Doob implies that the Gaussian random process  $v(t)$  is a Markoff process. Note that, as have been discussed in section 3.3, this Ohmic damping should be equivalent to the case of pure random process. In reality, any one realistic spectral function  $J(\omega)$  falls off in the limit  $\omega \rightarrow \infty$ . Otherwise, certain physical quantities would diverge. Clearly, there is always some microscopic memory time setting the time scale for inertia effects in the reservoir. The Drude-regularized retarded friction  $\gamma(t)$  with a memory time  $\tau_D = 1/\omega_D$  has the form  $\gamma(t) = \gamma\omega_D \exp(-\omega_D t)$  which, from eq. (3.68), has the corresponding spectral function,

$$J(\omega) = \frac{\eta\omega}{1 + \omega^2/\omega_D^2} \quad ; \eta = M\gamma \quad (3.90)$$

Notice that when the relevant frequencies of a system are much less than the "Drude cutoff frequency"  $\omega_D$ , the reservoir describing by eq. (3.90) behaves effectively like an Ohmic heat bath. Moreover, there is a generalized form of spectral function which is widely used in many papers such as ref. [17], [19]. It has the following form:

$$J(\omega) = \eta\omega^s \exp(-\omega/\omega_c), \quad (3.91)$$

with  $\omega_c$  the cutoff frequency whenever needed. In accordance with ref. [17],  $s > 1$  is the "super-Ohmic case",  $s = 1$  the "Ohmic case", and  $0 \leq s < 1$  the "sub Ohmic case".

Note that the reduced density matrix in this section (as in chapter II) is derived in the situation of thermal equilibrium. In general, the quantum Brownian motion problem frequently concerns with the non equilibrium case so the reduced density matrix is divided into two kinds, equilibrium and "non equilibrium" density matrix. We will not discuss about the non equilibrium density matrix here since our application of quantum Brownian motion in chapter IV just requires only in the equilibrium case. There are many papers dealing with quantum Brownian motion in the non equilibrium case such as ref [20], developed by Feynman and Vernon, which describes the quantum Brownian motion based on the assumption of initial state which is called the "factorize assumption" (no correlation

between the system and reservoir at the beginning) and ref. [21] which deals with the general initial state. A system in the quantum Brownian motion problem is sometimes called the "quantum dissipative system" or "open quantum system" since the quantum system we are interested in can't be regarded as isolated from the rest of the physical universe.