CHAPTER II

QUALITATIVE SURVEY

In proceeding to evaluate the polaron energy, the basic ideas of constructing the Feynman path integral and the determination of a forced harmonic oscillator propagator in the path integral formalism will be presented. The relationship between the propagator and the density matrix, and the polaron ground state energy, will also be considered in this chapter.

II.1 Feynman Path Integral

Consider the motion of a particle starting from one point to another. In quantum mechanics, we cannot specify its exact position at any chosen time but we can only indicate the probability of finding it at any given time and place. In this case there are many possible paths that the particle has the probability to take. In contrast, in classical mechanics the particle can move along one particular path for which the action $S = \int L dt$ is a minimum, where L is the Lagrangian of the system. For simplicity, we shall restrict ourselves to the case of the particle moving in one dimension with the position at any given time specified by a coordinate x and the path x(t). If the particle at an initial time t_a starts from the point x_a and goes to a final point x_b at time t_b, then the classical path $\bar{x}$ is that for which the principle of least action is satisfied, i.e.,

$$\delta S = 0, \tag{2.1}$$

and the classical action is given by

$$S_{cl} = \int_{t_a}^{t_b} L(\dot{\bar{x}}, \bar{x}, t)\, dt \ . \tag{2.2}$$

In quantum mechanics, there is not only just the classical path but there are many possible paths which the particle can take. The probability that the particle goes from a point x_a at time t_a to the point x_b at time t_b is given by the absolute square of an amplitude $K(b,a)$ which is the sum of the contributions $\phi[x(t)]$, one from each path $x(t)$, viz.,

$$K(b,a) = \sum_{\substack{\text{over all} \\ \text{paths from} \\ a \text{ to } b}} \phi[x(t)] \ , \tag{2.3}$$

where the contribution of a path $x(t)$ has a phase proportional to the action S,

$$\phi[x(t)] = \text{const.} \exp\left[\frac{i}{\hbar} S[x(t)]\right] . \tag{2.4}$$

To determine the probability amplitude $K(b,a)$, we have to compute the sum in (2.3) over all paths of infinite number, and it is thus more appropriate to replace the infinite summation by path integration. In order to do this, we first choose a subset of all paths by dividing the independent time variable into a series of small intervals ϵ. This gives a set of values $t_a, t_1, t_2, \ldots\ldots, \ldots$

t_{N-1}, t_b where $\epsilon = t_{i+1} - t_i$, $N\epsilon = t_b - t_a$, $t_0 = t_a$ and $t_N = t_b$. At each time t_i we select some special point x_i with $x_0 = x_a$, $x_N = x_b$ and then construct a path by connecting all the points with straight lines as shown in Fig.3.

A sum over all paths constructed in this manner can be defined by taking a multiple integral over all values of x_i for i between 1 and N-1 so that the propagator in Eq.(2.3) becomes

$$K(b,a) \sim \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \cdots\cdots \int_{-\infty}^{\infty} \phi[x(t)]\, dx_1\, dx_2 \cdots\cdots dx_{N-1} \quad , \qquad (2.5)$$

where the integrations over x_0 and x_N are not involved since these are the fixed end points x_a and x_b. A more representative sample of the complete set of all possible paths between a and b can be obtained by making ϵ infinitesimal and by introducing some normalizing factor, which is expected to depend on ϵ, into Eq.(2.5). The probability amplitude can then be written as

$$K(b,a) = \lim_{\epsilon \to 0} \frac{1}{A} \int\int \cdots\cdots \int \exp\left[\frac{i}{\hbar} S[x(t)]\right] \frac{dx_1}{A} \cdots\cdots \frac{dx_{N-1}}{A} \,. \qquad (2.6)$$

The integration in Eq.(2.6) can be written in a less restrictive notation as

$$K(b,a) = \int_{x_a}^{x_b} \exp\left[\frac{i}{\hbar} S[x(t)]\right] \mathcal{D}x(t) \quad , \qquad (2.7)$$

which is called a "path integral", and the probability amplitude of this form is known as the <u>Feynman propagator</u>.

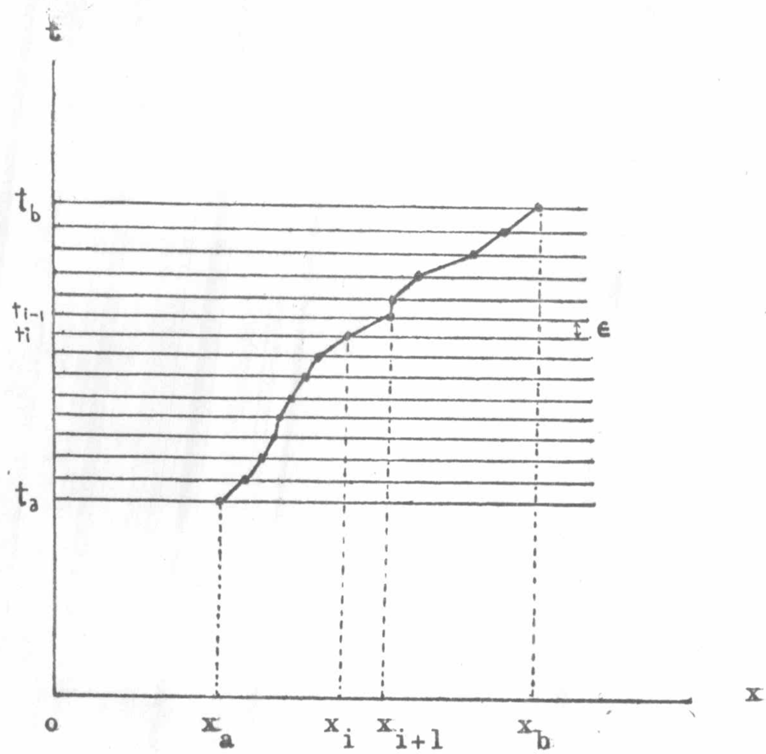

Fig. 3 The construction of the path integral.

II.2 Forced Harmonic Oscillator Propagator

In this section, we shall determine the Feynman propagator of a forced harmonic oscillator for the reason that not only it is a particularly interestig and simple example for the evaluation of the path integral but also it is of much importance in the solution of the polaron problem to be presented in the next chapter. We thus consider a system whose Lagrangian has the form

$$L = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2x^2 + f(t)x \qquad (2.8)$$

and for which the integration over all paths from (x,t) to (x,t) of the propagator

$$K(x'',x') = \int_{x'}^{x''} \exp\left[\tfrac{i}{\hbar} S[x(t)]\right] \mathcal{D}x(t) \quad , \qquad (2.\ )$$

where

$$S[x(t)] = \int_{t'}^{t''} \left[\tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2x^2 + f(t)x\right] dt \quad , \qquad (2.10)$$

must be carried out.

To accomplish this , we first describe the path x(t) by means of the classical path $\bar{x}(t)$ and the deviation y(t) from the classical path, viz.,

$$x(t) = \bar{x}(t) + \bar{y}(t) \quad . \qquad (2.11)$$

Thus, in a path integral, the path differential x(t) can now be represented by y(t), and the action (2.10) then becomes

$$S[\bar{x}(t)] = \int_{t'}^{t''} \left[\left[\tfrac{1}{2}m\dot{\bar{x}}^2 - \tfrac{1}{2}m\omega^2\bar{x}^2 + f(t)\bar{x}\right] + \left[\tfrac{1}{2}m\dot{y}^2 - \tfrac{1}{2}m\omega^2y^2 + m\omega^2\bar{x}y + f(t)y\right]\right]dt \qquad (2.12)$$

$$= S_{cl} + \int_{t'}^{t''} \left[\tfrac{1}{2}m\dot{y}^2 - \tfrac{1}{2}m\omega^2y^2\right] dt \quad , \qquad (2.13)$$

where the resulting integral of $S[\bar{x}(t)]$ is S_{cl} and the resulting integral for all terms which contain y as linear factor in the integrand vanishes. This simple integral is called the <u>Gaussian integral</u>[18].

On substituting Eq. (2.13) into Eq. (2.9) we obtain

$$K(x'',x') = \exp[\tfrac{i}{\hbar} S_{cl}] \int_0^0 \exp[\tfrac{i}{\hbar}\int_{t'}^{t''}[\tfrac{m}{2}\dot{y}^2 - \tfrac{m}{2}\omega^2 y^2]\,dt]\,\mathcal{D}y(t)$$

$$= \exp[\tfrac{i}{\hbar} S_{cl}]\, F(t',t'') \quad , \qquad (2.14)$$

where

$$F(t',t'') = \int_0^0 \exp[\tfrac{i}{\hbar}\int_{t'}^{t''}(\tfrac{m}{2}\dot{y}^2 - \tfrac{m}{2}\omega^2 y^2)\,dt]\,\mathcal{D}y(t)$$

is only a function of the times at the end points, since all paths y(t) start from and return to the point y=0. The path integrand $F(t',t'')$ can be evaluated by writing y(t) as a Fourier sine series,

$$y(t) = \sum_n a_n \sin\frac{n\pi t}{(t''-t')} \quad , \qquad (2.15)$$

and then by considering the paths as functions of the coefficients a_n instead of functions of y(t). The result is[19]

$$F(t',t'') = \left(\frac{m\omega}{2\pi i\hbar \sin\omega(t''-t')}\right)^{\frac{1}{2}} \quad . \qquad (2.16)$$

The problem of finding the propagator in the form of Eq. (2.9) or Eq. (2.14) is reduced to merely that of

---

18 See Reference (4) P. 58

19 See Reference (4) P. 72

determining the classical action of the system, which we shall now consider. In Eq.(2.13) the classical action of the system can be represented as

$$S_{cl} = \int_{t'}^{t''} \left[\frac{m}{2}\dot{\bar{x}}^2 - \frac{m}{2}\omega^2\bar{x}^2 + f(t)\bar{x} \right] dt \quad . \qquad (2.17)$$

We must first evaluate the classical path of the system by using the principle of least action, according to which the classical path $\bar{x}$ has to satisfy the condition

$$\delta S = 0 = \int_{t'}^{t''} \left[\frac{m}{2} \cdot 2\dot{\bar{x}}\,\delta\dot{\bar{x}} - \frac{m\omega^2}{2} \cdot 2\bar{x}\,\delta\bar{x} + f(t)\,\delta\bar{x} \right] dt$$

$$= m\dot{\bar{x}}.\delta\bar{x} \Big|_{t'}^{t''} + \int_{t'}^{t''} \left[-m\ddot{\bar{x}} - m\omega^2\bar{x} + f(t) \right] \delta\bar{x}\, dt \quad . \qquad (2.18)$$

Since the end points of the paths are fixed, the first term of (2.18) vanishes. Therefore we obtain

$$\ddot{\bar{x}}(t) + \omega^2\bar{x}(t) = \frac{f(t)}{m} \quad . \qquad (2.19)$$

To solve the differential equation of $\bar{x}(t)$, we shall use the Green function method. The Green function equation satisfying (2.19) is defined by

$$\left(\frac{d^2}{ds^2} + \omega^2\right) G(s,t) = \delta(s-t) \quad , \qquad (2.20)$$

with the boundary conditions

$$G(t',t) = G(t'',t) = 0 \quad . \qquad (2.21)$$

The solution of Eq.(2.20) when s is not equal to t is given by

$$G(s,t) = A\sin\omega s + B\cos\omega s \quad , \qquad (2.22)$$

where A and B are constants.

By applying the conditions (2.21) to Eq. (2.22) we obtain

$$G(s,t) = G_1(s,t)H(t-s) + G_2(s,t)H(s-t) \quad , \qquad (2.23)$$

where

$$G_1(s,t) = B\,(\cos\omega s - \cot\omega t'\sin\omega s) \quad , \qquad (2.24)$$

and $$G_2(s,t) = B'(\cos\omega s - \cot\omega t''\sin\omega s) \quad . \qquad (2.25)$$

The constants B and B' can be determined by using certain properties of the Green function, the first of which is that G(s,t) must be continuous at s = t,

$$G_1(t,t) = G_2(t,t) \quad . \qquad (2.26)$$

We thus obtain

$$B = B'\,\frac{(\cos\omega t - \cot\omega t''\sin\omega t)}{(\cos\omega t - \cot\omega t'\sin\omega t)} \quad . \qquad (2.27)$$

The second property of G(s,t) to be used is that its derivative must satisfy the equation

$$\Big[G_2'(s,t) - G_1'(s,t)\Big]_{s=t} = 1 \quad , \qquad (2.28)$$

where G' is the derivative of the Green function with respect to the variable s. On substituting the derivative of G_1 and G_2 from Eq.(2.24) and Eq.(2.25) into the above equation, we obtain

$$\Big[B'\omega(-\sin\omega t - \cot\omega t''\cos\omega t) - B\omega(-\sin\omega t - \cot\omega t'\cos\omega t)\Big] = 1 \quad . \qquad (2.29)$$

By making use of the value of B from Eq.(2.27) in Eq.(2.29), the constant B' can be determined as

$$B' = \frac{[\cos\omega t - \cot\omega t' \sin\omega t]}{\omega[\cot\omega t' - \cot\omega t'']} , \quad (2.30)$$

and hence

$$B = \frac{[\cos\omega t - \cot\omega t'' \sin\omega t]}{\omega[\cot\omega t' - \cot\omega t'']} . \quad (2.31)$$

By substituting the values of B and B' into Eq.(2.24) and Eq.(2.25), we obtain

$$G_1(s,t) = -\frac{\sin\omega(s-t')\sin\omega(t''-t)}{\omega\sin\omega(t''-t')} , \quad (2.32)$$

and

$$G_2(s,t) = -\frac{\sin\omega(t-t')\sin\omega(t''-s)}{\omega\sin\omega(t''-t')} . \quad (2.33)$$

Thus the Green function (2.23) is readily found to be

$$G(s,t) = -\frac{\sin\omega(s-t')\sin\omega(t''-t)}{\omega\sin\omega(t''-t')} . H(t-s) - \frac{\sin\omega(t-t')\sin\omega(t''-s)}{\omega\sin\omega(t''-t')} . H(s-t) . \quad (2.34)$$

The classical path $\bar{x}(t)$ can be determined by considering the two equations

$$\ddot{\bar{x}}(s) + \omega^2\bar{x}(s) = \frac{f(s)}{m} , \quad (2.35)$$

and

$$\left(\frac{d^2}{ds^2} + \omega^2\right) G(s,t) = \delta(s-t) , \quad (2.36)$$

which lead to

$$\int_{t'}^{t''} \left[\bar{x}(s)\left(\frac{d^2}{ds^2}+\omega^2\right)G(s,t) - G(s,t)\left(\frac{d^2}{ds^2}+\omega^2\right)\bar{x}(s)\right] ds = \int_{t'}^{t''} \left[\bar{x}(s)\delta(s-t) - \frac{f(s)}{m}G(s,t)\right] ds$$

and
$$\bar{x}(s)\frac{dG(s,t)}{ds}\Bigg|_{t'}^{t''} - G(s,t)\frac{d\bar{x}(s)}{ds}\Bigg|_{t'}^{t''} = \bar{x}(t) - \frac{1}{m}\int_{t'}^{t''} f(s)G(s,t)\,ds\,. \quad (2.37)$$

Then we have an explicit solution for $\bar{x}(t)$ as
$$\bar{x}(t) = \frac{1}{m}\int_{t'}^{t''} f(s)\,G(s,t)\,ds + \bar{x}(s)\frac{dG(s,t)}{dt}\Bigg|_{t'}^{t''}\,, \quad (2.38)$$

After substitution of the second term we obtain
$$\bar{x}(t) = \frac{1}{m}\int_{t'}^{t''} f(s)\,G(s,t)\,ds + \frac{[x''\sin\omega(t-t') + x'\sin\omega(t''-t)]}{\sin\omega(t''-t')}\,, \quad (2.39)$$

where we put the boundary conditions of the classical path $\bar{x}(t)$ in general form as
$$\bar{x}(t'') = x''\,, \quad \bar{x}(t') = x'\,. \quad (2.40)$$

To find the classical action (2.17), we integrate by parts
$$S_{cl} = \frac{m}{2}[\dot{\bar{x}}\,\bar{x}]_{t'}^{t''} - \int_{t'}^{t''}\left\{\left[\frac{m}{2}\ddot{\bar{x}} + \frac{m}{2}\omega^2\bar{x} - \frac{f(t)}{2}\right]\bar{x} - \frac{f(t)}{2}\bar{x}\right\}dt\,,$$

and since $\quad m\ddot{\bar{x}} + m\omega\bar{x} - f(t) = 0\,,$

it follows that
$$S_{cl} = \frac{m}{2}\left[x''\dot{\bar{x}}(t'') - x'\dot{\bar{x}}(t')\right] + \frac{1}{2}\int_{t'}^{t''} f(t)\bar{x}\,dt\,. \quad (2.41)$$

Differentiating Eq. (2.39) with respect to t, we obtain
$$\dot{\bar{x}}(t'') = \frac{\omega}{\sin\omega(t''-t')}\left[x''\cos\omega(t''-t') - x'\right] + \frac{1}{m\sin\omega(t''-t')}\int_{t'}^{t''} ds\, f(s)\sin\omega(s-t')\,, \quad (2.42)$$

and
$$\dot{x}(t') = \frac{\omega}{\sin\omega(t''-t')}\left[x''-x'\cos\omega(t''-t')\right]+\frac{1}{m\sin\omega(t''-t')}\int_{t'}^{t''}ds\,f(s)\sin\omega(t''-s). \tag{2.43}$$

By substituting Eqs. (2.42),(2.43), and (2.39) into (2.41), the desired classical action of the system can thus be determined as

$$S_{cl} = \frac{m\omega}{2\sin\omega(t''-t')}\Big[(x''^2+x'^2)\cos\omega(t''-t') - 2x'x'' + \frac{2x''}{m\omega}\int_{t'}^{t''}dt\,f(t)\sin\omega(t-t')$$
$$+\frac{2x'}{m\omega}\int_{t'}^{t''}dt\,f(t)\sin\omega(t''-t) + \frac{\sin\omega(t''-t')}{m^2\omega}\cdot 2\int_{t'}^{t''}dt\,f(t)\int_{t'}^{t}ds\,f(s)\,G_1(s,t)\Big]. \tag{2.44}$$

After substituting $G_1(s,t)$ from Eq. (2.32) into Eq. (2.44), we obtain the classical action

$$S_{cl} = \frac{m\omega}{2\sin\omega(t''-t')}\Big[(x''^2+x'^2)\cos\omega(t''-t') - 2x'x'' + \frac{2x''}{m\omega}\int_{t'}^{t''}dt\,f(t)\sin\omega(t-t')$$
$$+\frac{2x'}{m\omega}\int_{t'}^{t''}dt\,f(t)\sin\omega(t''-t) - \frac{2}{m^2\omega^2}\int_{t'}^{t''}dt\,f(t)\sin\omega(t''-t)$$
$$\int_{t'}^{t''}ds\,f(s)\sin\omega(s-t)\Big]. \tag{2.45}$$

Recalling the expressions (2.14) and (2.16) for the propagator $K(x'',x')$, we finally obtain the forced harmonic oscillator propagator based on the Feynman path integral, the Gaussian integral and the Green function method, as

$$K(x'',x') = \left(\frac{m\omega}{2\pi i\hbar\sin\omega(t''-t')}\right)^{\frac{1}{2}}\exp\left[\frac{i}{\hbar}S_{cl}\right], \tag{2.46}$$

where the classical action is given by (2.45).

II.3 Density Matrix

In this section, the relation between the density matrix and the propagator, including their asymptotic forms which are related to the ground state energy, will be presented.

Consider a system, initially in a given state $\Psi(x',t')$ at time t', which develops into any state $\psi(x'',t'')$ at time t'' as a consequence of the action of the propagator $K(x'',t''; x',t')$ for the time development of the state of the system.The final state is given as follows

$$\Psi(x'',t'') = \int K(x'',t''; x',t')\,\Psi(x',t')\,dx' . \quad (2.47)$$

For a stationary system, the Hamiltonian does not have an explicit time dependence, and in this case the solution of the Schrödinger equation

$$H\Psi(x',t') = \frac{i}{\hbar}\,\frac{\delta\Psi(x',t')}{\delta t} \quad , \quad (2.48)$$

is of the form

$$\Psi(x',t') = \sum_n C_n\, e^{-\frac{i}{\hbar}E_n t'}\,\Psi_n(x') = \sum_n a_n \Psi_n(x') , \quad (2.49)$$

where E_n and Ψ_n are, respectively, the eigenfuntions and eigenvalues of H for the time independent Schrödinger equation

$$H\Psi_n = E_n\Psi_n \quad . \quad (2.50)$$

The coefficient a_n are easily obtained by multiplication of (2.49) by the function $\psi_m^*(x')$ followed by integration over all x', thus

$$a_n = \int_{-\infty}^{\infty} \psi_n^*(x')\,\Psi(x',t)\,dx' \quad . \qquad (2.51)$$

Then the final state $\Psi(x'',t'')$ can be written in terms of the initial state $\Psi(x',t')$ as

$$\begin{aligned}\Psi(x'',t'') &= \sum_n C_n\, e^{-\frac{i}{\hbar}E_n t''}\psi_n(x'') \\ &= \sum_n a_n\, e^{-\frac{i}{\hbar}E_n(t'-t'')}\psi_n(x'') \\ &= \int_{-\infty}^{\infty}\sum_n \psi_n^*(x')\psi_n(x'')\, e^{-\frac{i}{\hbar}E_n(t'-t'')}\Psi(x',t')\,dx' . \qquad (2.52)\end{aligned}$$

By comparing the above equation with (2.47), we finally obtain the desired expression for the propagator,

$$\begin{aligned}K(x'',t'';x',t') &= \sum_n \psi_n^*(x')\psi_n(x'')\, e^{-\frac{i}{\hbar}E_n(t''-t')} \\ &= K(x'',x',t''-t') \quad . \qquad (2.53)\end{aligned}$$

In statistical mechanics, a stationary system in thermal equilibrium with its surroundings is described by a canonical ensemble with the density matrix at any temperature T defined by

$$\rho(x'',x';\beta) = \sum_n \psi_n^*(x')\psi_n(x'')\, e^{-\beta E_n} , \qquad (2.54)$$

where $\beta = \frac{1}{kT}$, and k is the Boltzmann constant.
By comparing the expression (2.53) and (2.54), we obtain the relation between the density matrix and the propagator as

$$\begin{aligned}\rho(x'',x';\beta) &= K(x'',-i\hbar\beta\,;x',0) \\ &= K(x'',x',-i\hbar\beta) \quad . \qquad (2.55)\end{aligned}$$

This result is particularly useful since it provides an easy method for finding the ground state energy of a quantum mechanical system. When the system is considered at very low temperatures, i.e., as β approaches an infinite value, the exponential terms of (2.54) survive only for the lowest E_n, say E_g, the ground state energy. Therefore Eq.(2.54) becomes

$$\rho(x'', x'; \beta)_{\beta \to \infty} = e^{-E_g \beta} \quad . \tag{2.56}$$

The quantum mechanical form of (2.56) can be obtained by taking the imaginary time interval $(0, -i\hbar\vartheta)$ in (2.53). Thus, for very large ϑ , we obtain

$$K(x'', -i\hbar\vartheta; x', 0)_{\vartheta \to \infty} = e^{-E_g \vartheta} \quad . \tag{2.57}$$

This result leads to an effective evaluation of the polaron ground state energy.