CHAPTER III

A VARIATIONAL METHOD

OVERVIEW

In general, a lot of path integrals cannot be integrated out and this problem is one in this case. Then an approximation method is needed inevitably. The most widely used methods in path integral formalism are perturbation and variational methods. Since this problem is not a perturbative-type problem, we shall choose a variational method.

The concept of this method is that the appropriate trial action with parameter(s) can be adjusted such that the required path integral can be obtained with high accuracy. There are two criteria that tell the chosen trial action suitable or not. First, the path integral of this action should be carried out easily and exactly. Second, the physical meaning of the "real" and trial action must be likely.

Of course, the last step of this method is to adjust the parameter(s). In doing this, it must have a rule or principle which enable us to find out the appropriate value of parameter(s). This is known as a variational principle. The discussion about the principle could not be considered yet in this chapter.

In this chapter, we shall construct a trial action from the model proposed first by Samathiyakanit (1974), which is similar to that of Feynman used in the polaron problem. Then the path integrals will be performed within the first cumulant approximation by using the constructed trial action in next chapter. Two variational principles will be considered in chapter V.

CONSTRUCTING A TRIAL ACTION

First, we shall model a system which is called a "two-particle" system. Here after, as we regard this system, it will mean a system of an electron and a fictitious particle where the mutual interaction is proportional to a distance between them squared, as well as the position of the fictitious particle at the beginning and end time are coincident.

The Lagrangian of this system can be written as

$$L_2 = \frac{1}{2}m\dot{\mathbf{x}}^2(\tau) + \frac{1}{2}M\dot{\mathbf{y}}^2(\tau) + \frac{1}{2}\kappa|\mathbf{x}(\tau) - \mathbf{y}(\tau)|^2, \tag{3.1}$$

where the electron of mass m is at position $\mathbf{x}(\tau)$, the fictitious particle of mass M is at position $\mathbf{y}(\tau)$, and κ is the force constant. Then the two-particle propagator is

$$K_0(\mathbf{x}_2, \mathbf{x}_1, \mathbf{y}_0, \mathbf{y}_0; t, 0) = \int D(\mathbf{x}(\tau))\int D(\mathbf{y}(\tau))\exp\left[-\frac{i}{\hbar}S_2[\mathbf{x}(\tau), \mathbf{y}(\tau)]\right], \tag{3.2}$$

where $S_2[\mathbf{x}(\tau), \mathbf{y}(\tau)]$ is the two-particle action, $S_2 = \int_0^t L_2 d\tau$.

We now turn to regard of a model for constructing a trial action. In this model, we suppose that the propagator of the trial action is proportional to the summation over all the fictitious particle's positions of the two-particle propagator.

That is,

$$K_0(\mathbf{x}_2,\mathbf{x}_1;t,0)=\int D(\mathbf{x}(\tau))\exp\left[-\frac{i}{\hbar}S_0[\mathbf{x}(\tau)]\right]$$

$$=A\int d\mathbf{y}_0 K_0(\mathbf{x}_2,\mathbf{x}_1,\mathbf{y}_0,\mathbf{y}_0;t,0), \tag{3.3}$$

where S_0, K_0 are the trial action and its propagator, respectively, and A is the proportional constant. By substituting the two-particle propagator from (3.2) in (3.3) and interchanging the order of integration between $\mathbf{x}(\tau)$ and $\mathbf{y}_0$, we get

$$\exp\left[\frac{i}{h}S_0[\mathbf{x}(\tau)]\right]=A\int d\mathbf{y}_0\int D(\mathbf{y}(\tau))\exp\left[\frac{i}{h}S_2[\mathbf{x}(\tau),\mathbf{y}(\tau)]\right]. \tag{3.4}$$

Reconsider the two-particle Lagrangian (3.1). Expand the interaction term, we have

$$L_2=\frac{1}{2}m\dot{\mathbf{x}}^2(\tau)+\frac{1}{2}\kappa\mathbf{x}^2(\tau)+\frac{1}{2}M\dot{\mathbf{y}}^2(\tau)+\frac{1}{2}M\mathbf{y}^2(\tau)+\kappa\mathbf{x}(\tau)\cdot\mathbf{y}(\tau). \tag{3.5}$$

Since the exponential of the first two terms can be moved out from both $\mathbf{y}_0$ and $\mathbf{y}(\tau)$-integrations in (3.4) then the path summation of $\mathbf{y}(\tau)$ can be performed easily. The relation (3.4) becomes

$$\exp\left[\frac{i}{h}S_0[\mathbf{x}(\tau)]\right]=A\left(\frac{M\omega}{2\pi i\hbar\sin\omega t}\right)^{3/2}\exp\left[\frac{i}{\hbar}\int_0^t\left(\frac{1}{2}m\dot{\mathbf{x}}^2(\tau)+\frac{1}{2}M\mathbf{x}^2(\tau)\right)d\tau\right]$$

$$\int d\mathbf{y}_0\exp\left[\frac{i}{h}S_{cl}^{[\mathbf{x}(\tau)]}(\mathbf{y}_0,t)\right], \tag{3.6}$$

where

$$S_{cl}^{[x(\tau)]}(\mathbf{y}_0,t) = -\frac{M\omega}{\sin\omega t}\left[2\mathbf{y}_0^2 \sin^2\frac{1}{2}\omega t - \frac{2\mathbf{y}_0}{M\omega}\cdot\int_0^t d\tau\,\kappa\mathbf{x}(\tau)\sin\frac{1}{2}\omega t\cos\frac{1}{2}\omega(t-2\tau)\right.$$

$$\left.+\frac{1}{M^2\omega^2}\int_0^t d\tau\int_0^t d\sigma\,\kappa^2\mathbf{x}(\tau)\cdot\mathbf{x}(\sigma)\sin\omega(t-\sigma)\sin\omega\sigma\right], \qquad (3.7)$$

is the classical action of a "forced" harmonic oscillator between $(\mathbf{y}_0,t)$ and $(\mathbf{y}_0,0)$, and $\omega^2 = \frac{\kappa}{M}$.

The $\mathbf{y}_0$-integration is a Gaussian type in three dimensions so it can be integrated by using the well-known formula,

$$\int_{-\infty}^{\infty}\exp\left[-ax^2+bx\right]dx = \sqrt{\frac{\pi}{a}}\exp\left[\frac{b^2}{4a}\right]. \qquad (3.8)$$

The result is

$$\int d\mathbf{y}_0\exp\left[\frac{i}{\hbar}S_{cl}^{[x(\tau)]}(\mathbf{y}_0,t)\right] = \left(\frac{\pi\hbar\cot\frac{1}{2}\omega t}{iM\omega}\right)^{3/2}\exp\left[\frac{i\kappa\omega}{2\hbar}\int_0^t d\tau\int_0^\tau d\sigma\,\mathbf{x}(\tau)\cdot\mathbf{x}(\sigma)\right.$$

$$\left.\times\frac{\cos\omega\left(\frac{1}{2}t-|\tau-\sigma|\right)}{\sin\frac{1}{2}\omega t}\right]. \qquad (3.9)$$

Substituting (3.9) into (3.6), we have

$$\exp\left[\frac{i}{\hbar}S_0[\mathbf{x}(\tau)]\right] = A\left(2i\sin\frac{1}{2}\omega t\right)^{-3}\exp\left[\frac{i}{\hbar}\int_0^t d\tau\,\left(\frac{1}{2}m\dot{\mathbf{x}}^2(\tau)\right.\right.$$

$$\left.\left.-\frac{1}{8}\kappa\omega\int_0^t d\sigma\left|\mathbf{x}(\tau)-\mathbf{x}(\sigma)\right|^2\frac{\cos\omega\left(\frac{1}{2}t-|\tau-\sigma|\right)}{\sin\frac{1}{2}\omega t}\right)\right]. \quad (3.10)$$

Therefore, if

$$A = \left(2i\sin\frac{1}{2}\omega t\right)^3, \quad (3.11)$$

then

$$S_0[\mathbf{x}(\tau)] = \int_0^t d\tau\,\left(\frac{1}{2}m\dot{\mathbf{x}}^2(\tau)-\frac{1}{8}\kappa\omega\int_0^t d\sigma\left|\mathbf{x}(\tau)-\mathbf{x}(\sigma)\right|^2\frac{\cos\omega\left(\frac{1}{2}t-|\tau-\sigma|\right)}{\sin\frac{1}{2}\omega t}\right). \quad (3.12)$$

It is advantageous to consider work adding due to a force acting on the electron into the two-particle Lagrangian,

$$L_2^f = \frac{1}{2}m\dot{\mathbf{x}}^2(\tau)+\frac{1}{2}\kappa\mathbf{x}^2(\tau)+\mathbf{f}(\tau)\cdot\mathbf{x}(\tau)+\frac{1}{2}M\dot{\mathbf{y}}^2(\tau)+\frac{1}{2}\kappa\mathbf{y}^2(\tau)+\kappa\mathbf{x}(\tau)\cdot\mathbf{y}(\tau), \quad (3.13)$$

which is called a forced two-particle Lagrangian. Since the added term does not depend on the fictitious particle's coordinates, it is easy to verify that the trial action obtained using this Lagrangian is different from our trial action only the time integral of the forced term. In notations,

$$S_0^{\mathbf{f}}[\mathbf{x}(\tau)] = S_0[\mathbf{x}(\tau)] + \int_0^t d\tau\ \mathbf{f}(\tau)\cdot\mathbf{x}(\tau)\,, \tag{3.14}$$

Where $S_0^{\mathbf{f}}$ is the forced trial action resulting from the contributions of the forced two-particle systems. From a hint of this equation, we can conversely find the trial action by setting $\mathbf{f} = 0$ in the expression of the forced one.

THE TRIAL PROPAGATOR

In order to calculate the propagator of the trial system which is represented by the trial action (3.12), we shall follow the standard method. The method begins with expanding all possible paths around the classical one. This makes us enable to separate the path integral into two parts: one is the classical contribution and the other is the fluctuation or quantum contribution called the prefactor or multiplicative factor. In certain systems, the prefactor depends only on the flight time. Hence, such a propagator can be written as

$$K(\mathbf{x}_2,\mathbf{x}_1;t,0) = F(t)\exp\left[\frac{i}{\hbar}S_{cl}(\mathbf{x}_2,\mathbf{x}_1;t,0)\right], \tag{3.15}$$

where S_{cl} is the classical action, F the prefactor.

Since the trial action is derived from the two-particle propagator, (3.3). Finding the classical trial action through the classical two-particle action is also possible. The transformation is then given by using (3.3) and (3.15),

$$F_0(t)\exp\left[S_{0,cl}(\mathbf{x}_2,\mathbf{x}_1;t,0)\right] = A\int d\mathbf{y}_0 F_2(t)\exp\left[\frac{i}{\hbar}S_{2,cl}(\mathbf{x}_2,\mathbf{x}_1,\mathbf{y}_0,\mathbf{y}_0;t,0)\right], \quad (3.16)$$

where the index 0 and 2 are referred as belonging to the trial and two-particle systems.

Based on the last section note, if we change the classical action and prefactor of a two-particle system to those of its corresponding forced system, each trial term will be replaced by the corresponding forced trial term. That is,

$$K_0^f(\mathbf{x}_2,\mathbf{x}_1;t,0) = F_0^f(t)\exp\left[\frac{i}{\hbar}S_{0,cl}^f(\mathbf{x}_2,\mathbf{x}_1;t,0)\right]$$

$$= A\int d\mathbf{y}_0 F_2^f(t)\exp\left[\frac{i}{\hbar}S_{2,cl}^f(\mathbf{x}_2,\mathbf{x}_1,\mathbf{y}_0,\mathbf{y}_0;t,0)\right]. \quad (3.17)$$

Along this line, we are able to get the wanted trial propagator in alternative way, beginning at a different point. Because we will have to use the classical forced trial action, hence, the chosen calculation reduces our task greatly. In other words, rather than finding both $S_{0,cl}$ and $S_{0,cl}^f$, obtaining only $S_{0,cl}^f$ is enough. Therefore the following consideration will be focused on the classical forced two-particle action and its prefactor.

As you know, the classical action is the action which its path satisfies the Hamilton's principle. On the other hand, the classical trajectory must obey a set of Lagrangian's equations,

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = 0. \quad (3.18)$$

It is obviously seen that the equations of motion are a set of coupled equations which is not easy to solve. Such a problem was attacked by transforming the Lagrangian into the center of mass coordinate system. The transformations are given by

$$\mathbf{r} = \mathbf{x} - \mathbf{y}, \tag{3.19a}$$

$$\mathbf{R} = \frac{m\mathbf{x} + M\mathbf{y}}{m + M}, \tag{3.19b}$$

$$m_0 = m + M\,, \tag{3.19c}$$

and

$$\mu = \frac{mM}{m + M}. \tag{3.19d}$$

Now, the Lagrangian (3.13) becomes

$$\frac{1}{2}\mu\,\dot{\mathbf{r}}^2(\tau) + \frac{1}{2}\kappa\mathbf{r}^2(\tau) + \frac{\mu}{m}\mathbf{f}(\tau)\cdot\mathbf{r}(\tau) + \frac{1}{2}m_0\dot{\mathbf{R}}^2(\tau) + \mathbf{f}(\tau)\cdot\mathbf{R}(\tau).$$

In this way, this can be interpreted that there are two non-interacting forced harmonic oscillators: one of mass μ has frequency $\left(\frac{\mu}{m}\right)^{1/2}$ and is acted by force $\frac{\mu\,\mathbf{f}(\tau)}{m}$, but the other has mass m_0, no frequency, and is acted by force $\mathbf{f}(\tau)$. With the help of above interpretation, the classical action then can be obtained easily. The result is

$$S^{t}_{2,cl} = \frac{\mu}{2\sin\nu t}\Bigg[\left(\mathbf{x}_1^2 + \mathbf{x}_2^2\right)\cos\nu t - 2\mathbf{x}_1\cdot\mathbf{x}_2 + \frac{2\mathbf{x}_2}{m\nu}\cdot\int_0^t d\tau\;\mathbf{f}(\tau)\sin\nu(t)$$

$$+\frac{2\mathbf{x}_1}{m\nu}\cdot\int_0^t d\tau\;\mathbf{f}(\tau)\sin\nu(t-\nu) - \frac{2}{m^2\nu^2}\int_0^t d\tau\int_0^\tau d\sigma\,\mathbf{f}(\tau)\cdot\mathbf{f}(\sigma)\sin\nu(t-\tau)\sin\nu\sigma\Bigg]$$

$$
+\frac{m^2}{2m_0 t}\left(\mathbf{x}_2-\mathbf{x}_1\right)^2+\frac{m\mathbf{x}_2}{m_0 t}\cdot\int_0^t d\tau\,\mathbf{f}(\tau)\tau+\frac{m\mathbf{x}_2}{m_0 t}\cdot\int_0^t d\tau\,\mathbf{f}(\tau)(t-\tau)
$$

$$
-\frac{1}{m_0 t}\int_0^t d\tau\int_0^\tau d\sigma\,\mathbf{f}(\tau)\cdot\mathbf{f}(\sigma)(t-\tau)\sigma+\frac{M\mathbf{y}_0}{m_0}\cdot\int_0^t d\tau\,\mathbf{f}(\tau)
$$

$$
-\frac{\mu\nu}{2\sin\nu t}\left[4\sin^2\frac{1}{2}\nu t\left(\mathbf{y}_0^2-\mathbf{y}_0\cdot\left(\mathbf{x}_2+\mathbf{x}_1\right)\right)+\frac{4\mathbf{y}_0}{m\nu}\cdot\int_0^t d\tau\,\mathbf{f}(\tau)\sin\frac{1}{2}\nu t\cos\nu(t-2\tau)\right],
$$

(3.20)

and

$$
F_2^t=\left(\frac{\mu\nu}{2\pi i\hbar\sin\nu t}\right)^{3/2}\left(\frac{m_0}{2\pi i\hbar}\right)^{3/2}, \tag{3.21}
$$

where $\nu^2=\frac{\kappa}{\mu}$. Substituting $A, S_{2,cl}^t, F_2^t$ from (3.11), (3.20), and (3.21), respectively, into (3.17) and performing $\mathbf{y}_0$-integration, we have

$$
F_0^t=\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\left(\frac{\nu\sin\frac{1}{2}\omega t}{\omega\sin\frac{1}{2}\nu t}\right)^3 \tag{3.22}
$$

and

$$
S_{0,cl}^t=\left(\frac{\mu\nu}{4}\cot\tfrac{1}{2}\nu t+\frac{m\mu}{2Mt}\right)\left(\mathbf{x}_2-\mathbf{x}_1\right)^2
$$

$$
+\mathbf{x}_2\cdot\int_0^t d\tau\,\mathbf{f}(\tau)\left(\frac{\mu}{m}\frac{\cos\frac{1}{2}\nu(t-\tau)\sin\frac{1}{2}\nu t}{\sin\frac{1}{2}\nu t}+\frac{\mu\tau}{mt}\right)
$$

$$
+\mathbf{x}_1\cdot\int_0^t d\tau\,\mathbf{f}(\tau)\left(\frac{\mu}{m}\frac{\sin\frac{1}{2}\nu(t-\tau)\cos\frac{1}{2}\nu t}{\sin\frac{1}{2}\nu t}+\frac{\mu(t-\tau)}{mt}\right)
$$

$$-\int_0^t d\tau \int_0^\tau d\sigma\, \mathbf{f}(\tau)\cdot \mathbf{f}(\sigma)\left(\frac{\mu}{mM}\frac{(t-\tau)\sigma}{t}\right.$$

$$\left.+\frac{2\mu}{m^2\nu}\frac{\sin\frac{1}{2}\nu(t-\tau)\sin\frac{1}{2}\nu\sigma\cos\frac{1}{2}\nu(t-\tau)}{\sin\frac{1}{2}\nu t}\right). \qquad (3.23)$$

By setting $\mathbf{f}=0$ in the forced trial propagator, then it will change to be the trial one. So, the trial propagator can be written as

$$K_0\left(\mathbf{x}_2,\mathbf{x}_1;t,0\right)=\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\left(\frac{\nu\sin\frac{1}{2}\omega t}{\omega\sin\frac{1}{2}\nu t}\right)^3$$

$$\exp\left[\frac{i}{\hbar}\left\{\left(\frac{\mu\nu}{4}\cot\frac{1}{2}\nu t+\frac{m\mu}{2Mt}\right)\left(\mathbf{x}_2-\mathbf{x}_1\right)^2\right\}\right]. \qquad (3.24)$$

Remark that this propagator has the translational symmetry.