CHAPTER III

FEYNMAN PATH INTEGRAL APPROACH TO THE POLARON AT ABSOLUTE ZERO TEMPERATURE

In this chapter, we shall present the detailed evaluation of the polaron ground state energy at absolute zero temperature by using the Feynman path integration approach. The original idea of this formulation was given by Feynman[6] in 1954.

III.1 Elimination of the Field Coordinates

Consider the Fröhlich idealized polaron model introduced in Chapter I and the classical Lagrangian of the system (1.20) which is given by

$$L = \frac{1}{2} m^* \dot{\underset{\sim}{r}}_{el}^2 + \frac{1}{2}\gamma \int [\dot{\underset{\sim}{P}}_{ir}^2(\underset{\sim}{r}) - \omega_L^2 \underset{\sim}{P}_{ir}^2(\underset{\sim}{r})] d^3\underset{\sim}{r} + \int \underset{\sim}{D}(\underset{\sim}{r}, \underset{\sim}{r}_{el}) \cdot \underset{\sim}{P}_{ir}(\underset{\sim}{r}) d^3\underset{\sim}{r} , \quad (3.1)$$

where $\underset{\sim}{P}_{ir}(\underset{\sim}{r})$ is the polarization field induced by the electron, which is implicitly dependent on the position vector $\underset{\sim}{r}_{el}$. The constant γ depends on the frequency ω_L, and the static and high frequency dielectric constants ϵ_s and ϵ_∞, as follows

$$\gamma = \frac{4\pi}{\omega_L^2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right)^{-1} , \quad (3.2)$$

$\underset{\sim}{D}(\underset{\sim}{r}, \underset{\sim}{r}_{el})$ is the dielectric displacement arising from the electronic charge, as defined by (1.3).

For simplicity, $\underset{\sim}{P}_{ir}(\underset{\sim}{r})$ is replaced by a Fourier sum of standing waves with real amplitudes

$$P_{ir}(\mathbf{r},t) = \sqrt{\frac{2}{V}} \sum_{\mathbf{k}} \mathbf{e}_{\mathbf{k}} q_{\mathbf{k}}(t) \begin{Bmatrix} \cos \mathbf{k}\cdot\mathbf{r} \\ \sin \mathbf{k}\cdot\mathbf{r} \end{Bmatrix} , \qquad (3.3)$$

where

$$\mathbf{e}_{\mathbf{k}} = \frac{\mathbf{k}}{|\mathbf{k}|} , \qquad \begin{Bmatrix} \cos \mathbf{k}\cdot\mathbf{r} \\ \sin \mathbf{k}\cdot\mathbf{r} \end{Bmatrix} \equiv \begin{cases} \cos \mathbf{k}\cdot\mathbf{r} & k_x > 0 \\ \sin \mathbf{k}\cdot\mathbf{r} & k_x < 0 . \end{cases} \qquad (3.4)$$

Then the Lagrangian(3.1) becomes

$$L = \frac{1}{2} m^* \dot{\mathbf{r}}_{el}^2 + \sum_{\mathbf{k}} \frac{1}{2} \gamma (\dot{q}_{\mathbf{k}}^2 - \omega_L^2 q_{\mathbf{k}}^2) + 4\pi e \left(\frac{2}{V}\right)^{\frac{1}{2}} \sum_{\mathbf{k}} \frac{q_{\mathbf{k}}}{\mathbf{k}} \begin{Bmatrix} \cos \mathbf{k}\cdot\mathbf{r} \\ \sin \mathbf{k}\cdot\mathbf{r} \end{Bmatrix}, \qquad (3.5)$$

which consists of the three components arising,respectively, from the electronic part, the lattice vibrational modes and the electron-lattice interaction.With the condition that the lattice vibrational modes are each coupled only to the electron, and not to the other modes, we can write the Lagrangian of the arbitary mode for any given path of the electron $\mathbf{r}_{el}(t)$ separately as

$$L_{\mathbf{k}} = \frac{m}{2} (\dot{q}_{\mathbf{k}}^2 - \omega_L^2 q_{\mathbf{k}}^2) + \Gamma_{\mathbf{k}}(t) q_{\mathbf{k}} , \qquad (3.6)$$

where $m = \gamma$, (3.7)

and
$$\Gamma_{\mathbf{k}}(t) = 4\pi e \left(\frac{2}{V}\right)^{\frac{1}{2}} \frac{1}{\mathbf{k}} \begin{Bmatrix} \cos \mathbf{k}\cdot\mathbf{r}_{el} \\ \sin \mathbf{k}\cdot\mathbf{r}_{el} \end{Bmatrix} . \qquad (3.8)$$

Obviously,$L_{\mathbf{k}}$ is the Lagrangian for a forced harmonic oscillator comparable with the Lagrangian(2.8), for which the classical action,including the propagator, has been provided in Section II.2 .

Furthermore, it is justifiable to represent the polaron system by a system of independent harmonic oscillators with coordinates $q_{\underset{\sim}{k}}$ and action S_o, each oscillator interacting with an electron with action S_{el} through the Lagrangian $q_{\underset{\sim}{k}}(t)\Gamma_{\underset{\sim}{k}}(t)$ and the action

$$S_{\underset{\sim}{k}I} = \int q_{\underset{\sim}{k}}(t)\,\Gamma_{\underset{\sim}{k}}(t)\,dt \quad . \tag{3.9}$$

If at some time t'' the electron is at $\underset{\sim}{r}''_{el}$, and the oscillators are in the eigenstate Q_m, when at a previous time t' the electron was at $\underset{\sim}{r}'_{el}$ and the oscillators were in the eigenstate Q_n, the propagator can then be written as

$$K(\underset{\sim}{r}''_{el}, Q_m(q''_1), \ldots\ldots, Q_m(q''_N); \underset{\sim}{r}'_{el}, Q_n(q'_1), \ldots, Q_n(q'_N)) = \langle \underset{\sim}{r}''_{el}, Q_m(q''_1), \ldots, Q_m(q''_N) | 1 | \underset{\sim}{r}'_{el}, Q_n(q'_1), \ldots, Q_n(q'_N) \rangle_{S_{el}+S_o+S_I} \; . \tag{3.10}$$

In general, the problem concerning an interaction of matter and field can be solved easily by first eliminating the field variables from the equation of motion of the matter so that the behaviour of the matter can then be discussed separately. Such a formulation has been found to be very useful in solving quantum electrodynamical problems.[(20)]

For the polaron system, it is also possible to integrate the field coordinates of the oscillator part from the system, and then we can concentrate our interest on the

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[20] R.P. Feynman, "Mathematical Formulation of the Quantum Theory of Electromagnetic Interaction", Physical Review, 20 (1950), 440.

behaviour of the electron alone. This is the advantage acquired through using a Lagrangian form of quantum mechanics to describe the polaron. Here, we are going to integrate the paths of the oscillators out by expressing the propagator in two parts as

$$\langle \underset{\sim}{r}''_{el}, Q_m(q_1''), \ldots, Q_m(q_N'') |1| \underset{\sim}{r}'_{el}, Q_n(q_1'), \ldots, Q_n(q_n') \rangle_{S_{cl}+S_o+S_I} = \langle \underset{\sim}{r}''_{el} | G_{mn} | \underset{\sim}{r}'_{el} \rangle_{S_{cl}} \quad (3.11)$$

where G_{mn} is a functional of the path of the electron alone, given by

$$G_{mn} = \prod_{\underset{\sim}{k}} \langle Q_m(q''_{\underset{\sim}{k}}) |1| Q_n(q'_{\underset{\sim}{k}}) \rangle_{S_{\underset{\sim}{k}}^{o} + S_{\underset{\sim}{k}}^{I}}$$

$$= \prod_{\underset{\sim}{k}} G_{mn}^{\underset{\sim}{k}} , \quad (3.12)$$

where $G_{mn}^{\underset{\sim}{k}}$ is the propagator of each oscillator

$$G_{mn}^{\underset{\sim}{k}} = \int \cdots \int Q_m^*(q''_{\underset{\sim}{k}}) \exp\left[\frac{i}{\hbar}(S_{\underset{\sim}{k}o} + S_{\underset{\sim}{k}I})\right] Q_m(q'_{\underset{\sim}{k}})\, dq'_{\underset{\sim}{k}}\, dq''_{\underset{\sim}{k}}\, \mathcal{D} q_{\underset{\sim}{k}}(t). \quad (3.13)$$

By using the path integration technique, $\mathcal{D} q_{\underset{\sim}{k}}(t)$ can be written explicitly as

$$G_{mn}^{\underset{\sim}{k}} = \int \cdots \int Q_m^*(q_{\underset{\sim}{k}}^{j}) \exp\left[\frac{i}{\hbar}\epsilon \sum_{i=1}^{j-1} \left[\frac{m}{2} \frac{(q_{\underset{\sim}{k}}^{i+1} - q_{\underset{\sim}{k}}^{i})^2}{\epsilon^2} - \frac{m\omega_L^2}{2} q_{\underset{\sim}{k}}^{i\,2} + \Gamma_{\underset{\sim}{k}}(t)\, q_{\underset{\sim}{k}}^{i}\right]\right] \cdot$$

$$Q_n(q_{\underset{\sim}{k}}^{o}) \cdot \frac{dq_{\underset{\sim}{k}}^{o}}{A} \cdot \frac{dq_{\underset{\sim}{k}}^{1}}{A} \cdots\cdots \frac{dq_{\underset{\sim}{k}}^{j-1}}{A} \cdot dq_{\underset{\sim}{k}}^{j} , \quad (3.14)$$

where $t''-t' = j\epsilon$, $q''_{\underset{\sim}{k}} = q_{\underset{\sim}{k}}^{j}$ and $q'_{\underset{\sim}{k}} = q_{\underset{\sim}{k}}^{o}$.

Eq.(3.14) is reduced to

$$G_{mn}^{\underset{\sim}{k}} = \iint Q_m^*(q_{\underset{\sim}{k}}^{j})\, K(q_{\underset{\sim}{k}}^{j}, t''; q_{\underset{\sim}{k}}^{o}, t')\, Q_n(q_{\underset{\sim}{k}}^{o})\, dq_{\underset{\sim}{k}}^{o}\, dq_{\underset{\sim}{k}}^{j} , \quad (3.15)$$

where $K(q_{\underset{\sim}{k}}^{j}, t''; q_{\underset{\sim}{k}}^{o}, t')$ is the propagator of a forced harmonic oscillator, initially at time t' at $q_{\underset{\sim}{k}}^{o}$ and finally at $q_{\underset{\sim}{k}}^{j}$ at time t", and was determined in Section II.2 with the explicit result given by (2.46) and (2.45). It is obtained by replacing x" and x' by $q_{\underset{\sim}{k}}j$ and $q_{\underset{\sim}{k}}o$ respectively; the result is

$$K(q_{\underset{\sim}{k}}j, t''; q_{\underset{\sim}{k}}o, t') = \left(\frac{m\omega_L}{2\pi i\hbar \sin\omega_L(t''-t')}\right)^{\frac{1}{2}} \exp\left[\frac{i}{\hbar} S_{cl}^{\underset{\sim}{k}}\right], \quad (3.16)$$

where $S_{cl}^{\underset{\sim}{k}}$ is the classical action calculated along the classical path between end points $(q_{\underset{\sim}{k}}j, t'')$ and $(q_{\underset{\sim}{k}}o, t')$, given by

$$\begin{aligned} S_{cl}^{\underset{\sim}{k}} = \frac{m\omega_L}{2\sin\omega_L(t''-t')} \Big[& (q_{\underset{\sim}{k}}^2 j + q_{\underset{\sim}{k}}^2 o)\cos\omega_L(t''-t') - 2q_{\underset{\sim}{k}}j\, q_{\underset{\sim}{k}}o \\ & + \frac{2q_{\underset{\sim}{k}j}}{m\omega_L}\int_{t'}^{t''} dt\, \Gamma_{\underset{\sim}{k}}(t)\sin\omega_L(t-t') \\ & + \frac{2q_{\underset{\sim}{k}o}}{m\omega_L}\int_{t'}^{t''} dt\, \Gamma_{\underset{\sim}{k}}(t)\sin\omega_L(t''-t) \\ & - \frac{2}{m^2\omega_L^2}\int_{t'}^{t''} dt\, \Gamma_{\underset{\sim}{k}}(t)\sin\omega_L(t''-t)\int_{t'}^{t} ds\, \Gamma_{\underset{\sim}{k}}(s)\, \times \\ & \sin\omega_L(s-t) \Big]. \end{aligned} \quad (3.17)$$

As the polaron state under consideration is at absolute zero temperature, all oscillators are in their ground states initially and also finally. Therefore the propagator of each oscillator, $G_{oo}^{\underset{\sim}{k}}$, is given by

$$G_{oo}^{\underset{\sim}{k}} = \iint Q_o^*(q_{\underset{\sim}{k}}j)\, K(q_{\underset{\sim}{k}}j, t''; q_{\underset{\sim}{k}}o, t')\, Q_o(q_{\underset{\sim}{k}}o)\, dq_{\underset{\sim}{k}}o\, dq_{\underset{\sim}{k}}j, \quad (3.18)$$

where $Q_o(q_{\underset{\sim}{k}}j)$ and $Q_o(q_{\underset{\sim}{k}}o)$ are the ground state harmonic oscillator wave functions obtained from the solutions of the quantum mechanical problem as

$$Q_o(q_{\underset{\sim}{k}}j) = \left(\frac{m\omega_L}{\hbar\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{2}\frac{\omega_L m}{\hbar} q_{\underset{\sim}{k}}^2 j\right) \exp\left(-\frac{1}{2} i\omega_L t''\right), \quad (3.19)$$

and $$Q_0(q_{\underset{\sim}{k}}{}^{o}) = \left(\frac{m\omega_L}{\hbar\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{2}\,\frac{\omega_L m\, q^2_{\underset{\sim}{k}}{}^{o}}{\hbar}\right)\exp\left(-\frac{1}{2}\,i\omega_L t'\right). \quad (3.20)$$

In order to determine $G^{\underset{\sim}{k}}_{oo}$, we substitute $Q^*_o(q_{\underset{\sim}{k}}j)$, $K(q_{\underset{\sim}{k}}j, t''; q_{\underset{\sim}{k}}{}^{o}, t')$ and $Q_o(q_{\underset{\sim}{k}}{}^{o})$ from(3.19),(3.20) and(3.16) into(3.18), and thus obtain

$$G^{\underset{\sim}{k}}_{oo} = \frac{\omega_L}{\pi}\left(\frac{m^2}{2i\hbar^2 \sin\omega_L T}\right)^{\frac{1}{2}} \exp\left(\frac{i\omega_L T}{2}\right)\exp(ie)\iint \exp\left[-aq^2_{\underset{\sim}{k}}{}^{o} - aq^2_{\underset{\sim}{k}}j - bq_{\underset{\sim}{k}}{}^{o}q_{\underset{\sim}{k}}j + icq_{\underset{\sim}{k}}{}^{o} + idq_{\underset{\sim}{k}}j\right] dq_{\underset{\sim}{k}}{}^{o}\, dq_{\underset{\sim}{k}}j, \quad (3.21)$$

where

$$T = t''-t',$$

$$a = -\frac{\omega_L m}{2\hbar}(i\cot\omega_L T - 1),$$

$$b = \frac{im\omega_L}{\hbar\sin\omega_L T},$$

$$c = \frac{1}{\hbar\sin\omega_L T}\int_{t'}^{t''} dt\, \Gamma_{\underset{\sim}{k}}(t)\sin\omega_L(t''-t),$$

$$d = \frac{1}{\hbar\sin\omega_L T}\int_{t'}^{t''} dt\, \Gamma_{\underset{\sim}{k}}(t)\sin\omega_L(t-t'),$$

and $$e = -\frac{1}{\hbar m\omega_L \sin\omega_L T}\int_{t'}^{t''} dt\, \Gamma_{\underset{\sim}{k}}(t)\sin\omega_L(t''-t)\int_{t'}^{t} ds\, \Gamma_{\underset{\sim}{k}}(s)\sin\omega_L(s-t'). \quad (3.22)$$

The integration of the form (3.21) can then be carried out by using standard mathematical techniques;(21) the result is

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[21] B.Friedman, " Principles and Techniques of Applied Mathematics.", New York : John Wiley &Sons, (1956),105.

$$G^{k}_{00} = \frac{\omega_L}{\pi}\left(\frac{m^2}{2i\hbar^2\sin\omega_L T}\right)^{\frac{1}{2}}\exp\left(\frac{i\omega_L T}{2}\right)\exp(ie)\cdot\sqrt{\frac{\pi^2}{\det A}}\exp\left[\frac{-\langle t, A^{-1}t\rangle}{A}\right], \tag{3.23}$$

where

$$A = \begin{pmatrix} a & \frac{b}{2} \\ \frac{b}{2} & a \end{pmatrix}, \quad t = \begin{pmatrix} c \\ d \end{pmatrix}. \tag{3.24}$$

On substituting the coefficient of (3.23), G^{k}_{00} becomes

$$G^{k}_{00} = \exp(ie)\exp\left[\frac{-\langle t, A^{-1}t\rangle}{4}\right].$$

Since

$$A^{-1} = \frac{1}{a^2 - \frac{b^2}{4}}\begin{pmatrix} a & -\frac{b}{2} \\ -\frac{b}{2} & a \end{pmatrix},$$

and

$$\langle t, A^{-1}t\rangle = \left\langle \begin{pmatrix} c \\ d \end{pmatrix}, \frac{1}{a^2 - \frac{b^2}{4}}\begin{pmatrix} ac & -\frac{bd}{2} \\ ad & -\frac{bc}{2} \end{pmatrix}\right\rangle = \frac{a}{a^2 - \frac{b^2}{4}}\left(c^2 + d^2 - \frac{bcd}{a}\right),$$

we have

$$G^{k}_{00} = \exp(ie)\exp\left[-\frac{a}{4a^2 - b^2}\left(c^2 + d^2 - \frac{bcd}{a}\right)\right].$$

Now, consider the factor $\frac{a}{4a^2-b^2}$. If we substitute into this the value of a and b from(3.22), it becomes $\frac{\hbar}{4\omega_L m}$.

Thus

$$G^{k}_{00} = \exp(ie)\exp\left[\frac{-\hbar}{4\omega_L m}\left(c^2 + d^2 - \frac{bcd}{a}\right)\right]. \tag{3.27}$$

By substituting the value of e, c^2, d^2 and $\frac{bcd}{a}$ into the above equation we obtain after some simple mathematical manipulation,

$$G^{k}_{00} = \exp\Big[-\frac{1}{2\hbar m\omega_L\sin^2\omega_L T}\int_{t'}^{t''}\int_{t'}^{t} dt\,ds\,\Gamma_k(t)\,\Gamma_k(s)\big[2\cos\omega_L T\sin\omega_L(t''-t)\sin\omega_L(s-t') + \sin\omega_L(t''-t)\sin\omega_L(t''-s) + \sin\omega_L(t-t')\sin\omega_L(s-t')\big]\Big]. \tag{3.28}$$

If the circular functions are re-expressed in the exponential forms, (3.28) then becomes

$$G^{k}_{00} = \exp\left[-\frac{1}{2\hbar m\omega_L}\int_{t'}^{t''}\int_{t'}^{t} dt\,ds\,\Gamma_k(t)\,\Gamma_k(s)\exp\left[-i\omega_L(t-s)\right]\right]. \tag{3.29}$$

Finally, recalling (3.11),(3.12) and (3.29), we can write the polaron propagator at absolute zero temperature as

$$K_{00}(\underset{\sim}{r}''_{el},t'';\underset{\sim}{r}'_{el},t') = \int \mathcal{D}\underset{\sim}{r}_{el}(t)\exp\left[\frac{i}{\hbar}\frac{m^*}{2}\int_{t'}^{t''}\dot{\underset{\sim}{r}}^2_{el}\,dt\right]\prod_{\underset{\sim}{k}} G^{\underset{\sim}{k}}_{00}$$

$$= \int \mathcal{D}\underset{\sim}{r}_{el}(t)\exp\left[\frac{i}{\hbar}\frac{m^*}{2}\int_{t'}^{t''}\dot{\underset{\sim}{r}}^2_{el}\,dt - \frac{1}{4\hbar m\omega_L}\int_{t'}^{t''}\int_{t'}^{t''}dt\,ds\,e^{-i\omega_L|t-s|}\sum_{\underset{\sim}{k}}\Gamma_{\underset{\sim}{k}}(t)\Gamma_{\underset{\sim}{k}}(s)\right]. \quad (3.30)$$

In computing the ground state energy, the following transformations are made: $it \to \tau$, $is \to \sigma$. Therefore (3.30) becomes

$$K_{00}(\underset{\sim}{r}''_{el},\tau'';\underset{\sim}{r}'_{el},\tau') = \int \mathcal{D}\underset{\sim}{r}_{el}(\tau)\exp\left[-\frac{m^*}{2\hbar}\int\left(\frac{d\underset{\sim}{r}_{el}}{d\tau}\right)^2 d\tau + \frac{1}{4\hbar m\omega_L}\iint d\tau\,d\sigma\,e^{-\omega_L|\tau-\sigma|}\sum_{\underset{\sim}{k}}\Gamma_{\underset{\sim}{k}}(\tau)\Gamma_{\underset{\sim}{k}}(\sigma)\right]. \quad (3.31)$$

The summation $\sum_{\underset{\sim}{k}}\Gamma_{\underset{\sim}{k}}(\tau)\Gamma_{\underset{\sim}{k}}(\sigma)$ is readily performed

$$\sum_{\underset{\sim}{k}}\Gamma_{\underset{\sim}{k}}(\tau)\Gamma_{\underset{\sim}{k}}(\sigma) = 4\pi e^2\left(\frac{2}{V}\right)\sum_{\underset{\sim}{k}}\frac{1}{k^2}\begin{Bmatrix}\cos\underset{\sim}{k}\cdot\underset{\sim}{r}_{el}(\tau).\cos\underset{\sim}{k}\cdot\underset{\sim}{r}_{el}(\sigma)\\ \sin\underset{\sim}{k}\cdot\underset{\sim}{r}_{el}(\tau).\sin\underset{\sim}{k}\cdot\underset{\sim}{r}_{el}(\sigma)\end{Bmatrix}$$

$$= 4\pi e^2 . \frac{1}{|\underset{\sim}{r}(\tau)-\underset{\sim}{r}(\sigma)|} . \quad (3.32)$$

Thus (3.31) becomes

$$K_{00}(\underset{\sim}{r}''_{el},\tau'';\underset{\sim}{r}'_{el},\tau') = \int \mathcal{D}\underset{\sim}{r}_{el}(\tau)\exp\left[-\frac{m^*}{2\hbar}\int\left(\frac{d\underset{\sim}{r}_{el}}{d\tau}\right)^2 d\tau + \frac{4\pi e^2}{4\hbar m\omega_L}\iint d\tau\,d\sigma\,\frac{e^{-\omega_L|\tau-\sigma|}}{|\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)|}\right]. \quad (3.33)$$

On substituting m from (3.7) and (3.2) into (3.33) and introducing the dimensionless coupling constant α , we obtain

$$\alpha = \frac{1}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)\frac{e^2}{\hbar\omega}\left(\frac{2m^*\omega}{\hbar}\right)^{\frac{1}{2}} .$$

Then the polaron propagator at absolute zero temperature becomes

$$K_{oo}(\underset{\sim}{r}''_{el},\tau'';\underset{\sim}{r}'_{el},\tau') = \int \mathcal{D}\underset{\sim}{r}_{el}(\tau)\exp\left[-\frac{1}{2}\int\left(\frac{d\underset{\sim}{r}_{el}}{d\tau}\right)^2 d\tau + \frac{\alpha}{2^{3/2}}\iint d\tau d\sigma \frac{e^{-|\tau-\sigma|}}{|\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)|}\right], \quad (3.34)$$

where our units are such that $\hbar\omega_L$ and the effective mass m^* are unity.

The polaron action after the phonon field is averaged, is given by the above equation as

$$S = -\frac{1}{2}\int\left(\frac{d\underset{\sim}{r}_{el}}{d\tau}\right)^2 d\tau + \frac{\alpha}{2^{3/2}}\iint d\tau d\sigma \frac{e^{-|\tau-\sigma|}}{|\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)|}, \quad (3.35)$$

which describes the electron at any particular time interacting with the produced field at a past time as a retarded, nonlocal coulomb potential with exponentially decaying time factor. The disturbance that acts back on the electron in the past time dies out since it takes some time for the lattice ions to relax.

III.2 Variational Principle

The polaron action after the phonons of the lattice field have been averaged is given by (3.35) as

$$S = -\frac{1}{2}\int\left(\frac{d\underset{\sim}{r}_{el}}{dt}\right)^2 dt + \frac{\alpha}{2^{3/2}}\iint dt ds \frac{e^{-|t-s|}}{|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|}, \quad (3.36)$$

where the time variables τ and σ are now replaced by t and s.

It is difficult to evaluate the path integration of this action which is not quadratic in $\underset{\sim}{r}$ and $\dot{\underset{\sim}{r}}$, since only quadratic actions will lead to integrable path integrals.

To determine the polaron ground state energy, an action which is simple, integrable, and imitates the action S in rough approximation, must be supposed, and then the variational method can be applied.

Feynman introduced the trial action in the form of

$$S_1 = -\frac{1}{2}\int\left(\frac{d\underset{\sim}{r}_{el}}{dt}\right)^2 dt - \frac{c}{2}\iint dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2\, e^{-\omega|t-s|} , \qquad (3.37)$$

where the kinetic energy part is the same as that of the exact action (3.36) and the potential energy part resembles the harmonic oscillator potential with the strength and frequency which can be varied by the two adjustable parameters C and ω.

Now consider

$$K_{oo}(\underset{\sim}{r}''_{el}, t''; \underset{\sim}{r}'_{el}, t') = \int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S} = \frac{\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1} \cdot e^{(S-S_1)}}{\int \mathcal{D}\underset{\sim}{r}_{el}(t) \cdot e^{S_1}} \int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}$$

$$= \langle e^{S-S_1} \rangle \int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1} . \qquad (3.38)$$

By using the general inequality for any variable x

$$\langle e^{x} \rangle \geq e^{\langle x \rangle} ,$$

then (3.38) becomes

$$K_{oo}(\underset{\sim}{r}''_{el}, t''; \underset{\sim}{r}'_{el}, t') \geq e^{\langle S-S_1 \rangle} \int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1} . \qquad (3.39)$$

Recalling (2.57), we have

$$K_{oo}(\underset{\sim}{r}''_{el}, t''; \underset{\sim}{r}'_{el}, t') = \int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S} \sim e^{-E_g \mathcal{J}} , \qquad (3.40)$$

where the imaginary time interval is $(0, \mathcal{J})$ with $\mathcal{J} \to \infty$, and E_g is the exact ground state energy.

Similarly,

$$\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1} \sim e^{-E_1 \mathcal{J}} , \qquad (3.41)$$

where E_1 is the ground state energy corresponding to the trial action S_1.

Since, for large $\mathcal{J}$, $S-S_1$ is proportional to $\mathcal{J}$,

$$\langle S - S_1 \rangle = \mathcal{S}\mathcal{J} \quad . \qquad (3.42)$$

Substituting (3.40), (3.41) and (3.42) into (3.39), we then obtain the very useful expression

$$E_g \leq E_1 - \mathcal{S} \qquad (3.43)$$

This is the <u>variational principle</u>, which provides an upper bound on the exact ground state energy. The problem is thus to determine $E_1 - \mathcal{S}$ and then to minimize it by means of the adjustable parameters C and ω.

III.3 Ground State Energy

In order to evaluate an upper bound to the ground state energy, we must determine both E_1 and $\mathcal{S}$. Let us consider first

$$\mathcal{S} = \frac{\langle S - S_1 \rangle}{\mathcal{J}} = A + B \quad , \qquad (3.44)$$

where

$$A = \frac{\alpha}{2^{3/2}} \int_0^{\mathcal{J}} ds \; e^{-|t-s|} \left\langle \frac{1}{|\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|} \right\rangle \quad , \qquad (3.44a)$$

$$B = \frac{c}{2} \int_0^{\mathcal{J}} ds \; e^{-\omega|t-s|} \left\langle |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 \right\rangle \quad . \qquad (3.44b)$$

We are concerned with the imaginary time, initially at $t'=o$, and finally at $t''=\mathcal{J}$ which is very large.

Our first object is to determine the A term of (3.44a). In it we can express $\frac{1}{|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|}$ by a Fourier transform,

$$\frac{1}{|\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)|} = \int \frac{d^3\underset{\sim}{K}}{2\pi K^2} \exp\left[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))\right] . \quad (3.45)$$

Then we need to study

$$\left\langle \exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)]\right\rangle = \frac{\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1} \exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)]}{\int \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}}$$

$$= \int \mathcal{D}\underset{\sim}{r}_{el}(t) \exp\left[-\frac{1}{2}\int\left(\frac{d\underset{\sim}{r}_{el}}{dt}\right)^2 dt - \frac{c}{2}\iint dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 \times e^{-\omega|t-s|} + \int \underset{\sim}{f}(t)\cdot\underset{\sim}{r}_{el}(t)\,dt\right] , \quad (3.46)$$

where $\underset{\sim}{f}(t) = i\underset{\sim}{K}(\delta(t-\tau)-\delta(t-\sigma))$, and where a normalization factor is dropped out.

Since the three rectangular components of (3.46) can be separated, we need to consider only one component, say the x-component. Therefore (3.46) is reduced to

$$\left\langle \exp[iK_x(x(\tau)-x(\sigma))]\right\rangle = \int \mathcal{D}x(t) \exp\left[-\frac{1}{2}\int\left(\frac{dx}{dt}\right)^2 dt - \frac{c}{2}\iint dt\,ds\,[x(t)-x(s)]^2 \cdot e^{-\omega|t-s|} + \int f_x(t)\,x(t)\,dt\right] . \quad (3.47)$$

The path integration of (3.47) can be carried out by substituting for $x(t)$ the classical path $\bar{x}(t)$ and its variation $y(t)$, and by using the method described in Section II.2. The result can be separated into two parts, viz., the terms that are directly dependent on the classical path, and the integration terms of $y(t)$ that give an unimportant constant depending on T only. Then we obtain

$$\left\langle \exp\left[iK_x(X(\tau)-X(\sigma))\right]\right\rangle = \exp\left[-\frac{1}{2}\int\left(\frac{d\bar{x}(t)}{dt}\right)^2 dt - \frac{c}{2}\iint dt\,ds\left[\bar{x}(t)-\bar{x}(s)\right]^2 e^{-\omega|t-s|} + \int f_x(t)\,\bar{x}(t)\,dt\right]. \tag{3.48}$$

The action corresponding to this expression can be written as

$$S = -\frac{1}{2}\int\left(\frac{d\bar{x}}{dt}\right)^2 dt - \frac{c}{2}\iint dt\,ds\left[\bar{x}(t)-\bar{x}(s)\right]^2 e^{-\omega|t-s|} + \int f_x(t)\bar{x}(t)\,dt. \tag{3.49}$$

The classical path $\bar{x}(t)$ is given by that function which satisfies the principle of least action $\delta S=0$.

Hence

$$\delta S = -\frac{1}{2}\int 2\left(\frac{d\bar{x}(t)}{dt}\right)\delta\dot{\bar{x}}(t)\,dt - \frac{c}{2}\iint dt\,ds\,2\left[\bar{x}(t)-\bar{x}(s)\right]e^{-\omega|t-s|}\delta\left[\bar{x}(t)-\bar{x}(s)\right] + \int f_x(t)\,\delta\bar{x}(t)\,dt$$

$$= \int\left[\frac{d^2\bar{x}(t)}{dt^2} - 2c\int ds\left[\bar{x}(t)-\bar{x}(s)\right]e^{-\omega|t-s|} + f_x(t)\right]\delta\bar{x}(t)\,dt = 0 ,$$

which gives the equation of motion for the classical path

$$\frac{d^2\bar{x}(t)}{dt^2} = 2c\int ds\left[\bar{x}(t)-\bar{x}(s)\right]e^{-\omega|t-s|} - f_x(t) , \tag{3.50}$$

under the boundary conditions $\bar{x}(0)=\bar{x}(\beta)=0$ which are chosen for convenience.

Thus (3.48) can be simplified by using (3.50) to

$$\left\langle \exp\left[iK_x(x(\tau)-x(\sigma))\right]\right\rangle = \exp\left[-\frac{1}{2}\frac{d\bar{x}(t)}{dt}.\bar{x}(t)\Big|_0^\beta + \frac{1}{2}\int\frac{d^2\bar{x}(t)}{dt^2}.\bar{x}(t)\,dt - \frac{c}{2}\iint dt\,ds\left[\bar{x}(t)-\bar{x}(s)\right]^2 e^{-\omega|t-s|} + \int f_x(t)\bar{x}(t)\,dt\right]$$

$$= \exp\left[\frac{iK_x}{2}\left(\bar{x}(\tau)-\bar{x}(\sigma)\right)\right] . \tag{3.51}$$

To obtain the above quantity, we must solve the equation of motion (3.50) and substitute $\bar{x}(\tau)$ and $\bar{x}(\sigma)$ into (3.51). To do this we define

$$Y(t) = \frac{\omega}{2}\int e^{-\omega|t-s|}\,\bar{x}(s)\,ds \quad . \tag{3.52}$$

Then the classical path equation of motion (3.50) can be written in the form involving y(t) as

$$\frac{d^2\bar{x}(t)}{dt^2} = \frac{4c}{\omega}\left[\bar{x}(t) - Y(t)\right] - f_x(t) \quad , \tag{3.53}$$

where we have substituted $\int ds\, e^{-\omega|t-s|}$ by $\frac{2}{\omega}$, the validity of which assumption will be discussed in Chapter VI.
By performing the second order differentiation with respect to time t on (3.52), we obtain the differential equation of Y(t) as

$$\frac{d^2Y(t)}{dt^2} = \omega^2\left[Y(t) - \bar{x}(t)\right] \quad . \tag{3.54}$$

It is desired to eliminate the Y(t) term in (3.53) in order to convert the classical path integro- differential equation into an ordinary differential equation. To do this, we multiply(3.53) by $\frac{\omega}{4C}(D^2-\omega^2)$ (where $D=\frac{d}{dt}$), whereupon we obtain

$$D^2(D^2 - v^2)\,\bar{x}(t) = -(D^2 - \omega^2)\,f_x(t) \quad , \tag{3.55}$$

where we have used

$$v^2 = \omega^2 + \frac{4C}{\omega} \quad . \tag{3.56}$$

Finally, we can solve for the classical path $\bar{x}(t)$ in the ordinary fourth order differential equation (3.55) by applying Laplace transform.

Thus Eq.(3.55) becomes

$$p^4 f(p) - p^3\bar{x}(0) - p^2\dot{\bar{x}}(0) - p\ddot{\bar{x}}(0) - \dddot{\bar{x}}(0) - v^2(p^2 f(p) - p\bar{x}(0) - \dot{\bar{x}}(0)) = - \int_0^\infty e^{-pt}(D^2-\omega^2) f_x(t)\, dt \ . \quad (3.57)$$

The transient terms in the solution at the end points can be neglected, since the time interval $(0,\mathcal{J})$ is very large and most of the contribution is certainly not from here. Then (3.57) is reduced to

$$p^2(p^2-v^2) f(p) = - iK_x \int_0^\infty e^{-pt}(D^2-\omega^2)(\delta(t-\tau)-\delta(t-\sigma))\, dt$$

$$f(p) = -\frac{iK_x(e^{-p\tau}-e^{-p\sigma})}{p^2-v^2} + \frac{iK_x\omega^2(e^{-p\tau}-e^{-p\sigma})}{p^2(p^2-v^2)} . \quad (3.58)$$

The classical path can be obtained directly from (3.58) by taking inverse Laplace transform. The result is that

$$\begin{aligned}\bar{x}(t) = & -\frac{iK_x}{v}\left[\sinh v(t-\tau)H(t-\tau) - \sinh v(t-\sigma)H(t-\sigma)\right] \\ & + \frac{iK_x}{v^3}\left[\sinh v(t-\tau)H(t-\tau) - \sinh v(t-\sigma)H(t-\sigma)\right] \\ & - \frac{iK_x\omega^2}{v^2}\left[(t-\tau)H(t-\tau) - (t-\sigma)H(t-\sigma)\right] . \quad (3.59)\end{aligned}$$

Now $\bar{x}(t)$ must satisfy the following boundary condition :

$$\begin{aligned}\bar{x}(\mathcal{J}) = 0 = & \left(-\frac{iK_x}{v} + \frac{iK_x}{v^3}\right)\left[\sinh v(\mathcal{J}-\tau) - \sinh v(\mathcal{J}-\sigma)\right] \\ & - \frac{iK_x\omega^2}{v^2}\left[(\mathcal{J}-\tau) - (\mathcal{J}-\sigma)\right] .\end{aligned}$$

As ξ approaches ∞,

$$0 = -\left(-\frac{iK_x}{V} + \frac{iK\omega^2}{V^3}\right)\left[2\cosh\frac{V}{2}(2\xi-\tau-\sigma)\sinh\frac{V}{2}(\tau-\sigma)\right] - 0 ,$$

whereupon we obtain a condition

$$\cdot \sinh\frac{V}{2}(\tau-\sigma) = 0 \quad \text{or} \quad \cosh V|\tau-\sigma| = 1 \qquad . \; (3.60)$$

By using (3.59), Eq.(3.51) leads to

$$\left\langle \exp[iK_x(X(\tau)-X(\sigma))]\right\rangle = \exp\left[-\frac{2cK_x^2}{V^3\omega}\left(\cosh V|\tau-\sigma| - e^{-V|\tau-\sigma|}\right) - \frac{K_x^2\omega^2}{2V^2}|\tau-\sigma|\right]$$

$$= \exp\left[-\frac{2cK_x^2}{V^3\omega}\left(1-e^{-V|\tau-\sigma|}\right) - \frac{K_x^2\omega^2}{2V^2}|\tau-\sigma|\right], \; (3.61)$$

so that

$$\left\langle \exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s))]\right\rangle = \exp\left[-\frac{2cK^2}{V^3\omega}\left(1-e^{-V|t-s|}\right) - \frac{K^2\omega^2}{2V^2}|t-s|\right]. \; (3.62)$$

We have obtained the result that is correctly normalized, since it is certainly valid for $\underset{\sim}{K}=0$. Now we can determine the A term by substitution of (3.62) and (3.45) into (3.44a), thus

$$A = \frac{\alpha}{2^{3/2}}\int_0^{\xi} ds\, e^{-|t-s|}\int_{-\infty}^{\infty}\frac{d^3K}{2\pi^2K^2}\exp\left[-\frac{2cK^2}{V^3\omega}\left(1-e^{-V|t-s|}\right) - \frac{K^2\omega^2}{2V^2}|t-s|\right]$$

$$= \frac{\alpha V}{\pi^{1/2}}\int_0^{\infty} d\tau\, e^{-\tau}\left[\frac{(V^2-\omega^2)(1-e^{-V\tau})}{V} + \omega^2\tau\right]^{-\frac{1}{2}} \qquad . \; (3.63)$$

Our next purpose is to find B; therefore we need the value of $\langle|\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2\rangle$. To obtain this we apply second order differentiation with respect to K_x to (3.61), and then take the limit K_x to zero, thus

$$\langle | \underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^2 \rangle = 3\langle (x(t) - x(s))^2 \rangle = \frac{12C}{v^3\omega}(1 - e^{-v|t-s|}) + \frac{3\omega^2}{v^2}|t-s|. \quad (3.64)$$

The B term can now be easily integrated out by using (3.64). The result is

$$B = \frac{3C}{v\omega}, \qquad (3.65)$$

where we have used the equality $\int_0^\infty e^{-a|t-s|} ds = \frac{2}{a}$, for any arbitary a which is independent of s, in performing the integration.

The final object is to evaluate the ground state energy E_1 that corresponds to the trial action S_1. To effect this, we recall (3.41)

$$\int \mathcal{D}\, \underset{\sim}{r}_{el}(t)\, e^{S_1} \sim e^{-E_1 \mathcal{J}}.$$

After differentiating both sides of this equation, we obtain

$$\frac{\frac{1}{2}\int \mathcal{D}\, \underset{\sim}{r}_{el}(t)\, e^{S_1}\left[\iint dt\, ds\, [\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)]^2 e^{-\omega|t-s|}\right]}{\int \mathcal{D}\, \underset{\sim}{r}_{el}(t)\, e^{S_1}} = \mathcal{J}\frac{dE_1}{dC}$$

$$\frac{3}{v\omega} = \frac{dE_1}{dC}. \qquad (3.66)$$

By substituting dC obtained from (3.56) into the above equation, it follows that

$$dE_1 = \frac{3}{2}dv + 3\frac{(v^2 - 3\omega^2)}{4v\omega}\, d\omega. \qquad (3.67)$$

Comparing (3.67) with

$$dE_1 = \frac{\delta E_1}{\delta v}.dv + \frac{\delta E_1}{\delta \omega}.d\omega,$$

we obtain

$$\frac{\delta E_1}{\delta v} = \frac{3}{2},$$

and hence

$$E_1 = \frac{3}{2}v + f(\omega). \qquad (3.68)$$

By using the condition $E_1=0$ when $C=0$, we can find $f(\omega)$ explicitly as $-\frac{3}{2}\omega$. Therefore, the ground state energy E_1 can be determined, i.e.,

$$E_1 = \frac{3}{2}(v-\omega) \quad , \qquad (3.69)$$

Finally, the expression for the upper-bound of the ground state energy can be evaluated by employing the results that are readily determined from (3.44), (3.63), and (3.65). We obtain

$$E = E_1 - \mathcal{S}_1 = \frac{3}{2}(v-\omega) - \frac{3}{v}\left(\frac{v^2-\omega^2}{4}\right) - A$$

$$= \frac{3}{4v}(v-\omega)^2 - A \quad , \qquad (3.70)$$

where A is given by (3.63).

We remark that the adjustable parameters C and ω are now replaced by v and ω which can be varied separately to minimize E. The complete evaluation of E requires numerical integration of A, which cannot be performed in closed form. The numerical work has been carried out by Schultz by using a digital computer. He has calculated the values of v, ω and E for several values of α, and his results will be presented in Chapter VII.