CHAPTER II

FEYNMAN PATH INTEGRAL FORMULATION OF QUANTUM MECHANICS

Before applying Feynman path integral to the polaron problem, in order to offer a clearer picture of his approach to those who are not familiar with this new formalism, we provide in this chapter the mathematical formulation of the quantum-mechanical transformation function or the propagator, in a form of the path integration. Then as an illustration and as it will be frequently referred to, we apply this method to the forced harmonic oscillator. In the last section, we relate the Feynman propagator to the density matrix.

II.1 Feynman Propagator[13]

Consider a quantum-mechanical system initially at time t' at a position $\vec{r}'$, the development of the system to a position $\vec{r}''$ at time t'' is described by the so-called transformation function.

$$K(\vec{r}''t'';\vec{r}'t') \equiv \langle\vec{r}''t''/\vec{r}'t'\rangle \qquad \text{for} \quad t''>t', \qquad (2.1)$$

where $/\vec{r}'t'\rangle$ represents the eigenstate of the Heisenberg operator $\vec{r}(t')$ with eigenvalue $\vec{r}'$. In other words K is the probability amplitude, the absolute square of K specifies the probability of finding the system initially in $(\vec{r}',t')$ to be in $(\vec{r}'',t'')$ subsequently. Recalling some interesting properties of $K(\vec{r}''t'';\vec{r}'t')$:

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[13] T.D. Schultz, "Feynman's Path Integral Method Applied to the Equilibrium Properties of Polarons and Excitons.", in Polarons and Excitons, Eds. C.G. Kuper, and G.D. Whitfield, Edinburgh and London : Oliver and Boyd (1972) 71.

For a system with the Hamiltonian H not dependent on time explicitly, the time development of the eigenstates of H is

$$\phi_n(\vec{r}''t'') = e^{i\frac{E_n}{\hbar}t''}\phi_n(\vec{r}''), \tag{2.1}$$

and those ϕ_n form a complete set, viz.,

$$\sum_n \overset{*}{\phi}_n(\vec{r})\phi_n(\vec{r}') = \delta(\vec{r}-\vec{r}'). \tag{2.2}$$

Consequently, K can be expanded in these states as

$$\begin{aligned} K(\vec{r}''t'';\vec{r}'t') &\equiv \langle \vec{r}''| e^{-\frac{i}{\hbar}H(t''-t')} |\vec{r}'\rangle \\ &= \sum_n e^{-\frac{i}{\hbar}E_n(t''-t')} \phi_n(\vec{r}'')\phi_n^*(\vec{r}'), \end{aligned} \tag{2.3}$$

assuming the energy spectrum of H is discrete.

The ground state energy E_g of the system can be obtained directly from (2.3), if we set $\tau = i(t''-t')\to\infty$, since then

$$K(\vec{r}''t''/\vec{r}'t') \underset{\tau\to\infty}{\sim} e^{-\frac{E_g}{\hbar}\tau}. \tag{2.4}$$

Considering K as a matrix; it possesses the composition property which is

$$\langle \vec{r}''t''|\vec{r}'t'\rangle = \int d\vec{r}_1 \langle \vec{r}''t''|\vec{r}'t_1\rangle\langle \vec{r}_1 t_1/\vec{r}'t_1\rangle, \tag{2.5a}$$

for any t_1 .

The transformation function on the right hand side can be further decomposed into subsequent states. Repeating the process indefinitely, we arrive at the general relation:

$$\langle \vec{r}''t''|\vec{r}'t'\rangle = \int\cdots\cdots\int d\vec{r}_1\cdots\cdots d\vec{r}_n \langle \vec{r}''t''/\vec{r}_n t_n\rangle \cdots\cdots\langle \vec{r}_1 t_1|\vec{r}'t'\rangle. \tag{2.5b}$$

For the system with one degree of freedom, (2.5b) reduces to:

$$\langle x''t''|x't'\rangle = \int \cdots\cdots \int dx_1 \cdots\cdots dx_n \langle x''t''|x_n t_n\rangle \cdots\cdots \langle x_1 t_1|x't'\rangle . \qquad (2.5c)$$

If the time difference in any transition j to $j+1$, $t_{j+1}-t_j = \varepsilon_j$, is infinitesimal, the transformation can be obtained explicitly. For a single particle moving in a potential $V(x)$, it has been found that

$$\langle x_{j+1}, t_j+\varepsilon|x_j t_j\rangle = \langle x_{j+1}|e^{-\frac{i}{\hbar}\varepsilon\left(\frac{p^2}{2m}+V(x)\right)}|x_j\rangle . \qquad (2.6)$$

Neglecting the noncommutativity of p^2 and $V(x)$, eq. (2.6) becomes

$$\langle x_{j+1}, t_j+\varepsilon|x_j t_j\rangle = \langle x_{j+1}|e^{-\frac{i}{\hbar}\varepsilon\frac{p^2}{2m}}|x\rangle e^{-\frac{i}{\hbar}\varepsilon V(x_j)} . \qquad (2.7)$$

The transformation function on the right is simply that of a free particle, in fact, it is the Schrödinger equation with $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$. It is well known to be

$$\langle x_{j+1}|e^{-\frac{i}{\hbar}\varepsilon\frac{p^2}{2m}}|x_j\rangle = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\varepsilon}\right)^2\varepsilon} . \qquad (2.8)$$

Recalling that $\left(\frac{x_{j+1}-x_j}{\varepsilon}\right)$ is just $\dot{x}_j$, the average velocity of a particle going from x_{j+1} to x_{j+1} , eq. (2.7) is generally,

$$\langle x_{j+1}, t_j+\varepsilon|x_j t_j\rangle = \frac{1}{A} e^{\frac{i}{\hbar}\varepsilon\mathcal{L}(x_j,\dot{x}_j,t_j)} , \qquad (2.9)$$

where

$$A = \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{\frac{1}{2}} \qquad (2.10)$$

and $\mathcal{L}$ is the classical Lagrangian. If the time interval (t', t'') is evenly divided into $(n+1)$ subintervals of width ε , $\varepsilon = \frac{(t''-t')}{(n+1)}$

then (2.5c) attains

$$\langle x''t''|x't'\rangle = \lim_{n\to\infty} \frac{1}{A}\int \cdots\cdots \int \frac{dx_1}{A}\cdots\cdots\frac{dx_n}{A}\, e^{\frac{i}{\hbar}\varepsilon\sum_{j=0}^{n}\mathcal{L}(x_j,\dot{x}_j,t_j)} \quad , \qquad (2.11)$$

where now $x_0 = x'$ and $x_{n+1} = x''$. Thus we are now dealing with the set of space-time coordinates $(x't', x_1t_1, \cdots, x_nt_n, x''t'')$ which specify an approximation to a path or ' history ' of the particle. Setting $n\to\infty$ or $\varepsilon\to 0$ means that the ability of choosing the points $x_1, \cdots\cdots, x_n$ to represent any path from x' to x'' is ultimately improved (see Fig II). The integration over all space for each x_j then becomes an integral over all paths . For the system with one degree of freedom, the transformation function (2.11) is now re-formulated as

$$\begin{aligned}\langle x''t''/x't'\rangle &= \lim_{n\to\infty}\frac{1}{A}\int\cdots\cdots\int\frac{dx_1}{A}\cdots\cdots\frac{dx_n}{A}\, e^{\frac{i\varepsilon}{\hbar}\sum_j^n \mathcal{L}(x_j,\dot{x}_j,t_j)} \\ &= \int \mathcal{D}x(t)\, e^{\frac{i}{\hbar}\int_{t'}^{t''}dt\,\mathcal{L}(x,\dot{x},t)} \\ &= \int \mathcal{D}x(t)\, e^{\frac{i}{\hbar}S[x(t)]} \quad , \qquad (2.12)\end{aligned}$$

which has been written in Feynman's path-integral notation, where

$$S = \int_{t'}^{t''} dt\,\mathcal{L}(x,\dot{x},t)$$

is the classical action, a functional of the path $x(t)$, and $Dx(t)$ stands for the product of differentials in the space of all paths together with A factors and the limits. Alternately, the probability amplitude written in path-integral formalism as in (2.12) is recognized as the " Feynman propagator."

Physically, the probability amplitude for the system to go from " ' state " to " "state" is the sum of contribution $\phi[x(t)]$ from each path, viz.,

$$\langle x''t''|x't'\rangle = \sum_{\substack{\text{over all paths} \\ \text{from ' to ''}}} \phi[x(t)] , \qquad (2.13)$$

and the contribution of a path has a phase proportional to the action S of the corresponding classical system,

$$\phi[x(t)] = \text{Const.}e^{\frac{i}{\hbar}S[x(t)]} . \qquad (2.14)$$

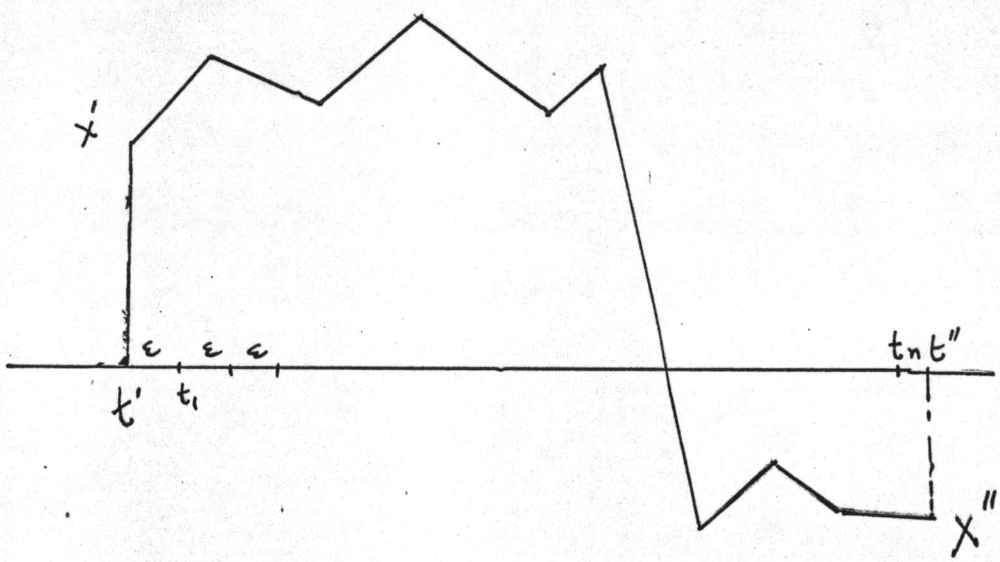

Fig. II Construction of the path integral.

II.2 Forced Harmonic Oscillator Propagator

Consider a one-dimensional forced harmonic oscillator with Lagrangian generally in the form:

$$\mathcal{L} \;=\; \frac{m}{2}(\dot{x}^2 - \omega^2 x^2) + f(t)x\,, \tag{2.15}$$

where $f(t)$ is any function of t .

Set

$$x(t) \;=\; \bar{x}(t) + y(t), \tag{2.16}$$

that is, we now represent the path $x(t)$ by the classical path $\bar{x}(t)$ going from $(x't')$ to $(x''t'')$, and the deviation $y(t)$ from the classical path. Consequently, we have to integrate over the paths $y(t)$ constrained by the conditions

$$y(t') \;=\; y(t'') \;=0 \tag{2.17}$$

From (2.15) and (2.16) the resulting action shows

$$S[\bar{x}(t)] \;=\; \int_{t'}^{t''}\Big\{\big[\tfrac{1}{2}m\dot{\bar{x}}^2 - \tfrac{1}{2}m\omega^2\bar{x}^2 + f(t)\bar{x}\big] + \big[\tfrac{1}{2}m\dot{y}^2 - \tfrac{1}{2}m\omega^2 y^2 + m\omega^2\bar{x}y + f(y)y\big]\Big\}dt \tag{2.18}$$

$$= \;\bar{S} + \int_{t'}^{t''}\tfrac{1}{2}m\,[\,\dot{y}^2 - \omega^2 y^2\,]\,dt \tag{2.19}$$

where

$$\bar{S} \;\equiv\; \int_{t'}^{t''}\tfrac{1}{2}m\,[\,\dot{\bar{x}}^2 - \omega^2\bar{x}^2 + f(t)\bar{x}\,]\,dt$$

corresponding to the classical action of the system and the terms linear in $y(t)$ vanish since S is stationary for small variation from $x(t)$. Our problem thus turns to the evaluation of the propagator $K(x''t'';x't')$,

$$K(x''t'';x't') = e^{\frac{i}{\hbar}\bar{S}} \int_0^0 e^{\frac{i}{\hbar}\int_{t'}^{t''} \frac{m}{2}[\dot{y}^2-\omega^2 y^2]dt} \mathcal{D}y(t)$$

$$= e^{\frac{i}{\hbar}\bar{S}} \eta(t',t''), \qquad (2.20)$$

where

$$\eta(t',t'') = \int_0^0 \mathcal{D}y(t) e^{\frac{i}{\hbar}\int_{t'}^{t''} \frac{m}{2}[\dot{y}^2-\omega^2 y^2]dt} \qquad (2.21)$$

is simply a Gaussian integral. The condition (2.17) implies that it is independent of end-point position, in other words, it depends only on the times at end points. This path integral can be performed either directly using Fourier series method as shown by Feynman[14] or indirectly through the knowledge of $\bar{S}$.

We now determine $\bar{S}$ explicitly, recalling

$$\bar{S} = \int_{t'}^{t''} \frac{m}{2}[\dot{\bar{x}}^2-\omega^2\bar{x}^2+f(t)\bar{x}]dt, \qquad (2.22)$$

where the classical path $\bar{x}(t)$ must satisfy the principle of least action, viz.,

$$\delta\bar{S} = 0 = m\dot{\bar{x}}\delta\bar{x}\Big|_{t'}^{t''} + \int_{t'}^{t''}[-m\ddot{\bar{x}} - m\omega^2\bar{x} + f(t)]\delta\bar{x}dt \qquad (2.23)$$

The first term of (2.23) vanishes in virtue of the fixed end-point condition. Consequently $\bar{x}(t)$ is the solution of the resulting classical equation of motion:

$$\ddot{\bar{x}} + \omega^2\bar{x} = \frac{f(t)}{m} \qquad (2.24)$$

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14 See Reference (1) P. 71

Solving for $\bar{x}(t)$, the Green function method can be employed. The Green function equation corresponding to (2.29) is

$$\left(\frac{d^2}{ds^2}+\omega^2\right)G(s,t) \quad = \quad \delta(s-t) \qquad (2.25a)$$

with the boundary conditions

$$G(t',t) \quad = \quad G(t'',t) \quad = 0. \qquad (2.25b)$$

To relate $G(s,t)$ to $\bar{x}(t)$, we consider

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

Integration by parts with the conditions (2.30b) yields

$$\bar{x}(s)\frac{dG(s,t)}{ds}\bigg|_{t'}^{t''} \quad = \quad \bar{x}(t)-\frac{1}{m}\int_{t'}^{t''}f(s)G(s,t)\,ds. \qquad (2.26)$$

Thus, we obtain a solution for $\bar{x}(t)$ for arbitrary $f(t)$:

$$\bar{x}(t) \quad = \quad \frac{1}{m}\int_{t'}^{t''}f(s)G(s,t)\,ds+x''\dot{G}(t'',t)-x'\dot{G}(t',t), \qquad (2.27)$$

where the boundary conditions on $\bar{x}(t)$:

$$x(t'') \equiv x'' \qquad \text{and} \qquad x(t') = x'$$

have been imposed.

Following the standard method of solving Green function equation, the solution of (2.25a,b) is readily found to be

$$G(s,t) \quad = -\frac{\sin\omega(s-t')\sin\omega(t''-t)}{\omega\sin\omega(t''-t)}\cdot H(t-s)-\frac{\sin\omega(t-t')\sin\omega(t'-s)}{\omega\sin\omega(t''-t')}, \qquad (2.28)$$

where

$$H(t-s) \quad = \begin{cases} 1\ , & t>s \\ 0\ , & t<s\ . \end{cases}$$

Inserting $\dot{G}(t'',t)$ and $\dot{G}(t',t)$ into (2.27), the full expression of $\bar{x}(t)$ reads

$$x(t) = \frac{1}{m}\int_{t'}^{t''} f(s)G(s,t)ds + \frac{[x''\sin\omega(t-t') + x'\sin\omega(t''-t)]}{\sin\omega(t''-t')} \qquad (2.29)$$

We are now able to evaluate the action along the classical path, $\bar{S}$, given in (2.22). Integration by parts simplifies $\bar{S}$ to

$$\bar{S} = \frac{m}{2}[\bar{x}(t)\dot{\bar{x}}(t)]_{t'}^{t''} + \frac{1}{2}\int_{t'}^{t''} dt\, f(t)\bar{x}(t), \qquad (2.30)$$

where we have used the identity (2.24):

$$m\ddot{\bar{x}} + m\omega^2\bar{x} - f(t) = 0.$$

It follows from (2.29) that

$$\dot{\bar{x}}(t'') = \frac{\omega}{\sin\omega(t''-t')}[x''\cos\omega(t''-t') - x'] + \frac{1}{m\sin\omega(t''-t')}\int_{t'}^{t''} ds\, f(s)\sin\omega(s-t') \qquad (2.31)$$

and

$$\dot{\bar{x}}(t') = \frac{\omega}{\sin\omega(t''-t')}[x'' - x'\cos\omega(t''-t')] + \frac{1}{m\sin\omega(t''-t')}\int_{t'}^{t''} ds\, f(s)\sin\omega(t''-s) \qquad (2.32)$$

Substitution of (2.31), (2.32) and (2.28) into (2.30) gives the desired classical action as

$$\bar{S} = \frac{m\omega}{2\sin\omega(t''-t')}\Big[(x''^2 - x'^2)\cos\omega(t''-t') - 2x'x'' + \frac{2x''}{m\omega}\int_{t'}^{t''} dt\, f(t)\sin\omega(t-t') +$$

$$+ \frac{2x'}{m\omega}\int_{t'}^{t''} dt\, f(t)\sin\omega(t''-t) - \frac{2}{m^2\omega^2}\int_{t'}^{t''} dt\, f(t)\sin\omega(t''-t)\int_{t'}^{t} ds\, f(s)\sin\omega(s-t')\Big]$$

$$(2.33)$$

Our remaining work is to obtain the multiplicative factor $\eta(t',t'')$ which is defined by (2.26) as

$$\eta(t',t'') \equiv \int_0^0 \mathcal{D}y(t)\, e^{\frac{i}{\hbar}\int_{t'}^{t''}\frac{m}{2}[\dot{y}^2-\omega^2 y^2]dt}$$

To accomplish this indirectly, recall (2.20)

$$\langle x''t''|x't'\rangle \equiv K(x''t'';x't') = e^{\frac{i}{\hbar}\bar{S}}\,\eta(t',t'')$$

with $\bar{S}$ given by (2.33).

Set $f(t) = 0$, thus

$$\langle x''t''|x't'\rangle = e^{\frac{i}{\hbar}\frac{m\omega}{2\sin\omega(t''-t')}\left[(x''^2+x'^2)\cos\omega(t''-t')-2x''x'\right]}\,\eta(t',t''). \tag{2.34}$$

Since $\langle x''t''|x't'\rangle$ is unitary, then

$$\int dx''\langle xt'|x''t''\rangle\langle x''t''|x't'\rangle = \delta(x-x') \tag{2.35}$$

Insertion of (2.34) in (2.35) gives

$$|\eta(t',t'')|^2 = \frac{m\omega}{2\pi\hbar\sin\omega(t''-t')} \text{ or } \eta(t',t'') = \sqrt{\frac{m\omega}{2\pi\hbar\sin\omega(t''-t')}} \times \text{arbitrary phase factor}$$

For infinitesimal time interval the problem reduces to that of a free particle whose propagator is readily known as

$$\langle x''t''|x't'\rangle \underset{(t''-t')\to 0}{\sim} e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x''-x')^2}{(t''-t')}} \times \sqrt{\frac{m}{2\pi i\hbar(t''-t')}} \tag{2.36}$$

The phase factor is thus determined and we have explicitly,

$$\eta(t',t'') \equiv \eta(t''-t') = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega(t''-t')}} \tag{2.37}$$

In conclusion, the one-dimensional forced harmonic oscillator propagator is found to be

$$K(x''t'',x't') = \left(\frac{m\omega}{2\pi i\hbar \sin\omega(t''-t')}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\bar{S}}, \tag{2.38}$$

where the classical action $\bar{S}$ is given by (2.33).

II.3 Density Matrix

A stationary system in statistical mechanics is one which is in equilibrium with a heat bath, or alternately, when it is in the canonical ensemble. In such a system the density matrix at any temperature is defined by

$$\begin{aligned} \rho(\vec{r}'',\vec{r}';\beta) &\equiv \langle \vec{r}''| e^{-\beta H} | \vec{r}' \rangle \\ &= \sum_n e^{-\beta E_n} \phi_n(\vec{r}'') \phi_n^*(\vec{r}'), \end{aligned} \tag{2.39}$$

where $\beta = \frac{1}{k_B T}$ and k_B is the Boltzmann constant. Comparing with the transformation function for the same system as given in (2.3):

$$K(\vec{r}''t'';\vec{r}'t') = \sum_n e^{-\frac{i}{\hbar}E_n(t''-t')} \phi_n(\vec{r}'')\phi_n^*(\vec{r}') \tag{2.40}$$

We note that it is closely related together by

$$\rho(\vec{r}''r';\beta) = K(\vec{r}'', t'-i\beta; \vec{r}'t') \tag{2.41}$$

Thus knowledge of either ρ or K for a time-independent system leads at once to the evaluation of the other by analytic continuation.

The partition function Z of the system can be found providing

ρ is already known, since

$$Z \equiv \int d\vec{r}\,\rho(\vec{r}\,\vec{r};\beta) = \sum_n e^{-\beta E_n} \tag{2.42}$$

Recalling (2.4)

$$K(\vec{r}''t'';\vec{r}'t') \underset{\tau = i(t''-t')\to\infty}{\sim} e^{-\frac{1}{\hbar}E_g\tau}.$$

or

$$\rho(\vec{r}''\vec{r}';\beta) \underset{\beta=\frac{1}{k_BT}\to\infty}{\sim} e^{-\beta E_g}.$$

Thus it is now clear that for large imaginary time difference in the transformation, the only lowest energy state or the ground state energy will survive, this is just equivalent to the statement that a system will be in its ground state at 0 K.