CHAPTER II

FUNCTIONAL INTEGRATIONS AND QUANTUM STATISTICAL MECHANICS

2.1 A BRIEF HISTORY OF FUNCTIONAL INTEGRATION

The systematic development of functional analysis began with Volterra, his work contributing a general method of handing functional operations.

However, he first application of functional integration as a means of solving partial differential equtions of stochastic type was made by Wiener in the early 1920s.

In general, integration of a function over all variables by analogy to the integration of multivariable functions leads to divergence. The remedy lies in the introduction of a weighting factor per variable of integration. The joint weight for all variables constitutes the measure of integration.

However, the major step in the formulation of Quantum Mechanics, via functional integration, was undertaken by Feynman (1948) [21] with his work on *Space-Time Approach to Non-Relativistic Quantum Mechanics*. In a series of publications following this paper, Feynman developed the Theory of Quantum Electrodynamics and the Statistical Mechanics treatment of liquid helium.

2.2 PROPAGATOR AND PARTITION FUNCTION

Starting at the one body problem, which has Lagrangian as

$$L=\frac{m\dot{\bar{x}}^2}{2}-V(\bar{x}) \tag{2.1}$$

and which corresponds to the Hamiltonian, H

$$L=p\dot{x}-H\,, \tag{2.2}$$

the Feynman propagator is

$$K(\bar{x},t;\bar{x}',0)=\frac{1}{A}\int D[\bar{x}(t)]Exp\left[\frac{i}{\hbar}\int_0^t L(\tau)d\tau\right]. \tag{2.3}$$

If L from equation (2.2) is replaced, the result is

$$K(\bar{x},t;\bar{x}',0)=\frac{1}{A}\int D[\bar{x}(t)]Exp\left[\frac{i}{\hbar}\int_0^t\left(\frac{m\dot{\bar{x}}^2(\tau)}{2}-V(\bar{x})\right)d\tau\right] \tag{2.4}$$

where, $D[\bar{x}(\tau)]=\left(\frac{m}{2\pi\hbar dt}\right)^{3/2}\prod_{i=1}\left(\frac{m}{2\pi i\hbar dt}\right)^{3/2}d\bar{x}_i(\tau)$.

The Feynman propagator $K(\bar{x},t;\bar{x}',0)$ can be expressed in terms of the Schr dinger wave function ϕ_n and its energy eigen value E_n by the following [22]

$$K(\bar{x},t;\bar{x}',0)=\sum_{n=1}^{\infty}\phi_n(\bar{x})\phi_n^*(\bar{x}')Exp\left[-\frac{i}{\hbar}E_n t\right],\quad t>0. \tag{2.5}$$

If the Feynman propagator over all space is integrated, then

$$\int K(\bar{x},t;\bar{x}',0)d\bar{x}=\sum_{n=1}^{\infty}Exp\left[-\frac{i}{\hbar}E_n t\right]. \tag{2.6}$$

Let $t=-i\hbar\beta$ then,

$$\int K(\bar{x},-i\hbar\beta;\bar{x}',0)d\bar{x}=\sum_{n=1}^{\infty}Exp\left[-\frac{i}{\hbar}E_n(-i\hbar\beta)\right].$$

$$\int K(\bar{x},-i\hbar\beta;\bar{x}',0)d\bar{x}=\sum_{n=1}^{\infty}Exp\left[-\beta E_n\right]. \tag{2.7}$$

From the right hand side of the above equation partition function is evident. Therefore, the partition function in functional formalism can be rewritten by the expression

$$Q(\beta)=\int K(\bar{x},-i\hbar\beta;\bar{x}',0)d\bar{x}. \tag{2.8}$$

This is essentially an analytic continuation of the propagator in the lower half plane of a complex time.

As with one body problems the same idea to introduce the partition function of many body problems can be used. Papadopoulos [23] suggests that it is not difficulty to replace the one body Lagrangian by a many-bodied Lagrangian. Using his suggestion, the propagator of a many body problem takes the form:

$$K(\bar{x}_1,\bar{x}_2,\dots,\bar{x}_N,t;\bar{x}_1',\bar{x}_2',\dots,\bar{x}_N',0)=\int_{\bar{x}_1}\int_{\bar{x}_2}\dots\int_{\bar{x}_N} Exp\left\{\frac{i}{\hbar}\int_0^t (N-bodyLagrangian)d\tau\right\}$$
$$\times D[\bar{x}_1(\tau)]D[\bar{x}_2(\tau)]\dots D[\bar{x}_N(\tau)] \quad (2.9)$$

where, $D[\bar{x}(\tau)]=\left(\frac{m}{2\pi\hbar dt}\right)^{3/2}\prod_{i=1}\left(\frac{m}{2\pi i\hbar dt}\right)^{3/2} d\bar{x}_i(\tau)$.

And, then

$$Q_N=\int K(\bar{x}_1,\bar{x}_2,\dots,\bar{x}_N,t;\bar{x}_1',\bar{x}_2',\dots,\bar{x}_N',0)d\bar{x}_1 d\bar{x}_2\dots d\bar{x}_N \quad (2.10)$$

If N body Lagrangian of the system is

$$L_N=\sum_{i=1}^{N}\frac{m\dot{\bar{x}}^2}{2}-V(\bar{x}_1,\bar{x}_2,\dots,\bar{x}_N). \quad (2.11)$$

the partition function is obtained from the following propagator,

$$K(\bar{X},h\beta;\bar{X}',0)=\int_{\substack{\bar{x}_i(0)=\bar{x}_i'\\ \bar{x}_i(\hbar\beta)=\bar{x}}} Exp\left[\frac{1}{\hbar}\int_0^{\hbar\beta}\left\{\sum_i\frac{m\dot{\bar{x}}^2(s)}{2}+V(\bar{x}_1(s),\bar{x}_2(s),\dots,\bar{x}_N(s))\right\}ds\right]$$
$$\times D[\bar{x}_1(s)]D[\bar{x}_2(s)]\dots D[\bar{x}_N(s)] \quad (2.12)$$

where,

$$D[\bar{x}(s)] = \left(\frac{m}{2\pi\hbar ds}\right)^{3/2} \prod_{0<s<\hbar\beta} \left(\frac{m}{2\pi\hbar ds}\right)^{3/2} d\bar{x}(s).$$

The next step will include the effect of statistical mechanics about the permutation properties of particles

$$Q_N = \frac{1}{N!}\int\left[\sum_P (+)^P \int_{\bar{x}_1}\int_{\bar{x}_2}\ldots\int_{\bar{x}_N} Exp\left\{\frac{i}{\hbar}\int_0^t (N-bodyLagrangian)d\tau\right\}\right.$$
$$\left.\times D[\bar{x}_1(\tau)]D[\bar{x}_2(\tau)]\ldots D[\bar{x}_N(\tau)] - \right]\prod_i d\bar{x}_i \qquad (2.13)$$

for boson systems

and,

$$Q_N = \frac{1}{N!}\int\left[\sum_P (-)^P \int_{\bar{x}_1}\int_{\bar{x}_2}\ldots\int_{\bar{x}_N} Exp\left\{\frac{i}{\hbar}\int_0^t (N-bodyLagrangian)d\tau\right\}\right.$$
$$\left.\times D[\bar{x}_1(\tau)]D[\bar{x}_2(\tau)]\ldots D[\bar{x}_N(\tau)] - \right]\prod_i d\bar{x}_i \qquad (2.14)$$

for fermion systems.

Dealing with the quantum field operators or second quantization, the same idea of replacing the co-ordinate Lagrangian by the Lagrangian of each representation can be used. In field operator representation the Hamiltonian is written as

$$H(\tau) = \int d\bar{x}\left(\frac{\hbar^2}{2m}\nabla\psi^+(\bar{x},\tau)\nabla\psi(\bar{x},\tau) - \lambda\psi^+(\bar{x},\tau)\psi(\bar{x},\tau)\right)$$
$$+\frac{1}{2}\int d\bar{x}d\bar{y}U(\bar{x}-\bar{y})\psi^+(\bar{x},\tau)\psi^+(\bar{y},\tau)\psi(\bar{y},\tau)\psi(\bar{x},\tau), \qquad (2.15)$$

where, $U(\bar{x}-\bar{y})$ is the pair potential function and λ is the chemical potential coefficient. Especially $\psi^+(\bar{x},\tau)$ and $\psi(\bar{x},\tau)$ are the field operators which create and annihilate a particle at $\bar{x}$ at time τ, respectively. The Lagrangian can be evaluated by the expression

$$L = \int d\bar{x}\psi^+(\bar{x},\tau)\partial_\tau\psi(\bar{x},\tau) - H(\tau) \qquad (2.16)$$

Then, the partition function becomes

$$Q = \int Exp\left\{\frac{1}{\hbar}\int_0^t L(\tau)d\tau\right\}D\psi^+(\bar{x},\tau)D\psi(\bar{x},\tau). \qquad (2.17)$$