CHAPTER II

FEYNMAN PATH INTEGRATION

Introduction

In this chapter, we would like to show how we can formulate the Feynman propagator from evolution operators of Schrödinger quantum mechanics. The details of the calculations of propagator from *path summations* can be found in the text of Feynman and Hibbs[11]. Also, we show the formulation of the statistical operator in terms of path integrals. This statistical operator will be used in the calculation process of the quantum average in our work.

Propagator from Evolution Operator

The wave function $\Psi(t)$ of a quantum mechanical system with a Hamiltonian $\mathcal{H}$ evolves according to the Schrödinger equation

$$i\hbar\frac{\partial\Psi(t)}{\partial t} = \hat{\mathcal{H}}\Psi(t) \tag{31}$$

Its solution, developing from $\Psi(t_0)$ at t_0, may be presented in the form

$$\Psi(t) = \hat{\mathcal{U}}(t,t_0)\Psi(t_0), t \gg t_0, \tag{32}$$

where the unitary evolution operator, $\hat{\mathcal{U}}$, satisfies the equation

$$i\hbar\frac{\partial\hat{\mathcal{U}}(t,t_0)}{\partial t} = \hat{\mathcal{H}}\,\hat{\mathcal{U}}(t,t_0), \tag{33}$$

with $\hat{\mathcal{U}}(t_0, t_0) = 1$. It may be formally solved in terms of a time-ordered exponential

$$\hat{\mathcal{U}}(t, t_0) = \hat{T} \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \hat{\mathcal{H}}_s ds\right). \tag{34}$$

The time-ordering operator, $\hat{T}$, acts according to the following definition

$$\hat{T}\prod_{j=1}^{n} \hat{A}_{t_j}^{(i_n)} = \hat{A}_{t_{i_n}}^{(i_n)} \hat{A}_{t_{i_{n-1}}}^{(i_{n-1})} \ldots \hat{A}_{t_{i_2}}^{(i_2)} \hat{A}_{t_{i_1}}^{(t_1)},$$
$$t_{i_n} > t_{i_{n-1}} > \ldots > t_{i_2} > t_{i_1}, \tag{35}$$

where $(i_1, \ldots, i_n)$ is a permutation of the indices $(1, \ldots, n)$. Thus in the evolution operator eq.(34), time is the ordering parameter. If the Hamiltonian $\mathcal{H}(t)$ has an explicit time dependence, then the integrand in the evolution operator contains time both explicitly and as the ordering parameter

$$\hat{\mathcal{U}}(t, t_0) = \hat{T} \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \hat{\mathcal{H}}_s(s) ds\right). \tag{36}$$

It was shown by Feynman[12] that under the ordering operator sign in eq.(35) one may consider the operators to be commutative and handle them as numerical functions of the ordering parameter.

Path Integral in Phase Space

Let a system be described by a Hamiltonian function

$$\mathcal{H}(p,q;t) = \int e^{i(\alpha p+\beta q)}h(\alpha,\beta;t)d^n\alpha d^n\beta \tag{37}$$

in the phase space with the canonical coordinates $p=(p_1,...,p_n)$, $q=(q_1,...,q_n)$, analogously α,β are n-dimensional vectors, $\alpha p=\sum_{i=1}^n \alpha_i p_i$ and $d^n\alpha = d\alpha_1...d\alpha_n$, $d^n\beta = d\beta_1...d\beta_n$. The quantization is carried out by establishing the correspondence to this function of the operator (Hamiltonian) $\hat{\mathcal{H}}=\hat{\mathcal{H}}(\hat{p},\hat{q};t)$, where $\hat{p}=(\hat{p}_1,...,\hat{p}_n);\hat{q}=(\hat{q}_1,...,\hat{q}_n)$ are the momentum and coordinate operators. Unambiguity of the quantization is achieved by a certain ordering of the non-commutative operators $\hat{p}_i,\hat{q}_i(i=1,...,n)$. If it is chosen in the symmetric form

$$\hat{\mathcal{H}}(\hat{p},\hat{q};t) = \int e^{i(\alpha\hat{p}+\beta\hat{q})}h(\alpha,\beta;t)d^n\alpha d^n\beta, \tag{38}$$

the function in eq.(37) is a Weyl symbol of the Hamiltonian[13]. To any operator written in the symmetric form, its Weyl symbol is defined analogously.

For an operator $\hat{A}(\hat{p},\hat{q})$ its matrix elements in the coordinate representation and trace are determined by certain integral transform of its Weyl symbol

$$< q|\hat{A}(\hat{p},\hat{q})|q_0> = \frac{1}{(2\pi\hbar)^n}\int A(p,\frac{q+q_0}{2})\exp\left(\frac{i}{\hbar}p(q-q_0)\right)d^np, \tag{39}$$

$$\mathrm{Tr}\hat{A}(\hat{p},\hat{q}) = \frac{1}{(2\pi\hbar)^n}\int A(p,q)d^npd^nq. \tag{40}$$

From eq.(37) the composition rule follows: if $\hat{A}=\hat{A}_1\hat{A}_2$, then

$$A(p,q) = \frac{1}{(\pi\hbar)^{2n}}\int A_1(p_1,q_1)A_2(p_2,q_2)$$

$$\cdot \exp\left\{\frac{2i}{\hbar}(p_1(q-q_1)+p_2(q_1-q)+p(q_2-q))\right\}$$

$$\cdot d^n p_1 d^n q_1 d^n p_2 d^n q_2. \tag{41}$$

Using the Weyl symbol in eq.(37) of the Hamiltonian allows on the basis of eq.(41) to represent the matrix elements of the evolution operator, eq.(36),

$$< q|\hat{\mathcal{U}}(t,t_0)|q_0 > \;=\; \int_{q(t_0)=q_0}^{q(t)=q} \exp\left\{\frac{i}{\hbar}S(t,t_0)\right\} \prod_s \frac{dp(s)dq(s)}{(2\pi\hbar)^n} \tag{42}$$

in term of path integral in phase space, where a classical action functional is introduced

$$S[t,t_0] \;=\; \int_{t_0}^{t} [p(s)q(s) - \mathcal{H}(p(s),q(s))]ds, \quad \dot{q}(s) = \frac{dq(s)}{ds}. \tag{43}$$

Making a partition of the time segment $[t,t_0]$ into N parts:

$$t_0 \;=\; s_0 < s_1 < s_2 < ... < s_{N-1} < s_N = t \tag{44}$$

and introducing a set of approximative paths

$$q^{(N)}(s) \;=\; q_{j-1} + \frac{q_j - q_{j-1}}{s_j - s_{j-1}}(s - s_{j-1}), q_0 = q(t_0), q_N = q(t); \tag{45}$$

$$p^{(N)}(s) \;=\; p_j \tag{46}$$

for $s_{j-1} < s < s_j, j = 1,...,N$, we obtain a finite dimension from which after a limiting transition $N \to \infty$ (so that $\max_j(s_j - s_{j-1} \to 0)$ a path integral results:

$$\int_{q(t_0)}^{q(t)} F[q(s),p(s)] \prod_s \frac{dp(s)dq(s)}{(2\pi\hbar)^n}$$

$$= \lim_{N\to\infty} \int ... \int F[q^{(N)}(s),p^{(N)}(s)] \frac{d^n p_N}{(2\pi\hbar)^n} \prod_{j=1}^{N-1} \frac{d^n p_j d^n q_j}{(2\pi\hbar)^n} \tag{47}$$

For systems with Hamiltonian functions which are quadratic in p:

$$\mathcal{H}(p,q;s) \;=\; \frac{1}{2}\sum_{k,l=1}^{n} [p_k - a_k(q)]m_{kl}^{-1}[p_l - a_l(q)] + V(q,s) \tag{48}$$

the path integral in momentum space in eq.(42) may be accomplished explicitly[14]. Namely, after the change of variables

$$p_k(s) = a_k(q(s)) + \sum_{l=1}^{n} m_{kl}\dot{q}_l(s) + p'_k(s) \tag{49}$$

the action functional eq.(43) takes the form

$$\begin{aligned} S[t,t_0] &= \int_{t_0}^{t} \mathcal{L}(q(s),\dot{q}(s);s)ds \\ &\quad -\frac{1}{2}\sum_{k,l=1}^{n}\int_{t_0}^{t} p'_k(s)m^{-1}_{kl}p'_l(s)ds \end{aligned} \tag{50}$$

with a Lagrange function

$$\mathcal{L}(q,\dot{q};s) = \frac{1}{2}\sum_{k,l=1}^{n}\dot{q}_k m_{kl}\dot{q}_l + \sum_{k=1}^{n} a_k(q)\dot{q}_k - V(q,s). \tag{51}$$

After this the path integrals in the coordinate $q(s)$ and momentum $p'(s)$ spaces are separated, and the matrix elements of the evolution operator eq.(42) are represented

$$< q|\hat{\mathcal{U}}(t,t_0)|q_0 > = \int_{q_0}^{q} \mathcal{D}[g_s]\exp\left(\frac{i}{\hbar}\int_{t_0}^{t}\mathcal{L}(q(s),\dot{q}(s);s)ds\right) \tag{52}$$

in terms of Feynman path integrals[11], the propagator $K(q,q_0;t-t_0) =< q|\hat{\mathcal{U}}(t,t_0)|q_0 >$. Making use of a set of approximated paths eq.(45) one may formally carry out the integrals over momenta and obtain the Feynman path integral by the above described limiting transition in the finite-dimension approximation

$$\int_{t(t_0)}^{q(t)} F[q(s)]\mathcal{D}q(s) = \lim_{N\to\infty}\int\ldots\int F[q^{(N)}(s)]\frac{1}{A_N}\prod_{j=1}^{N-1}\frac{d^n q_j}{A_j}; \tag{53}$$

where on account of eqs.(47) and(51) the normalizing factors assume the form

$$\frac{1}{A_j} = \left\{\frac{\det||m_{kl}||}{[2\pi i\hbar(s_j,s_{j-1})]^n}\right\}^{1/2}. \tag{54}$$

Exceptionally important are path integrals of Gaussian functionals, with a Lagrange function which is quadratic in both $q(s)$ and $\dot{q}(s)$ (they constitute the basis of a constructive definition of a path integral) which have the form of eq.(52). Such path integrals may be expressed explicitly[11], through the stationary path $\bar{q}(s)$ obeying the Euler-Lagrange equations,

$$\frac{d}{ds}\frac{\partial \mathcal{L}}{\partial \dot{q}_k(s)} - \frac{\partial \mathcal{L}}{\partial q_k(s)} = 0, (k = 1, ..., n) \tag{55}$$

with boundary conditions $q(t_0) = q_0, q(t) = q$:

$$< q|\hat{\mathcal{U}}(t, t_0)|q_0 > = f(t, t_0) \exp\left(\frac{i}{\hbar}\int_{t_0}^{t} \mathcal{L}(\bar{q}(s), \dot{\bar{q}}(s); s)ds\right). \tag{56}$$

The time-dependent pre-exponential factor has been calculated on the basis of eq.(53) in a rather general form in refs.[15, 16], see also [17].

Path Integrals Representation for Density Matrix

The statistical operator $\hat{\rho}(t)$ of a mixed ensemble of systems with Hamiltonian $\hat{\mathcal{H}}$ obeys the von Neumann (or quantum Liouville) equation

$$i\hbar\frac{\partial\hat{\mathcal{H}}}{\partial t} = \left[\hat{\mathcal{H}},\hat{\rho}(t)\right]_{-}. \tag{57}$$

Its solution developing from $\hat{\rho}(t_0)$ at t_0 may be represented analogously to eq.(32), in the form

$$\begin{aligned}\hat{\rho}(t) &= \hat{\rho}\,[t,t_0;\hat{\rho}(t_0)] \\ &= \hat{\mathcal{U}}(t,t_0)\hat{\rho}(t_0)\hat{\mathcal{U}}^{-1}(t,t_0), t \gg t_0,\end{aligned} \tag{58}$$

where the operator which is the inverse of eq.(36)

$$\begin{aligned}\hat{\mathcal{U}}^{-1}(t,t_0) &= \hat{T}^{-1}\exp\left(\frac{i}{\hbar}\int_{t_0}^{t}\hat{\mathcal{H}}_s(s)ds\right) \\ &= \hat{\mathcal{U}}^{\dagger}(t,t_0)\end{aligned} \tag{59}$$

is expressed in terms of a reverse time-ordered exponential. The reverse time-ordering operator is defined by the expression

$$\begin{aligned}\hat{T}^{-1}\prod_{j=1}^{n}\hat{A}_{t_i}^{(i)} &= \hat{A}_{t_{i_n}}^{(i_n)}\hat{A}_{t_{i_{n-1}}}^{(i_{n-1})}...\hat{A}_{t_{i_2}}^{(i_2)}\hat{A}_{t_{i_1}}^{(i_1)}, \\ & t_{i_n} < t_{i_{n-1}} < ... < t_{i_2} < t_{i_1}.\end{aligned} \tag{60}$$

In terms of path integrals, the density matrix of eq.(58) may be written in the coordinate representation as

$$\begin{aligned}\rho(q,q') &= <q|\hat{\rho}|q'> \\ &= <q|\hat{\mathcal{U}}\hat{\rho}(t_0)\hat{\mathcal{U}}^{-1}|q'>\end{aligned} \tag{61}$$

Inserting the complete set $\int dq|q><q| = 1$ into eq.(61), then we get the result

$$\rho(q,q') = \int dq_0 \int dq_0' < q|\hat{\mathcal{U}}|q_0 >< q_0|\hat{\rho}(t_0)|q_0' >< q_0'|\hat{\mathcal{U}}^{-1}|q' > . \quad (62)$$

From the expression of $< q|\hat{\mathcal{U}}|q_0 >$ in eq.(52), we get

$$\begin{aligned}\rho(q,q') = & \int dq_0 \int dq_0' \rho(q_0,q_0') \\ & \cdot \int \mathcal{D}[q_s] \int \mathcal{D}[q_s'] \exp\{\frac{i}{\hbar}\int_0^T ds(\mathcal{L}(q,\dot{q};s) \\ & -\mathcal{L}(q',\dot{q}';s))ds\}. \end{aligned} \quad (63)$$

This is the expression of path integrals representation of density matrix and will be used extensively in our calculations of quantum transport problem.

Propagator for the Modeled System

From our modeled system discussed in the previous chapter, we would like to write down the expression of the propagator of such system. From the expression of the Hamiltonian in eq.(30), its corresponding Lagrangian is

$$\mathcal{L}(r,\dot{r};t) = \frac{1}{2}m\dot{r}^2 + \frac{e}{c}A\cdot\dot{r} - V(r) \quad (64)$$

The potential $V(r)$ depends on the kind and configuration of the imperfections. We would like to suppose that if the imperfections are being fixed scatterers of impurities and randomly distributed, this is called *random system* [18]. we also suppose that the scattering processes are two-body interactions, then we can write the potential term as

$$V(r) = \sum_i v(r-R_i) \quad (65)$$

where R_i is the site of impurity. With this Lagrangian, the propagator can be expressed as

$$K(r_T, r_0; T) = \int \mathcal{D}[r_t] \exp \frac{i}{\hbar} \int_0^T dt \mathcal{L}(r, \dot{r}; t) - \frac{i}{\hbar} \int_0^T dt V(r_t)\} \qquad (66)$$

To consider the dynamical properties of an electron, we would like to take an effect of scattering with impurities by averaging the propagator over all the scattering potential at all sites via the expression

$$K^{av}(r_T, r_0; T) = \int dV P(V) K(r_T, r_0; T) \qquad (67)$$

$P(V)$ is the potential distribution. Because the impurities are randomly distributed, then, for the system of the area A, the probability to find one impurity located in the small area dR is dR/A . Then for all impurities we get the distribution

$$P(V) = \int \frac{dR_1}{A} \cdots \int \frac{dR_N}{A} \delta \left(V - \sum_{i=1}^{\infty} v(r - R_i) \right) \qquad (68)$$

where the delta function is used to contraint that the scattering is a type we choose. With this expression of the potential distribution, the averaged propagator of eq.(67) becomes to be

$$\begin{aligned} K^{av}(r_T, r_0; T) &= \int dV P(V) \int \mathcal{D}[r_t] e^{\frac{i}{\hbar} \int_0^T \mathcal{L}(r, \dot{r}; t) dt - \frac{i}{\hbar} \int_0^T V(r_t) dt} \\ &= \int \mathcal{D}[r_t] e^{\frac{i}{\hbar} \int_0^T \mathcal{L}(r, \dot{r}; t) dt} \left[\int \frac{dR}{A} e^{-\frac{i}{\hbar} \int_0^T v(r_t - R) dt} \right]^N \end{aligned} \qquad (69)$$

where we have integrated the potential V and used the delta function. At this step of calculation, we would like to use the identity

$$[X]^N = [(X-1)+1]^N \xrightarrow[N->\infty]{} > e^{N(X-1)} \qquad (70)$$

The averaged propagator of eq.(69) comes into the form

$$K^{av}(r_T, r_0; T) = \int \mathcal{D}[r_t] e^{\frac{i}{\hbar}\int_0^T \mathcal{L}(r,\dot{r};t)dt} \cdot \exp\left\{ N\left(\int \frac{dR}{A} e^{-\frac{i}{\hbar}\int_0^T dt v(r_t - R)} - 1 \right) \right\} \tag{71}$$

At this stage, we further suppose that the scattering potential is weak, then we can expand the exponential term of scattering potential on the right hand side of eq.(71) into series and keep only the first non-vanishing term, then we get

$$K^{av}(r_T, r_0; T) = \int \mathcal{D}[r_t] e^{\frac{i}{\hbar}\int_0^T dt \mathcal{L}(r,\dot{r};t)} \cdot \exp\left\{ -\frac{1}{2\hbar^2} \int_0^T dt \int_0^T dt' W(r_t - r_{t'}) \right\} \tag{72}$$

where we have assumed that the configuration average of the scattering potential is zero, $\int \frac{dR}{N} v(r_t - R) = 0$, and define the potential correlation function

$$W(r_t - r_{t'}) = N \int dR v(r_t - R) v(r_{t'} - R) \tag{73}$$

which is a nonlocal function in time. For the second term on the right hand side of eq.(72) may be expressed it in terms of the *impurity influence function* $,\phi(r_t, r_{t'})$, as

$$\frac{i}{\hbar}\phi(r_t, r_{t'}) = -\frac{1}{2\hbar^2} \int_0^T dt \int_0^T dt' W(r_t - r_{t'}) \tag{74}$$

This term will cause the difficulty in the evaluation of the corresponding propagator in eq.(72). There are many ways to overcome this difficulty. What we expect to do here is using the model of influence functional instead of using the direct function from the Coulomb or screened Coulomb interactions. We would like to use the *gaussian model* of this potential correlation function[18]

$$W(r_t - r_{t'}) = \xi_l^2 e^{-(r_t - r_{t'})^2/L^2} \tag{75}$$

where we have put two parameters into this model. The first one is the strength of the scattering,ξ_L , which we call the correlation strength and the second one is the range of the correlation, L , which is called the correlation length. More details of our calculation will be shown in the subsequence chapter and in the next section we would like to discuss the expression of the density matrix in Feynman path integrals representaion for our chosen model.

Density Matrix for the Modeled System

From the Lagrangian of our model system in eq.(64), we can write down the density matrix, in path integrals representation ,eq.(63), as

$$\begin{aligned}\rho(r_T, r'_T) &= \int dr_0 \int dr'_0 \rho(r_0, r'_0) \\ &\cdot \int \mathcal{D}[r_t] \int \mathcal{D}[r'_t] \exp\left\{\frac{i}{\hbar}\int_0^T dt\,(\mathcal{L}(r,\dot{r};t) - V(r_t))\right\} \\ &\cdot \exp\left\{-\frac{i}{\hbar}\int_0^T dt\,(\mathcal{L}(r',\dot{r}';t) - V(r'_t))\right\} \qquad (76)\end{aligned}$$

The averaged density matrix can be evaluated with the scattering potential distribution in eq.(67), and results in the expression

$$\begin{aligned}\rho^{av}(r_T, r'_T) &= \int dr_0 \int dr'_0 \rho(r_0, r'_0) \\ &\cdot \int \mathcal{D}[r_t] \int \mathcal{D}[r'_t] \exp\left\{\frac{i}{\hbar}\int_0^T dt\,(\mathcal{L}(r,\dot{r};t) - \mathcal{L}(r',\dot{r}';t))\right\} \\ &\cdot \exp\{-\frac{1}{2\hbar^2}\int_0^T dt \int_0^T dt'(W(r_t - r_{t'}) - 2W(r_t - r'_{t'}) \\ &+ W(r'_t - r'_{t'}))\} \qquad (77)\end{aligned}$$

This expression is derived under using of identity of eq.(70) and the assumption of weak scattering potential. This resulting averaged density matrix will be used in the procedure of quantum averaging in our studying the quantum transport problem in subsequence chapters.