CHAPTER IV

FEYNMAN- VERNON THEORY

There are problems in nature in which several non-relativistic quantum systems are coupled together. But not every system is equally important. One separates a problem into two parts; an interesting system, and an environment of the interesting system or a heat bath surrounding the interesting system. A useful theory one uses to solve such problems is the Feynman-Vernon theory.[4] The theory is formulated by using Feynman path integrals of non-relativistic quantum mechanics where the behavior of the interesting system may be calculated in terms of its own variables only, and the effect of the environment can always be included in a general class of functional, influence functional.

Influence Functional

To make the discussion clear, supposing that there is a complete system composed of a general quantum system (non-relativistic) whose coordinate is specified by q , and a heat bath with general coordinate x. These two systems are coupled together through some interaction potential, which is, in general, a function of q, x and time t. It is well known that this problem can be analyzed by taking the total Hamiltonian $H=H_O(q)+H_E(x)+V(q,x,t)$ of the whole system, where H_0 is a Hamiltonian of the system of coordinate q and H_n for the heat bath, and forming the wave equation as follows:

$$\{H_O(q)+H_E(x)+V(q,x,t)\}\psi(q,x,t) = i\hbar\frac{\partial}{\partial t}\psi(q,x,t), \qquad (4.1)$$

and then solving this equation for $\psi(q,x,t)$. If one knows the wave function ψ, then one can know everything. But it is extremely difficult to solve this equation in general. Moreover, it is not easy to eliminate the variable x and to equivalently include its effects when describing everything directly in terms of q alone. So we use Feyman's formalism introduced in the previous chapter to solve this problem. Instead of a Hamiltonian, we use the Lagrangian L of the whole system as

$$L = L_0(\dot{q},q,t) + L_E(\dot{x},x,t) - V(q,x,t) \tag{4.2}$$

where $L_0(\dot{q},q,t)$ and $L_E(\dot{x},x,t)$ are the Lagranian of the interesting system and of the heat bath respectively. The corresponding action is

$$A = A_0(q) + A_E(x) - \int_s^S V(q,x,t)dt \tag{4.3}$$

Then the propagator $K(q_S,x_S;q_s,x_s)$ for the complete system, when the interesting system goes from q_s at $t = s$ to q_S at $t = S$, and the environment goes from x_s at $t = s$ to x_S at $t = S$, is

$$K(q_S,x_S;q_s,x_s) = \int Dq(t)Dx(t)\, \exp\frac{i}{\hbar}\left[A_0(q) + A_E(x) - \int_s^S V(q,x,t)dt\right]. \tag{4.4}$$

When system of variables q and x do not interact with each other, we assume $V=0$, the systems q and x can be described by the sets of wave functions $\phi_k(q)$ and $\chi_p(x)$ respectively. If the interesting system q goes from state $\phi_m(q_s)$ at initial time s to state $\phi_n(q_S)$ at final time S, and the heat bath x goes from state $\chi_i(x_s)$ at time s to state $\chi_f(x_S)$ at time S, the amplitude for this case is

$$K_{nf,mi} = \int dq_S dx_S dq_s dx_s \phi_n^*(q_S)\chi_f^*(x_S)K(q_S,x_S,S;q_s,x_s,s)\phi_m(q_s)\chi(x_s). \tag{4.5}$$

$$P_{nf,mi} = \left|K_{nf,mi}\right|^2$$

$$= \int dq_S dq'_S dx_S dx'_S dq_s dq'_s dx_s dx'_s \phi_n^*(q_S)\chi_f^*(x_S)\phi_n(q'_S)\chi_f(x'_S)$$
$$\times K^*(q'_S,x'_S;q'_s,x'_s)K(q_S,x_S;q_s,x_s)\phi_m(q_s)\chi_i(x_s)\phi_m^*(q'_s)\chi_i^*(x'_s) \qquad (4.6)$$

or in the form

$$P_{nf,mi} = \int dq_S dq'_S dx_S dx'_S dq_s dq'_s dx_s dx'_s DqDxDq'Dx'\phi_n^*(q_S)\chi_f^*(x_S)\phi_n(q'_S)\chi_f(x'_S)$$
$$\times \exp\left\{\frac{i}{\hbar}\left[A_O(q)-A_O(q')+A_E(x)-A_E(x')-\int_s^S dt[V(q,x,t)-V(q',x',t)]\right]\right\}$$
$$\times \phi_m(q_s)\chi_i(x_s)\phi_m^*(q'_s)\chi_i^*(x'_s). \qquad (4.7)$$

We see that in this equation all the variables of the heat bath can be eliminated by integration as follows

$$\int \chi_f^*(x_S)\chi_f(x'_S)\exp\left\{\frac{i}{\hbar}\left[A_E(x)-A_E(x')-\int_s^S dt[V(q,x,t)-V(q',x',t)]\right]\right\}$$
$$\chi_i(x_s)\chi_i^*(x'_s)DxDx'dx_s dx'_s dx_S dx'_S. \qquad (4.8)$$

This integral is dependent on paths $q(t)$ and $q'(t)$. It is a functional of paths $q(t)$ and $q'(t)$ and we represent it by $F[q(t),q'(t)]$. So, after eliminating all variables of the heat bath, the probability $P_{nf,mi}$ depends on coordinates of the interesting system only. We then write $P_{n,m}$ for $P_{nf,mi}$

$$P_{n,m} = \int \phi_n^*(q_S)\phi_n(q'_S)\exp\left\{\frac{i}{\hbar}\left[A_O(q)-A_O(q')\right]\right\}F[q,q']$$
$$\phi_m(q_s)\phi_m^*(q'_s)DqDq'dq_s dq'_s dq_S dq'_S. \qquad (4.9)$$

$F[q(t),q'(t)]$ can be written in terms of the propagator as follows

$$\int Dq Dq' \exp \frac{i}{\hbar} \left\{ A_O(q) - A_O(q') - \int_s^S dt [q(t) - q'(t)] V(t) \right\}$$

$$= K(q_S, S; q_s, s) K^*(q'_S, S; q'_s, s) \qquad (4.14)$$

which has two path integrals. One is

$$K(q_S, S; q_s, s) = \int Dq \exp \frac{i}{\hbar} \left\{ A_O(q) - \int_s^S dt\, q(t) V(t) \right\} \qquad (4.15)$$

and the other is

$$K(q'_S, S; q'_s, s) = \int Dq' \exp \frac{i}{\hbar} \left\{ A_O(q') - \int_s^S dt\, q'(t) V(t) \right\}. \qquad (4.16)$$

Each integral is over paths with appropriate end points. We shall call the expression (4.14) the double path integral (so the form of Eq.(4.13) is also a double path integral). But now we suppose the potential $V(t)$ is known only by its probability distribution P_I $[V(t)]DV(t)$. Then the probability of the interesting system q going from $\phi_m(q_s)$ to $\phi_n(q_S)$, given by Eq (4.13) could be calculated for each $V(t)$. Then we have to average over all $V(t)$ with the weight $P_I[V(t)]DV(t)$ for each $V(t)$,

$$P_{av}[\phi_m \to \phi_n] = \int dq_S dq'_S dq_s dq'_s \phi_n^*(q_S) \phi_n(q'_S) W(q_S, q'_S, q_s, q'_s) \phi_m(q_s) \phi_m^*(q'_s)$$

$$(4.17)$$

where W the average of (4.14) over all $V(t)$ with weight $P_I[V(t)]DV(t)$,

$$W(q_S, q'_S; q_s, q'_s) = \int \exp \left\{ \frac{i}{\hbar} \left[A_O(q) - A_O(q') - \int_s^S [q(t) - q'(t)] V(t) dt \right] \right\} P_I[V(t)]$$

$$\times Dq(t) Dq'(t) DV(t). \qquad (4.18)$$

In this form we can do the integral over $V(t)$ first. That is

$$F[q(t),q'(t)] = \int dx_S dx'_S dx_s dx'_s \, \chi_f^*(x_S)\chi_f(x'_S)K_q(x_S,x_s)K_{q'}^*(x'_S,x'_s)$$
$$\times \chi_i(x_s)\chi_i^*(x'_s).$$

(4.10)

where the subscript q in K mean that the propagator K contains the effect of a potential $V(q,x,t)$ acting on x during the time interval $s < t < S$. In the expression $F[q(t),q'(t)]$ as shown in Eq.(4.10), $F[q(t),q'(t)]$ is a functional whose form is dependent upon the physical system x, the initial and final states of x, and the coupling between q and x. If there is no interaction between q and x, then F does not contain variable q and q', and F is reduced to the probability transition of system x from state $\chi_i(x_s)$ to $\chi_f(x_S)$.

For system q which interacts with external potential $V(t)$ rather than system x, its action is

$$A = A_o(q) - \int_s^S q(t)V(t)dt.$$

(4.11)

The transition amplitude of state $\phi_m(q_s)$ at time s to $\phi_n(q_S)$ at time S is

$$K_{n,m} = \int dq_S dq_s Dq \phi_n^*(q_S) \left(\exp \frac{i}{\hbar} \left[A_o(q) - \int_s^S dt \, q(t)V(t) \right] \right) \phi_m(q_s),$$

(4.12)

and the probability of the transition is

$$P_{n,m} = |K_{n,m}|^2$$
$$= \int dq_S dq'_S dq_s dq'_s Dq Dq' \phi_n^*(q_S)\phi_n(q'_S)$$
$$\times \left(\exp \frac{i}{\hbar} \left\{ A_o(q) - A_o(q') - \int_s^S dt[q(t) - q'(t)]V(t) \right\} \right) \phi_m(q_s)\phi_m^*(q'_s).$$

(4.13)

This expression involves the path integral

$$\phi[q(t) - q'(t)] = \int \exp\left\{ -\frac{i}{\hbar} \int_s^s [q(t) - q'(t)] V(t) dt \right\} P_i[V(t)] DV(t) \qquad (4.19)$$

which is called the characteristic function.[2],[6]

To summarize, the behavior of the interesting system in any environment can be discussed in terms of a double path integral like Eq.(4.9), where F is a property of the environment. F contains all effects of the environment which influence the interesting system. We can understand F by analogue to the term "external force" which when used in classical mechanics, describes the effects of the surrounding which influences the system of interest. In classical mechanics we can only analyze the motion of an interesting system (coordinate q) in an environment by coordinate q provided that we know what force is produced by the environment. The equation of motion of q alone in classical mechanics, Newton's equation of motion $m\ddot{q} = f(t)$, is the rough analogue of Eq.(4.9); whereas Eq.(4.10) corresponds to the calculation of the force $f(t)$ produced by the heat bath. Two different heat baths which produce the same force $f(t)$ on q are equivalent. Actually, the analogue is only rough; say, F contains the entire effect of the heat bath including the change in behavior of the environment resulting from reaction with q. In our analogue to classical force $f(t)$, F would correspond to knowing not only what the force is as a function of time, but what it would be for every possible motion $q(t)$ of the object. The force of a given heat bath depends in general on the motion of the motion of the interesting system, of course, since the environmental system is affected by interaction with the system of interest q.

The General Properties of the Influence Functional

There are several properties of the influence functional which are of interest and very useful in practice. These properties can be derived from the definition of influence functional,

$$F[q,q'] = \int dx_S\, dx'_S\, dx_s\, dx'_s\; \chi_f^*(x_S)\chi_f(x'_S)K_q(x_S,x_s)K_{q'}^*(x'_S,x'_s)\chi_i(x_s)\chi_i^*(x'_s)_{S'}$$

(4.20)

i) Influence functional has the property

$$F[q,q'] = F^*[q',q]$$

(4.21)

This can be seen directly from (4.20).

ii) Some physical situations are not certain or not of interest, but we know their probability to occur. Supposing that we have the ith situation which is not of interest and the corresponding influence functional is F_i with probability w_i; then the effective influence functional is

$$F_{eff} = \sum_i w_i F_i \equiv \langle F \rangle .$$

(4.22)

If the final states of heat, for example, is not of interest and we do not measure on these states, then the probability $P_{n\,m}$ is $\sum_f w_f P_{nf\,mf}$. Because the summation involving the x variables, the sum over the influence functional for each possible final state leads to the average influence functional of the type $F_{eff} = \sum_f w_f F_f \equiv \langle F \rangle$.

iii) If the surroundings contain several sub-systems which do not interact with each other, but they all act on the interesting system, then the total influence functional is equal to the product of the influence functional of those sub-systems. Then we can write

$$F = \prod_k F_k, \tag{4.23}$$

where k represents the kth sub-system. This property can be seen directly from Eq (4.20).

iv) For the problem in which the final state of interaction system is arbitrary, these states are all summed over. If we let $q(t) = q'(t)$ for all $t > s$ then the influence functional does not depend on the actual value of $q(t)$ for $t > s$. We can analyze this property as follows : From the equation (4.20) in which $K_q(x_S, x_s)$ is

$$K_q(x_S, S; x_s, s) = \int Dx(t) \, \exp[\frac{i}{\hbar} \int_s^S dt \, L]. \tag{4.24}$$

We set $q(t) = q'(t)$ and sum over all states f, so the right hand side of (4.20) is

$$\sum_f \int dx_S dx'_S dx_s dx'_s \chi_f^*(x_S) \chi_f(x'_S) K_q(x_S, S; x_s, s) K_q^*(x'_S, S; x'_s, s) \chi_i^*(x'_s) \chi_i(x_s)$$

Because all of the wave functions $\chi_f(x_S)$ form the complete orthonormal set, the sum over all final states f becomes the Dirac delta function $\delta(x_S - x'_S)$, so that the above expression becomes:

$$\int dx_S dx'_S dx_s dx'_s \, \delta(x_S - x'_S) \, K_q(x_S, S; x_s, s) K_q^*(x'_S, S; x'_s, s) \chi_i^*(x'_s) \chi_i(x_s).$$

After integration with respect to the variable x'_S, one can get

$$\int dx_S dx_s dx'_s \; K_q(x_S, S; x_s, s) K_q^*(x_S, S; x'_s, s) \chi_i^*(x'_s) \chi_i(x_s).$$

By using the property of the propagator K the integration with respect to x_S equals the Dirac delta function $\delta(x_s - x'_s)$ so that this expression can be written in the form:

$$\int \delta(x_s - x'_s) \chi_i^*(x'_s) \chi_i(x_s) dx'_s dx_s.$$

We integrate this last expression with respect to x'_s and using the normalized condition $\int \chi_i^*(x'_s) \chi_i(x_s) dx_s = 1$, we shall have

$$F[q,q] = 1.$$

which is independent of q.

Influence Functional and Statistical Mechanics

For an environment which is composed of many particles, one can not know detail information such as positions of each particle at any time. One has to use statistical mechanics to treat the problem. In the sense of statistical mechanics all information of the system is included in a density matrix. So it is approximated to point out explicitly the significance of influence functional to study quantum statistical mechanics. We start by recalling the definition of a density matrix ρ of the complete system (the interesting system q plus the heat bath x) in the coordinates representation as follows :

$$\rho(q,x;q',x') = \langle \psi(q,x)\psi^*(q',x') \rangle \tag{4.26}$$

where $\psi(q,x)$ is the wave function of the complete system for one of the systems, an ensemble of systems each representing one of the possible states of the q, x system. The density matrix $\rho(q,x;q',x')$ contains more information of the heat bath, on the other hand we do not measure any properties of the environment, so we eliminate its coordinates by integration. Then $\rho(q,x;q',x')$ reduces to density matrix $\rho(q,q')$ which contains information of the interesting system in terms of its coordinates only, by the relation

$$
\begin{aligned}
\rho(q_t,q_t') &= \int dx_t dx_t' \, \delta(x_t - x_t') \rho(q_t,x_t;q_t',x_t') \\
&= \int dx_t dx_t' \, \delta(x_t - x_t') \langle \psi(q_t,x_t,t)\psi(q_t',x',t) \rangle .
\end{aligned}
\tag{4.27}
$$

At the time $t = S$

$$
\rho_S(q_S,q_S',S) = \int dx_S dx_S' \delta(x_S - x_S') \langle \psi(q_S,x_S,S)\psi(q_S',x_S',S) \rangle
\tag{4.28}
$$

We know from chapter III that the wave function $\psi(q_S,x_S,S)$ can be written in terms of the wave function $\psi(q_s,x_s,s)$ at time $t = s < S$ as

$$
\psi(q_S,x_S,S) = \int K(q_S,x_S,S;q_s,x_s,s)\psi(q_s,x_s,s)dx_s dq_s
$$

where the propagator $K(q_S,x_S,S;q_s,x_s,s)$ is

$$
K(q_S,x_S,S;q_s,x_s,s) = \int Dq Dx \, \exp\left\{ \frac{i}{\hbar}\left[A_O(q) + A_E(x) + A_I(q,x) \right] \right\} .
$$

Then the term $\langle \psi(q_S,x_S,S)\psi^*(q_S',x_S',S) \rangle$ is equal to

$$\left\langle \int dq_s dq'_s dx_s dx' Dq Dq' Dx Dx' \exp\left\{\frac{i}{\hbar}\left[A_0(q) - A_0(q')\right]\right\}\right.$$

$$\times \exp\left\{\frac{i}{\hbar}\left[A_E(x) - A_E(x') + A_I(q,x) - A_I(q',x')\right]\right\} \psi(q_s,x_s,s)\psi^*(q'_s,x'_s,s), \left.\vphantom{\int}\right\rangle$$

$$= \int dq_s dq'_s dx_s dx'_s Dq Dq' \exp\left\{\frac{i}{\hbar}\left[A_0(q) - A_0(q')\right]\right\}$$

$$\times K_q(x_S,S;x_s,s)K_{q'}^*(x_S,S;x_s,s)\langle\psi(q_s,x_s,s)\psi^*(q'_s,x'_s,s)\rangle$$

where the path integral $K_q(x_S,S;x_s,s)$ is

$$K_q(x_S,S;x_s,s) = \int Dx \exp\left\{\frac{i}{\hbar}\left[A_E(x) + A_I(q,x)\right]\right\}$$

and

$$\langle\psi(q_s,x_s,s)\psi^*(q'_s,x'_s,s)\rangle = \rho_s(q_s,x_s;q'_s,x'_s),$$

hence,

$$\rho_S(q_S,x_S;q'_S,x'_S) = \int dq_s dq'_s dx_s dx'_s Dq Dq' \exp\left\{\frac{i}{\hbar}\left[A_0(q) - A_0(q')\right]\right\}$$

$$\times K_q(x_S,S;x_s,s)K_{q'}^*(x'_S,S;x'_s,s)\rho_s(q_s,x_s;q'_s,x'_s). \quad (4.28)$$

For the initial time $t = s$, the interesting system q and heat bath x are independent of each other and their wave functions can be split into wave function of individual system only. For non-interaction, each system can be described by a set of eigenstates $\varphi(q_s)$ for the interesting system q at time s, and $\chi(x_s)$ for the heat bath at time s. Therefore, one writes

$$\psi(q_s,x_s,s) = \varphi(q_s)\chi(x_s) \quad (4.29)$$

and we get

$$\begin{aligned}
\rho_s &= \left\langle \varphi^*(q'_s)\chi^*(x'_s)\varphi(q_s)\chi(x_s) \right\rangle \\
&= \left\langle \varphi^*(q'_s)\varphi(q_s) \right\rangle \left\langle \chi^*(x'_s)\chi(x_s) \right\rangle \\
&= \rho_0(q_s,q'_s)\,\rho_E(x_s,x'_s).
\end{aligned} \tag{4.30}$$

Inserting Eq.(4.30) into Eq.(4.28), one obtains

$$\rho_S(q_S,x_S;q'_S,x'_S) = \int dq_s dq'_s dx_s dx'_s DqDq' \exp\left\{\frac{i}{\hbar}\left[A_O(q) - A_O(q')\right]\right\}$$
$$\times K_q(x_S,x_s)K_{q'}^*(x'_S,x'_s)\rho_0(q_s,q'_s)\rho_E(x_s,x'_s). \tag{4.31}$$

So the expression of $\rho_S(q_S,q'_S)$ is

$$\rho_S(q_S,q'_S) = \int J(q_S,q'_S;q_s,q'_s)\rho_0(q_s,q'_s)dq_s dq'_s. \tag{4.32}$$

where

$$J(q_S,q'_S;q_s,q'_s) = \int dx_S dx'_S dx_s dx'_s DqDq' \exp\left\{\frac{i}{\hbar}\left[A_0(q) - A_0(q')\right]\right\}$$
$$\times \delta(x_S - x'_S)K_q(x_S,x_s)K_{q'}^*(x'_S,x'_s)\rho_E(x_s,x'_s). \tag{4.33}$$

If we write

$$F(q,q') = \int dx_S dx'_S dx_s dx'_s \delta(x_S - x'_S)K_q(x_S,x_s)K_{q'}^*(x'_S,x'_s)\rho_E(x_s,x'_s). \tag{4.34}$$

then

$$J(q_S,q'_S;q_s,q'_s) = \int DqDq' \exp\left\{\frac{i}{\hbar}\left[A_0(q) - A_0(q')\right]\right\}F(q,q'). \tag{4.35}$$

We see that J looks like the propagator K. Then we can say that J is the propagator of the density matrix, if there is a transition of density matrix $\rho_0(q_s,q'_s)$ at initial time $t = s$ to the density matrix $\rho_S(q_S,q'_S)$ at the final time $t = S$. Moreover, J contains the effect of the heat bath x which influences the interesting system q. We see that we

include all effect of the heat bath in a functional $F(q,q')$, an influence functional, which we have discussed in the previous section.

Again we can describe the behaviors of the interesting system q in terms of its variables only as Eq.(4.33) or (4.35).