CHAPTER III

PATH INTEGRALS APPROACH TO THE FROEHLICH POLARON

This chapter is devoted to the description of the polaron theory by the method of path integration formulated by Feynman [26] which is also used in this problem[14]. This chapter is a very important basis for understanding the material in later chapters. Nevertheless, the author prefers a descriptive way rather detailed calculation since there are many good reviews available [27]. The advantage of Feynman's theory is that it is applicable for all value of the coupling constant with smooth interpolation of the energies and effective mass between weak, intermediate and strong couplings. Altogether we will include review of the method of Krivoglaz and Pekar [22] since it gives the same expression of ground state energy as those of Feynman. Moreover, we will show in the later chapter that the effective mass of the polaron defined by Krivoglaz and Pekar can be derived from the full density matrix (or the propagator)of the polaron.

3.1 Statement of the Problem

In the Froehlich model, the electron was supposed to move through the continuous field of polarization which has a constant frequency. Feynman has used his path integration method to eliminate the field coordinates and left only the electron

coordinate and gave the two-time (or non-local) action. Since the path integral of this action cannot be evaluated exactly, the variational principle will then be applied. That is a trial action chosen to be a representative of the polaron system and the ground state energy could be estimated from this action with an extremization condition called the Feynman-Jansen Inequality [28]. In the paper "Slow Electron in a Polar Crystal", Feynman started with the Froehlich Lagrangian

$$L=\frac{m\dot{\vec{x}}^2}{2}+\left[\sum_k\left(\frac{\mu}{2}\dot{Q}_k^2-\omega^2Q_k^2\right)+\gamma_k(t)Q_k\right] \tag{3.1}$$

where the polarization vector was decomposed into standing waves with real amplitudes. It is obvious that the terms in square bracket of equation (3.1) is the Lagrangian of the forced harmonic oscillators and we can find the path integral of this Lagrangian easily [9]. The phonon coordinates can be integrated out as an average and left out only a functional of the electron coordinates. Then the density matrix can be written as

$$\rho = \int \mathrm{D}x(\tau)\ \exp[S] \tag{3.2}$$

where

$$S=-\frac{1}{2}\int_0^\beta d\tau\ \dot{\vec{x}}(\tau)^2+\frac{\alpha}{2^{\frac{1}{2}}}\int_0^\beta\int_0^\beta d\tau d\sigma\frac{e^{-|\tau-\sigma|}}{|\vec{x}(\tau)-\vec{x}(\sigma)|}. \tag{3.3}$$

and α is the coupling constant defined in previous chapter. The action in equation (3.3) is really an effective one since all the effect of the phonon has been averaged out into this effective action. The second term in this action leads us to interpretation that

when an electron is moving in polar crystal at one time it produces a field that acts back to it at a later time. Due to the fact that this action is a Coulomb type and cannot be evaluated exactly, the variational method may be used to find the ground state energy of the polaron.

3.2 Variational Approach

By constructing an appropriate action with some variational parameters, we can use the path integral of this action to estimate the upper bound of the ground state energy. To be more clearly, consider the density matrix in the form of the sum over energy eigenstates

$$\rho(\vec{x}_2,\vec{x}_1;\beta)=\sum_n \Psi_n^*(\vec{x}_2)\Psi_n(\vec{x}_1)\exp[-E_n\beta]. \tag{3.4}$$

As the imaginary time goes to infinity i.e. temperature goes to zero, the higher order terms of the summation decays more rapidly than the first leading term or the term involving the ground state energy. So we can write

$$\rho \xrightarrow{\beta\to\infty} \exp(-E_0\beta). \tag{3.5}$$

Whenever we choose any trial action namely S_1 (where we can find its density matrix exactly), we can write the path integral

$$\rho=\int Dx(t)\, e^{S}=\int Dx(t)\, e^{(S-S_1)}e^{S_1}$$

$$=\langle e^{S-S_1}\rangle \int D\,x(t), \tag{3.6}$$

where we average with weighting factor e^{S_1} defined by

$$\langle F \rangle = \frac{\int \mathrm{D}x(t)\, e^{S_1} F}{\int \mathrm{D}x(t)\, e^{S_1}}. \tag{3.7}$$

In order to evaluate the energy as in equation (3.5), we must write the density matrix in the exponential form. To do this we apply the in equality

$$\langle e^{F} \rangle \geq \exp\langle F \rangle \tag{3.8}$$

called the Feynman-Jansen inequality. Then the density matrix in equation (3.5) can be approximated as

$$\rho \geq \exp\langle S - S_1 \rangle \int \mathrm{D}x(t)\, e^{S_1}. \tag{3.9}$$

Remember that the path integral of S_1 gives the ground state energy as

$$\rho_1 \approx \exp(-E_1\beta) \tag{3.10}$$

Then the equation (3.9) can be written as

$$\exp(-E_0\beta) \geq e^{\langle S-S_1 \rangle} e^{-E_1\beta}$$

$$E_0 \leq E_1 - \frac{\langle S - S_1 \rangle}{\beta}. \tag{3.11}$$

3.3 The Trial Action

The next problem is to determine the form of the trial action, S_1. Feynman has used the free particle action which yields the same result as the perturbation method when apply to the weak coupling limit [4,5]. If one use the Coulomb potential the result is the same as the strong coupling theory of the polaron [1]. However the good theory should cover all range of the coupling constant. The best choice would be the action of a particle bound by a potential of the form

$$V = k(\vec{x}-\vec{y})^2, \tag{3.12}$$

where $\vec{y}$ is the coordinate of a fictitious particle. This coordinate can be eliminated out in the same way as the polaron action leaving only the coordinate $\vec{x}$ of electron. That is

$$S_1 = -\frac{1}{2}\int \dot{\vec{x}}^2 dt - \frac{C}{2}\int\int dt\, ds[x(t)-x(s)]\, e^{-w|t-s|} \tag{3.13}$$

where C and w are the variational parameter chosen to minimize the ground state energy.

3.4 Evaluation of the Energy

Consider the last term of the right hand side of the equation (3.11)

$$\frac{1}{\beta}\langle S-S_1\rangle = \int ds\left[\frac{\alpha}{2^{\frac{1}{2}}}e^{-|t-s|}\left\langle|\vec{x}(t)-\vec{x}(s)|^{-1}\right\rangle + \frac{C}{2}\left\langle(x(t)-x(s))^2 e^{-w|t-s|}\right\rangle\right] \tag{3.14}$$

The first term in the integrand may be calculated by expressing the coordinate term in a Fourier transform

$$|\vec{x}(t)-\vec{x}(s)|^{-1}=\int\frac{d^3k}{(2\pi^2k^2)}\exp\left(i\vec{k}(\vec{x}(t)-\vec{x}(s))\right). \tag{3.15}$$

Averaging this quantity gives the generating functional that leads to the path integral of the action

$$S_f=-\frac{1}{2}\int\dot{\vec{x}}^2dt-\frac{C}{2}\int\int dt\,ds(\vec{x}(t)-\vec{x}(s))^2e^{-w|t-s|}+\int\vec{f}(t)\cdot\vec{x}(t)dt \tag{3.16}$$

where $\vec{f}(t)=i\vec{k}\delta(t-\tau)-i\vec{k}\delta(t-\sigma)$.

We can find its classical action by variation calculation of this action yielding the integro-diffential equation

$$\frac{d^2\vec{x}'}{dt^2}=2C\int(\vec{x}'(t)-\vec{x}'(s))\,e^{-w|t-s|}-f(t), \tag{3.17}$$

The generating functional can be simplified to

$$\int Dx(t)\,e^{S_f}=\exp\left[\frac{1}{2}\int\vec{f}(t)\,\vec{x}'(t)dt\right], \tag{3.18}$$

where $\vec{x}'(t)$ is the classical path. To solve equation (3.17), a new variable is introduced

$$Z(t)=\frac{w}{2}\int_0^t e^{-w|t-s|}\vec{x}'(s)ds \tag{3.19}$$

Then the equation (3.17) reads

$$\frac{d^2\vec{x}'(t)}{dt^2} = \frac{4C}{w}[\vec{x}'(t) - Z(t)] - f(t) \tag{3.20}$$

The solution of above equation is

$$\vec{x}'(t) = i\vec{k}\left(\frac{1}{\nu} - \frac{1}{\nu^3}\right)[\sinh\nu(t-\tau)H(t-\tau) - \sinh\nu(t-\sigma)H(t-\sigma)]$$

$$-i\vec{k}\frac{w^2}{\nu^2}[(t-\tau)H(t-\tau) - (t-\sigma)H(t-\sigma)] \tag{3.21}$$

Then the generating functional of equation (3.18) can be written as

$$\left\langle \exp\left(i\vec{k}\cdot(\vec{x}(\tau) - \vec{x}(\sigma))\right)\right\rangle = \exp\left[-\frac{2Ck^2}{\nu^2 w}\left(1 - e^{-\nu|\tau-\sigma|}\right) - \frac{w^2}{2\nu^2}k^2|\tau-\sigma|\right] \tag{3.22}$$

where $\nu^2 = w^2 + \frac{4C}{w}$.

From equation (3.14) and (3.15), the first term of the right hand side of (3.14) reads

$$\frac{\alpha}{2^{\frac{1}{2}}}\int ds\left\langle|\vec{x}(t) - \vec{x}(s)|^{-1}\right\rangle e^{-|t-s|} = \frac{\alpha\nu}{\sqrt{\pi}}\int_0^\infty d\tau\left[w^2\tau + \tfrac{\nu^2-w}{\nu}\left(1 - e^{-\nu\tau}\right)\right]^{-\frac{1}{2}} e^{-\tau}. \tag{3.23}$$

The second term of (3.14)is calculated by using equation (3.22) by expanding the exponential term of both sides and comparing terms by terms gives

$$\frac{1}{3}\left\langle(x(\tau) - x(\sigma))^2\right\rangle = \frac{4C}{\nu^3 w}\left(1 - e^{-\nu|\tau-\sigma|}\right) + \frac{w^2}{\nu^2}|\tau-\sigma| \tag{3.24}$$

The next quantity is the energy corresponds to the trial action S_1. Although we can calculate it by direct path integration but it is more easily to follow Feynman by differenting with respect to C both sides of the equation

$$\int Dx(t)\, e^{S_1} \approx e^{-E_1\beta}. \tag{3.25}$$

With some algebra, the energy for S_1 is

$$E_1 = \frac{3}{2}(v-w). \tag{3.26}$$

The ground state energy of the polaron is

$$E_0 = \frac{3}{2}(v-w)^2 - \frac{\alpha v}{\sqrt{\pi}}\int_0^\infty \frac{d\tau\, e^{-\tau}}{\sqrt{w^2\tau + v(1-\frac{w^2}{v^2})(1-e^{-v\tau})}} \tag{3.27}$$

Then the task left is finding the numerical value of the ground state energy which can be done by minimizing this equation with respect to the two parameter v and w.

3.5 The Effective Mass

To find the effective mass, Feynman considered the polaron properties at ground state near those of the free particle. Then its energy should be of the form $m_F V^2/2$ (V is the group velocity and m_F is the effective mass). The next assumption is that the velocity of the polaron is low enough, that we can use the same variational parameter to determine the value of the effective mass.

At the ground state, the density matrix is proportional to

$$\rho \approx \exp\left[-E_{\cdot}\beta - \frac{m_F\left(\vec{x}_2-\vec{x}_1\right)^2}{2\beta}\right] \tag{3.28}$$

Hence, we can determine the effective mass from the $\left(\vec{x}_2-\vec{x}_1\right)^2$ dependent term. Since there is some complications in solving the integro-differential equation so the approximation $\left(\vec{x}_2-\vec{x}_1\right)=\vec{U}\beta$ will be introduced. This means that the classical path from equation (3.16) is a straight line, so we can substitute $\vec{x}=\vec{U}\beta$ and then find the classical path from equation (3.16). Similar to previous section, we can find the generating functional as

$$\left\langle \exp\left(i\vec{k}\cdot\left(\vec{x}(\tau)-\vec{x}(\sigma)\right)\right)\right\rangle = \exp\left[-\frac{k^2}{2\nu^2}F(|\tau-\sigma|)+i\vec{k}\cdot\vec{U}(\tau-\sigma)\right] \tag{3.29}$$

where

$$F(\tau)=w^2\tau+\frac{\nu^2-w^2}{\nu}\left(1-e^{-\nu\tau}\right). \tag{3.30}$$

Then the energy of the excited state with small velocity (near the ground state) is

$$E_U=\frac{U^2}{2}+\frac{3}{4\nu}(\nu-w)^2-\frac{\alpha}{2^{\frac{1}{2}}}\int_0^{\infty}d\tau\int\frac{d^3k}{2\pi^2k^2}\,e^{-\tau}\exp\left[-\frac{k^2}{2\nu^2}F(\tau)+i\vec{k}\cdot\vec{U}\tau\right] \tag{3.31}$$

By expanding the exponential in the last term up to U^2 we find that

$$E_U=E_{\cdot}+\frac{m_F}{2}U^2 \tag{3.32}$$

where

$$m_F = 1 + \frac{\alpha v^3}{3\sqrt{\pi}} \int_0^\infty d\tau \frac{\tau^2 e^{-\tau}}{[F(\tau)]^{\frac{3}{2}}}. \tag{3.33}$$

The numerical value of this effective mass can be calculated by the parameter that minimizes the ground state energy. This is not a satisfaction assumption since we have no minimization condition for the effective mass as for the ground state energy (which has the Feynman-Jansen Inequality).