# CHAPTER VI

# SUMMARY

As previously mentioned, this thesis started by surveying the classical theory of Brownian motion which has been well-known for a long time because knowledge of the theory in the classical limit is very useful and important for studying quantum mechanical case.

One of the main purpose of this work is to analyze in detail both the mathematical and physical features of Feynman path integrals and to apply this powerful tool to the Brownian motion problem. One knows that the characteristic of the Brownian movement is a phenomenon that a particle moves in some surrounding and exhibits a random type of movement. We have to evaluate the reduced density matrix of the Brownian particle, since all information about this particle is contained in this quantity. In general case where an interesting system coupled to other general system or surrounding system, using the Feynman path integrals impose upon us to write the reduced density matrix of the interesting system in the more convenient form as discussed in Eq.(4.32). The function $J$ plays the same role as the propagator relating density matrices at different time or the transition probability for the density matrix. All surrounding effects acting on the particle are already included in the propagator $J$. Actually, these effects are collected in the influence functional which is hidden in the propagator $J$ (Feynman-Vernon theory). The density matrix in this form is written in terms of parameters of the interesting system, not in term of that of the surrounding. The Feynman method is more advantageous and convenient than other methods to solve problems like this one.

The quantum mechanical model under our consideration consists of the Brownian particle coupling to the bath of harmonic oscillators (or a bosonic heat bath) with linear coupling

$$L_I = -q\sum_{k=1}^{n} c_k x_k ,$$

where $c_k$ is the linear coupling constant for the Brownian particle and the $k^{th}$ oscillator. The Lagrangian and the action for the complete system are presented in Eq.(5.4) and (5.6) as follows:

$$L = \frac{1}{2}M\dot{q}^2 - V(q,t) - q\sum_{k=1}^{n} c_k x_k + \sum_{k=1}^{n}\left(\frac{1}{2}m\dot{x}_k^2 - \frac{1}{2}m\omega_k^2 x_k^2\right) \tag{6.1}$$

and

$$A = \int_0^{t_f} dt\left[\frac{1}{2}M\dot{q}^2 - V(q,t) - q\sum_{k=1}^{n} c_k x_k + \sum_{k=1}^{n}\left(\frac{1}{2}m\dot{x}_k^2 - \frac{1}{2}m\omega_k^2 x_k^2\right)\right]. \tag{6.2}$$

The moving of the Brownian particle produces the effect which has feedback on itself. This effect comes from the perturbation of the moving particle to the heat bath.

Feynman and Vernon have developed the theory to solve problem of these kinds by using Feynman path integrals. In this approach any variables of the heat bath can be eliminated and given in the influence functional $F$. To apply the Feyman-Vernon theory for the specific model of the Brownian motion, the influence functional is given in the form of

$$F[q(t),q'(t)] = \exp\left\{-\frac{1}{\hbar}\int_0^{t_f} dt\int_0^{t} ds\,[q(t)-q'(t)][\alpha(t-s)q(s)-\alpha^*(t-s)q'(s)]\right\}, \tag{6.3}$$

where

$$\alpha(t-s) = \sum_{j=1}^{n} \frac{c_j^2}{2m\omega_j} \coth\frac{\hbar\omega_j}{2kT} \cos\omega_j(t-s) - i\sum_{j=1}^{n} \frac{c_j^2}{2m\omega_j} \sin\omega_j(t-s). \tag{6.4}$$

This functional keep all interactions between the Brownian particle and the heat bath. Studying this functional in detail leads us to understand the interactions well.

The reduced density matrix in Eq.(5.12) is used for the particular case, not in general. The more general case is presented in Eq.(4.28). In this work, we are interested in the case that, for the initial time $t = 0$, our two subsystems (a particle and a heat bath) do not interact with one another, but the interaction will be switched on at the later time $t > 0$. For this case we assume that the wave function $\psi$ of the whole system can be split into two parts in the form

$$\psi(q_s, x_s, s) = \varphi(q_s)\chi(x_s),$$

where, at time $t = 0$, $\varphi(q_0)$ describing only the particle and $\chi(x_0)$ for the heat bath. From this reason, the initial density matrix

$$\rho_0 = \rho(q_0, x_0; q_0', x_0') = \langle \psi(q_0, x_0, 0)\psi^*(q_0', x_0', 0) \rangle$$

can be written in the form

$$\rho_0 = \rho_0(q_0, q_0')\,\rho_h(x_0, x_0').$$

Again at the beginning of time $t = 0$, $\rho_0(q_0, q_0')$ is the density matrix describing the Brownian particle alone and $\rho_h(x_0, x_0')$ for the heat bath.

We do not use the density matrix $\rho(q_u, q_u'; x_u, x_u')$ shown in Eq(5.9), for the complete system because we are not interested to measure any quantities of the heat bath at final states. Furthermore, because no one can know all information of the complete system in details, particularly the heat bath which compose of the large number of oscillators, we sum over all final states of the heat bath and reduce the complete final density matrix into the reduced density matrix. The density matrix $\tilde{\rho}(q_u, q'_u, u)$ for the model is obtained in the form

$$\tilde{\rho}(q_u, q'_u, u) = \int dq_0 dq'_0 J(q_u, q'_u; q_0, q'_0)\, \rho_B(q_0, q'_0, 0) \tag{6.5}$$

with the propagator $J$ written in the form

$$\begin{aligned} J[q_u, q'_u; q_0, q'_0] = \int Dq(t) Dq'(t)\ \exp\frac{i}{\hbar}\Big\{ & A_B[q] - A_B[q'] \\ & - \int_0^u dt \int_0^t ds\, [q(t) - q'(t)]\, \alpha_I(t-s) [q(s) + q'(s)]\ \Big\} \\ & \times \exp - \frac{1}{\hbar} \int_0^u dt \int_0^t ds\, [q(t) - q'(t)]\, \alpha_R(t-s) [q(s) - q'(s)]\,. \end{aligned} \tag{6.6}$$

To make our result reduce to the classical limit, we have compared the real part of Eq.(6.4) to the well-known correlation of force

$\langle F(t)F(s)\rangle = 2\eta\, kT\delta(t-s)$.

To do so, it is necessary to consider the continuum of oscillator with density $\rho_D(\omega)$, and to impose the condition:

$$\rho_D(\omega)c^2(\omega) = \begin{cases} \dfrac{2m\eta\omega^2}{\pi} & for \quad \omega \quad \Omega \\ 0 & for \quad \omega \quad \Omega \end{cases}$$

on our result. Finally, the propagator can be written in the form

$$J[q_u, q'_u; q_0, q'_0] = \int Dq(t)\,Dq'(t)\ \exp\frac{i}{\hbar}\Big\{ A_r[q] - A_r[q'] - M\gamma \int_0^{t_u} dt \left[q(t)\dot{q}(t) - q'(t)\dot{q}'(t) + q(t)\dot{q}'(t) - q'(t)\dot{q}(t)\right] \Big\}$$
$$\times \exp - \frac{1}{\hbar}\frac{2M\gamma}{\pi}\int_0^{\Omega} d\omega\ \omega \coth\frac{\hbar\omega}{2kT}\int_0^{t_u} dt \int_0^{t} ds \left[q(t) - q'(t)\right]\ \cos\omega(t-s)\ \left[q(s) - q'(s)\right] \qquad (6.7)$$

One can see that it is expressed in terms of the relaxation constant $\gamma = \frac{\eta}{2M}$ or on the other words in terms of the damping constant $\eta$ (the phenomenological viscosity coefficient).

As we have said above, the propagator $J$ plays itself the same role as the propagator $K$ for a wave function. That is, $J$ developes in time of the reduced density matrix. Using Eq.(6.5) and (6.7) one can obtain the well-known Fokker-Planck equation as

$$\frac{\partial w}{\partial t} = -\frac{1}{M}\frac{\partial pw}{\partial q} + \frac{\partial V'_r w}{\partial p} + 2\gamma\frac{\partial pw}{\partial p} + D\frac{\partial^2 w}{\partial p^2}, \qquad (6.8)$$

by considering the short time propagator $J$.