CHAPTER III

FEYNMAN PATH-INTEGRAL APPROACH TO THE POLARON AT ABSOLUTE ZERO TEMPERATURE

As it is the basis of our present research, the whole chapter will be given to a detailed study of Feynman's original work[14] on the ground state energy and effective mass of the polaron.

III.1 The Polaron Action

Recalling that in sec. I.2 the classical Lagrangian describing the motion of the Fröhlich idealized polaron is found to be

$$\mathcal{L} = m_{eff}\frac{\dot{\vec{r}}^2}{2} - e\int \nabla_{\vec{r}'}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\cdot\vec{F}(\vec{r}')\,d^3r' + \frac{M_f}{2}\int \dot{\vec{F}}^2(\vec{r}') - \omega_L^2\vec{F}^2(\vec{r}')\,d^3r' \tag{3.1}$$

which involves both electron coordinates $\vec{r}$ and field coordinates $\vec{r}'$. For further mathematical consideration of the problem, this needs to be reformulated quantum mechanically.

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[14] R.P. Feynman, " Slow Electrons in a Polar Crystal.", Physical Review, 97 (1955) 660.

Using Feynman path-integral formulation of quantum mechanics, it is possible to eliminate the field coordinates from the Lagrangian and then we are allowed to focus our attention on the behavior of the electron alone.

Now, if we represent the polarization field $\vec{F}(\vec{r})$ by a composition of standing waves with real amplitudes:

$$\vec{F}(\vec{r}',t) = \sqrt{\frac{2}{V}} \sum_{\vec{k}} \frac{\vec{k}}{|k|} Q_{\vec{k}}(t) \begin{Bmatrix} \cos\vec{k}\cdot\vec{r}' \\ \sin\vec{k}\cdot\vec{r}' \end{Bmatrix} \tag{3.2}$$

where symbolically,

$$\begin{Bmatrix} \cos\vec{k}\cdot\vec{r}' \\ \sin\vec{k}\cdot\vec{r}' \end{Bmatrix} \equiv \begin{cases} \cos\vec{k}\cdot\vec{r}' & \text{if} \quad k_x > 0 \\ \sin\vec{k}\cdot\vec{r}' & \text{if} \quad k_x < 0 \end{cases},$$

the expression (3.1) is simplified to be

$$\mathcal{L} = m_{eff}\frac{\dot{\vec{r}}^2}{2} - 4\pi e\sqrt{\frac{2}{V}} \sum_{\vec{k}} \frac{Q_{\vec{k}}}{k} \begin{Bmatrix} \cos\vec{k}\cdot\vec{r}' \\ \sin\vec{k}\cdot\vec{r}' \end{Bmatrix} + \frac{M_f}{2}\sum_{\vec{k}} (\dot{Q}_{\vec{k}}^2 - \omega_L^2 Q_{\vec{k}}^2). \tag{3.3}$$

As a result, the propagator under our consideration is now of the form:

$$\langle \vec{r}''Q_1''\cdots Q_N''t''/\vec{r}'Q_1'\cdots Q_N't'\rangle = \int\cdots\int \mathcal{D}\vec{r}(t)\mathcal{D}Q_1(t)\cdots\mathcal{D}Q_N(t)\exp\left\{\frac{i}{\hbar}\int_{t'}^{t''}\mathcal{L}(\vec{r},\dot{\vec{r}},Q_1\ldots Q_N,\dot{Q}_1\cdots\dot{Q}_N,t)\right\} \tag{3.4}$$

Providing that each lattice vibrational mode is coupled only to the electron and not to the other modes, for arbitrary paths of the electron $\vec{r}(t)$, the second and the third terms of the Lagrangian (3.3) can be combined and written separately as

$$\mathcal{L}_{\vec{k}} = \frac{M_f}{2}(\dot{Q}_{\vec{k}}^2 - \omega_L^2 Q_{\vec{k}}^2) + \gamma_{\vec{k}}(t)Q_{\vec{k}} \tag{3.5}$$

for the k^{th} mode, where

$$\gamma_{\vec{k}}(t) = -\frac{4\pi e}{k}\sqrt{\frac{2}{V}}\begin{Bmatrix}\cos\vec{k}\cdot\vec{r}(t)\\ \sin\vec{k}\cdot\vec{r}(t)\end{Bmatrix} \tag{3.6}$$

Clearly, the Lagrangian $\mathcal{L}_{\vec{k}}$ is just that of a forced harmonic oscillator of which the path integral we have already worked out in sec. II.2. Thus the effect of the polarization field is now represented by a system of mutually independent forced harmonic oscillators. Consequently, the polaron propagator becomes

$$\langle \vec{r}''Q_1''\cdots Q_N''t''|\vec{r}'Q_1'\cdots Q_N't'\rangle = \int \mathcal{D}\vec{r}(t)\, e^{\frac{i}{\hbar}\int_{t'}^{t''} m_{eff}\frac{\dot{\vec{r}}^2}{2}dt} \prod_{\vec{k}} \langle Q_{\vec{k}}''t''/Q_{\vec{k}}'t'\rangle_{\gamma_{\vec{k}}(t)}, \tag{3.7}$$

in which $\langle Q_{\vec{k}}''t''/Q_{\vec{k}}'t'\rangle_{\gamma_{\vec{k}}(t)}$ is the $\vec{k}^{th}$ mode forced harmonic propagator obtained explicitly by writing $Q_{\vec{k}}''$, $Q_{\vec{k}}'$, M_f and $\gamma_{\vec{k}}(t)$ instead of x'', x', and $f(t)$ respectively in (2.36) and (2.33).

Since we are now concerning with the polaron at absolute zero temperature, all oscillators are assumed to be in their ground state initially and finally. It is necessary to calculate the transformation function in which the lattice is the uncoupled phonon vacuum at t' and at t''. However, any linear transformation on the polaron propagator will not change its asymptotic decay rate, so we can replace $\langle Q_{\vec{k}}''t''/Q_{\vec{k}}'t'\rangle$ in (3.7) by

$$G_{00}^{\vec{k}} = \langle n_{\vec{k}}'' = 0, t''|n_{\vec{k}}' = 0, t'\rangle \equiv \langle vac\, t''|vac\, t'\rangle,$$

where

$$G_{00}^{\vec{k}} = \iint \phi_0^*(Q_{\vec{k}}''t'')\langle Q_{\vec{k}}''t''/Q_{\vec{k}}'t'\rangle_{\gamma_{\vec{k}}}\phi_0(Q_{\vec{k}}'t')\,dQ_{\vec{k}}''dQ_{\vec{k}}'. \tag{3.8}$$

Recalling that $\phi_0(Q_{\vec{k}},t)$ is the ground state harmonic-oscillator wave function which is readily obtained in quantum mechanics as

$$\phi_0(Q_{\vec{k}}t) = \left(\frac{M_f\omega_L}{\hbar\pi}\right)^{\frac{1}{4}} e^{\left(-\frac{1}{2\hbar}M_f\omega_L Q_{\vec{k}}^2\right)} e^{-\frac{1}{2}i\omega_L t} . \tag{3.9}$$

After some lengthy mathematical manipulation involving a kind of Gaussian integration, we arrive at

$$G_{00}^{\vec{k}} = \exp\left[-\frac{1}{2\hbar M_f\omega_L}\int_{t'}^{t''}\int_{t'}^{t} dt\,ds\,\gamma_{\vec{k}}(t)\gamma_{\vec{k}}(s)e^{-i\omega_L|t-s|}\right]. \tag{3.10}$$

It follow from (3.7), (3.8) and (3.10) that the field coordinates are now entirely eliminated and the resulting propagator is

$$\langle \vec{r}''Q_1''\ldots Q_N''t''|\vec{r}'Q_1'\ldots Q_N't'\rangle \equiv K_{00}(\vec{r}''t'';\vec{r}'t')$$

$$= \int \mathcal{D}\vec{r}(t)\, e^{\frac{i}{\hbar}\frac{m_{eff}}{2}\int_{t'}^{t''}\dot{\vec{r}}^2 dt} \prod_{\vec{k}} G_{00}^{\vec{k}}$$

$$= \int \mathcal{D}\vec{r}(t)\exp\left[\frac{i}{\hbar}\frac{m_{eff}}{2}\int_{t'}^{t''}\dot{\vec{r}}^2 dt - \frac{1}{4\hbar M_f}\int\int_{t'}^{t''} dt\,ds\, e^{-i\omega_L|t-s|} \sum_{\vec{k}}\gamma_{\vec{k}}(t)\gamma_{\vec{k}}(s) \ldots \right. \tag{3.11}$$

To estimate the ground state energy the real exponent is required, hence the time variables are transformed to

$$it' = \tau', \quad it'' = \tau'', \quad it = \tau \text{ and } is = \sigma . \tag{3.12}$$

Eq. (3.11) is then

$$K_{00}(\vec{r}'\tau'';\vec{r}'\tau') = \int \mathcal{D}\vec{r}(\tau)\exp\left[-\frac{m_{eff}}{2\hbar}\int\left(\frac{d\vec{r}}{d\tau}\right)^2 d\tau + \frac{1}{4M_f\omega}\int d\tau\, d\sigma\, e^{-\omega_L|\tau-\sigma|}\sum_{\vec{k}}\gamma_{\vec{k}}(\tau)\gamma_{\vec{k}}(\sigma)\right] \tag{3.13}$$

The factor $\sum_{\vec{k}}\gamma_{\vec{k}}(\tau)\gamma_{\vec{k}}(\sigma)$ is explicitly :

$$\sum_{\vec{k}} \gamma_{\vec{k}}(\tau)\gamma_{\vec{k}}(\sigma) = \frac{2(4\pi e)^2}{V}\sum_{\vec{k}}\frac{1}{k^2}\left\{\begin{array}{l}\cos\vec{k}\cdot\vec{r}(\tau)\cos\vec{k}\cdot\vec{r}(\sigma)\\ \sin\vec{k}\cdot\vec{r}(\tau)\sin\vec{k}\cdot\vec{r}(\sigma)\end{array}\right\}$$

$$= \frac{2(4\pi e)^2}{V}\sum_{k_x>0}\frac{1}{k^2}\cos\vec{k}\cdot(\vec{r}(\tau)-\vec{r}(\sigma))$$

$$= \frac{4\pi e^2}{|\vec{r}(\tau)-\vec{r}(\sigma)|}. \tag{3.14}$$

Employing the relations :

$$M_f = \frac{4\pi}{\omega_L^2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon}\right)^{-1}, \quad \alpha = \frac{e^2}{2}\frac{1}{\hbar\omega_L}\sqrt{\frac{2m_{eff}\omega_L}{\hbar}}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon}\right)$$

and setting for convenient $\hbar = \omega_L = m_{eff} = 1$, the polaron propagator reduces to

$$K_{oo}(\vec{r}''\tau'';\vec{r}'\tau') = \int \mathcal{D}\vec{r}(\tau)\, e^{-\frac{1}{2}\int\left(\frac{d\vec{r}}{d\tau}\right)^2 d\tau + \frac{\alpha}{2^{3/2}}\iint_{\tau'}^{\tau''} d\tau d\sigma \frac{e^{-|\tau-\sigma|}}{|\vec{r}(\tau)-\vec{r}(\sigma)|}} \tag{3.15}$$

Identifying $K_{\infty}(\vec{r}\tau'';\vec{r}'\tau')$ with $\int \mathcal{D}\vec{r}(\tau)\, e^S$ the effective action of the polaron after the phonon field has been averaged out reads

$$S = -\frac{1}{2}\int\left(\frac{d\vec{r}}{d\tau}\right)^2 + \frac{\alpha}{2^{3/2}}\iint_{\tau'}^{\tau''} d\tau\, d\sigma \frac{e^{-|\tau-\sigma|}}{|\vec{r}(\tau)-\vec{r}(\sigma)|} \tag{3.16}$$

which manifests the electron considered at any particular time " interacting " with its position at a past time by a reaction which is inversely proportional to the distance traveled between these two times and which dies out exponentially with the time difference.

III.2 Evaluation of the Ground State Energy

In accordance with the preceding section, the polaron propagator takes the form

$$K_{oo}(\vec{r}'',t'';\vec{r}',t') = \int e^{S}\mathcal{D}\vec{r}(t) \tag{3.17}$$

with S given by

$$S = -\frac{1}{2}\int\left(\frac{d\vec{r}}{dt}\right)^2 dt + \frac{\alpha}{2^{3/2}}\int\int_{t'}^{t''} dt\,ds\,\frac{e^{-|t-s|}}{|\vec{r}(t)-\vec{r}(s)|}\,. \tag{3.18}$$

We have discussed in sec.II.1 that for a large time interval $\mathcal{T}$, $\mathcal{T}=(t''-t')$, the asymptotic rate of decay of (3.16) is

$$\int e^{S}\mathcal{D}\vec{r}(t) \underset{\mathcal{T}\to\infty}{\sim} e^{-E_g\mathcal{T}} \tag{3.19}$$

Consequently, to obtain the exact ground-state energy E_g we must evaluate the path integral (3.17) for large $\mathcal{T}$.

Unfortunately, the action S is not quadratic in $\vec{r}$ and so far only the path integral with a quadratic action can be performed exactly. Feynman remedied this situation by introducing a quadratic trial action S_o,

$$S_o = -\frac{1}{2}\int\left(\frac{d\vec{r}}{dt}\right)^2 dt - \frac{1}{2}C\int\int dt\,ds\,[\vec{r}(t)-\vec{r}(s)]^2 e^{-\omega|t-s|} \tag{3.20}$$

with two adjustable parameters C and ω to closely approximate the actual action S. In fact, this S_o describes a simple physical system in which the electron is coupled by a harmonic force to a fictitious second particle. The physical picture and the significance of this system as applied to the polaron problem will be examined quantitatively in chapter V.

Now let us consider

$$\int e^{S}\mathcal{D}\vec{r}(t) = \int e^{(S-S_0)}e^{S_0}\mathcal{D}\vec{r}(t)$$

$$= \langle e^{(S-S_0)}\rangle \int \mathcal{D}\vec{r}(t)\, e^{S_0}, \qquad (3.21)$$

where we have defined the average for any functional f by

$$\langle f\rangle \equiv \int e^{S_0} f\, \mathcal{D}\vec{r}(t) \Big/ \int e^{S_0}\mathcal{D}\vec{r}(t) . \qquad (3.22)$$

It follows mathematically that for any random variable f the inequality

$$\langle e^{f}\rangle \geqslant e^{\langle f\rangle}$$

can be imposed. Thus if we replace $\langle e^{S-S_0}\rangle$ by $e^{\langle S-S_0\rangle}$ (3.21) becomes

$$\int e^{S}\mathcal{D}\vec{r}(t) \geqslant e^{\langle S-S_0\rangle}\int \mathcal{D}\vec{r}(t)\, e^{S_0} \qquad (3.23)$$

Since, as $\mathcal{T}\to\infty$, $\langle S-S_0\rangle$ is proportional to $\mathcal{T}$ we thus write

$$\langle S-S_0\rangle = s\mathcal{T} \qquad (3.24)$$

Furthermore, supposing that the asymptotic decay of the propagator corresponding to the action S_0 is,

$$\int \mathcal{D}\vec{r}(t)\, e^{S_0} \sim e^{-E_0\mathcal{T}} \qquad (3.25)$$

Obviously, E_0 is the lowest energy for the system with action S_0 . Therefore from (3.19), (3.23), (3.24) and (3.25), we have

$$e^{-E_g T} \geq e^{\Delta T} \cdot e^{-E_0 T} , \tag{3.26a}$$

or

$$E_g \leq E_0 - \Delta ,$$

which is the variational principle of Feynman.

If we let

$$E = E_0 - \Delta , \tag{3.26b}$$

eq. (3.25) then reads

$$E_g \leq E = E_0 - \Delta \tag{3.26c}$$

Our objective is to carry out E and then choose the best values of the parameters C and ω which yield a minimum value of E . The resulting E is thus an upper bound to the required ground state energy E_g .

To obtain E , it is necessary to evaluate precisely the following quantities :

$$E_0 = -\lim_{T\to\infty} \frac{\ln \int e^{S_0} \mathcal{D}\vec{r}(t)}{T} \tag{3.27}$$

and

$$\Delta = \lim_{T\to\infty} \frac{1}{T}\langle S - S_0\rangle = \lim_{T\to\infty} \frac{1}{T} \cdot \frac{\int e^{S_0}(S-S_0)\mathcal{D}\vec{r}(t)}{\int e^{S_0}\mathcal{D}\vec{r}(t)} \tag{3.28}$$

$$= \langle S\rangle + \langle S_0\rangle , \tag{3.29.a}$$

where $$\langle S\rangle \equiv 2^{-3/2}\alpha\int_{t'=0}^{t''=\mathcal{T}} \langle|\vec{r}(t)-\vec{r}(s)|^{-1}\rangle e^{-|t-s|}ds \tag{3.29b}$$

$$\langle S_o\rangle \equiv \frac{1}{2}c\int_{t'=0}^{t''=\mathcal{T}} \langle(\vec{r}(t)-\vec{r}(s))^2\rangle e^{-\omega|t-s|}ds\,. \tag{3.29c}$$

To determine $\langle S\rangle$, we first replace the factor $|\vec{r}_t-\vec{r}_s|^{-1}$ in it by a Fourier transform,

$$|\vec{r}_t-\vec{r}_s|^{-1} = \int d^3k\,\frac{1}{2\pi^2k^2}\cdot e^{i\vec{k}\cdot(\vec{r}_t-\vec{r}_s)} \tag{3.30}$$

This leads to

$$\langle e^{i\vec{k}\cdot(\vec{r}_\tau-\vec{r}_\sigma)}\rangle_{S_o} = \int\mathcal{D}\vec{r}(t)e^{S_o}\cdot e^{i\vec{k}\cdot(\vec{r}_\tau-\vec{r}_\sigma)}\Big/\int\mathcal{D}\vec{r}(t)e^{S_o} \tag{3.31a}$$

or $$\langle e^{i\vec{k}\cdot(\vec{r}_\tau-\vec{r}_\sigma)}\rangle = \int\mathcal{D}\vec{r}(t)\cdot\exp\Big[-\frac{1}{2}\Big(\frac{d\vec{r}}{dt}\Big)^2dt-\frac{1}{2}c\iint(\vec{r}_t-\vec{r}_s)^2e^{-\omega|t-s|}dt\,ds$$
$$+\int\vec{f}(t)\cdot\vec{r}(t)dt\Big] \tag{3.31b}$$

where

$$\vec{f}(t) = i\vec{k}\,\delta(t-\tau)-i\vec{k}\,\delta(t-\sigma) \tag{3.32}$$

and where we have neglected the normalization factor for the reason which will be seen later.

To find $\langle S_o\rangle$, we have to compute $\langle(\vec{r}_\tau-\vec{r}_\sigma)^2\rangle$ precisely, however, we notice that once (3.31b) is performed, it follows that this $\langle(\vec{r}_\tau-\vec{r}_\sigma)^2\rangle$ can be obtained immediately by

$$\langle(\vec{r}_\tau-\vec{r}_\sigma)^2\rangle = -\left[\nabla^2_{\vec{k}}\langle e^{i\vec{k}\cdot(\vec{r}_\tau-\vec{r}_\sigma)}\rangle\right]_{\vec{k}=0} \tag{3.33}$$

Furthermore, one can take an advantage from the definitions of E_0 and $\langle S_0\rangle$ to verify directly the relation between them as

$$C\left(\frac{\partial E_0(C,\omega)}{\partial C}\right)_\omega = \langle S_0\rangle \tag{3.34}$$

which is a linear differential equation for E_0 , providing that $\langle S_0\rangle$ is known, with the boundary condition that for $C=0$, i.e., in case of a free particle,

$$E_0(0,\omega) = 0 \quad . \tag{3.35}$$

Thus our problem reduces to the evaluation of $\langle e^{i\vec{k}\cdot(\vec{r}_\tau-\vec{r}_\sigma)}\rangle$ given by (3.31b). Since the effect of the motion along the three rectangular components contribute additively to the exponent of (3.31b), we can equivalently consider in terms of a scalar x . Therefore, we need full expression of

$$\langle e^{ik_x(x_\tau-x_\sigma)}\rangle = \int \mathcal{D}x(t)\exp\left[-\frac{1}{2}\int_0^{\mathcal{T}}\left(\frac{dx}{dt}\right)^2 dt - \frac{C}{2}\int_0^{\mathcal{T}}\int_0^{\mathcal{T}} dt\,ds\,(x_t-x_s)^2 e^{-\omega|t-s|} + \int_0^{\mathcal{T}} f_x(t)x(t)\,dt\right] \tag{3.36}$$

The path integration involved is then proceeded formally the same as that presented in Sec. II.2. The result consists of two terms, one is the exponent corresponding to the classical path $\bar{x}(t)$ and the unimportant multiplying factor depending on $\mathcal{T}$ only. Within such a factor

$$\langle e^{ik_x(X_\tau - X_\sigma)}\rangle = \exp\Big[-\tfrac{1}{2}\int \dot{\bar{X}}^2(t)\,dt - \tfrac{C}{2}\iint dt\,ds\,(\bar{X}_t - \bar{X}_s)^2 e^{-\omega|t-s|}$$

$$+\int f_x(t)\bar{X}(t)\,dt\ \Big] \qquad (3.37a)$$

$$= \exp\big[\bar{S}_o'\big], \qquad (3.37b)$$

where $\bar{X}(t)$ must satisfy the equation given by : $\delta\bar{S}_o' = 0$, i.e.,

$$\frac{d^2\bar{X}(t)}{dt^2} = 2C\int(\bar{X}_t - \bar{X}_s)e^{-\omega|t-s|}\,ds - f_x(t) \,. \qquad (3.38)$$

Since the initial and final positions do not affect the asymptotic decay rate, the classical equation of motion for $\bar{X}(t)$ can be solved explicitly with the boundary conditions :

$$\bar{X}(0) = \bar{X}(T) = 0 \qquad (3.39)$$

Integrating the first terms in $\bar{S}_o'$ by parts once, then using the identitie (3.37) and (3.39) , eq. (3.37a) can be simplified to

$$\langle e^{ik_x(X_\tau - X_\sigma)}\rangle = e^{\frac{1}{2}\int f(t)\bar{X}(t)\,dt} \qquad (3.40a)$$

or

$$= e^{i\frac{k_x}{2}(\bar{X}(\tau) - \bar{X}(\sigma))} \qquad (3.40b)$$

To solve the integro-differential equation (3.38) with (3.39) for arbitrary $\bar{X}(t)$, Feynman defined in addition

$$Z(t) = \frac{\omega}{2}\int e^{-\omega|t-s|}\bar{X}_s\,ds \,, \qquad (3.41)$$

so that

$$\frac{d^2Z(t)}{dt^2} = \omega^2\left[Z(t) - \bar{X}(t)\right] , \tag{3.42}$$

and in terms of $Z(t)$, (3.37) reduces to

$$\frac{d^2\bar{X}(t)}{dt^2} = \frac{4c}{\omega}\left[\bar{X}(t) - Z(t)\right] - f_x(t) , \tag{3.43}$$

in which the equality $\int_0^\infty ds\, e^{-\omega|t-s|} = \frac{2}{\omega}$ has been imposed. After $Z(t)$ is eliminated from (3.43) , we are left with the ordinary fourth order differential equation for $\bar{X}(t)$ which is readily solved. One comes out with

$$\begin{aligned}\bar{X}(t) &= -\frac{ik_x}{\nu}\left[\sinh\nu(t-\tau)H(t-\tau) - \sinh\nu(t-\sigma)H(t-\sigma)\right] \\ &+ \frac{ik_x}{\nu^3}\left[\sinh\nu(t-\tau)H(t-\tau) - \sinh\nu(t-\sigma)H(t-\sigma)\right] \\ &- \frac{ik_x\omega^2}{\nu^2}\left[(t-\tau)H(t-\tau) - (t-\sigma)H(t-\sigma)\right] ,\end{aligned} \tag{3.44}$$

where $\nu^2 = \omega^2 + 4c/\omega$

and where the transient terms at the end points have been ignored in assuming that over the large interval $(0, \mathcal{T})$ most of the contribution is during $\tau >> 0$, $\sigma << \mathcal{T}$.

Imposing the boundary equations given by (3.39) on the substitution of $\bar{X}(\tau)$ and $\bar{X}(\sigma)$ into (3.40) finally leads to

$$\left\langle e^{ik_x(X(\tau) - X(\sigma))}\right\rangle = e^{-\frac{2ck_x^2}{\nu^3\omega}(1 - e^{-\nu|\tau-\sigma|}) - \frac{\omega^2}{2\nu^2}k_x^2|\tau-\sigma|} \tag{3.45}$$

or

$$\left\langle e^{i\vec{k}\cdot(\vec{r}(t) - \vec{r}(s))}\right\rangle = e^{\left[-\frac{2ck^2}{\nu^3\omega}(1 - e^{-\nu|t-s|}) - \frac{k^2\omega^2}{2\nu^2}|t-s|\right]} . \tag{3.46}$$

It is now clear that the normalization factor in (3.31) can be dropped out since in this case $e^{\bar{S}}$ is correctly normalized, as we can check by setting $\vec{k}=0$ in (3.46).

Using (3.45) and recalling (3.29), (3.30), (3.33), (3.34) and (3.35) the calculation of $\langle S\rangle$, $\langle S_0\rangle$ and E_0 is now straightforward, in the limit $T\to\infty$, the consequent results are :

$$\langle S\rangle = \pi^{-\frac{1}{2}}\alpha\nu\int_0^\infty\left[\omega^2\tau+\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu\tau})\right]^{-\frac{1}{2}}e^{-\tau}d\tau, \qquad (3.47)$$

$$\frac{1}{3}\langle(\vec{r}_\tau-\vec{r}_\sigma)^2\rangle = \frac{4C}{\nu^3\omega}(1-e^{-|\tau-\sigma|})+\frac{\omega^2}{\nu^2}|\tau-\sigma|, \qquad (3.48)$$

$$\langle S_0\rangle = \frac{3C}{\nu\omega}, \qquad (3.49)$$

and

$$E_0 = \frac{3}{2}(\nu-\omega). \qquad (3.50)$$

It follows immediately from (3.26c) and (3.29) that the required energy expression reads

$$E = \frac{3}{4\nu}(\nu-\omega)^2-\langle S\rangle, \qquad (3.51)$$

with $\langle S\rangle$ given by (3.47). To obtain the best approximation for the actual ground state E_g, the two adjustable parameters ν and ω have to be varied separately to yield a minimum E. This can be accomplished generally by minimizing (3.51) with respect to both ν and ω. These $\frac{\delta E}{\delta\nu}=0$; $\frac{\delta E}{\delta\omega}=0$;

give two defining equations for the optimal ν and ω, viz.,

$$\frac{3}{2}\frac{(\nu-\omega)}{\nu}-\frac{3}{4}\frac{(\nu-\omega)^2}{\nu^2} = \frac{\langle S\rangle}{\nu}-\frac{1}{2}\pi^{-\frac{1}{2}}\alpha\nu\int_0^\infty d\tau[F(\tau)]^{-\frac{3}{2}}e^{-\tau}\left\{\frac{\nu^2+\omega^2}{\nu^2}(1-e^{-\nu\tau})+\frac{(\nu^2-\omega^2)}{\nu}\tau e^{-\nu\tau}\right\}$$

(3.52)

and

$$\frac{3}{2\nu}(\nu-\omega) = \pi^{-\frac{1}{2}}\alpha\nu\int_0^\infty [F(\tau)]^{-\frac{3}{2}} e^{-\tau}\left\{\omega\tau - \frac{\omega}{\nu}(1-e^{-\nu\tau})\right\}d\tau \tag{3.53}$$

where $\quad F(\tau) \equiv [\omega^2\tau + \frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu\tau})]$

Unfortunately, the integrations involved in these equations cannot be calculated in closed form and the numerical method must be employed in solving the exact values of ν and ω which in turn give general result of E. However, Feynman showed that it is possible to analytically estimate E in the two limiting case : the case of large α and small α.

For large α or strong coupling which corresponds to large ν, if we first choose $\omega = 0$, $\langle S \rangle$ reduces to

$$\langle S \rangle = \pi^{-\frac{1}{2}}\alpha\nu^{\frac{1}{2}}\int_0^\infty e^{-\tau}d\tau[1-e^{-\nu\tau}]^{-\frac{1}{2}}$$

$$= \pi^{-\frac{1}{2}}\alpha\nu^{\frac{1}{2}}\frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2})}{\nu\Gamma(\frac{1}{2}+\frac{1}{\nu})} \tag{3.54}$$

$$= \frac{\nu^{\frac{1}{2}}\alpha\Gamma(\frac{1}{2})}{\nu\Gamma(\frac{1}{2}+\frac{1}{\nu})}. \tag{3.55}$$

The asymptotic formula of (3.55), for $\nu >> 1$ can be considered as follows

$$\langle S \rangle = \frac{\alpha\nu^{\frac{1}{2}}\Gamma(\frac{1}{\nu})}{\nu\Gamma(\frac{1}{2}+\frac{1}{\nu})} = (\alpha\nu^{\frac{1}{2}})\frac{\Gamma(1+\frac{1}{\nu})}{\Gamma(\frac{1}{2}+\frac{1}{\nu})}$$

$$= (\alpha\nu^{\frac{1}{2}})\frac{\Gamma(1)}{\Gamma(\frac{1}{2})}\left\{\frac{1+\frac{1}{\nu}\frac{\Gamma'(1)}{\Gamma(1)}}{1+\frac{1}{\nu}\frac{\Gamma'(\frac{1}{2})}{\Gamma(\frac{1}{2})}}\right\}$$

$$= \frac{\alpha\nu^{\frac{1}{2}}}{\pi^{1/2}}\left\{\left(1+\frac{1}{\nu}\Psi(1)\right)\left(1-\frac{1}{\nu}\Psi(\tfrac{1}{2})\right)\right\}$$

$$\simeq \frac{\alpha \nu^{\frac{1}{2}}}{\pi^{1/2}}\left\{1+\frac{1}{\nu}\left(\psi(1)-\psi(\tfrac{1}{2})\right)\right\}$$

$$\simeq \frac{\alpha \nu^{1/2}}{\pi^{1/2}}\left\{1+\frac{1}{\nu}\cdot 2\ln 2\right\}, \qquad (3.56)$$

where $\Gamma(z)$ is a gamma function defined by

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt \quad ; \qquad (Re.Z>0)$$

$\psi(z)$ is a psi function given by

$$\psi(z) = \frac{d}{dz}[\ln \Gamma(z)] = \frac{\Gamma'(z)}{\Gamma(z)} \quad ,$$

and where we have applied a gamma function property : $\Gamma(1+z) = z\Gamma(z)$, and neglected terms of higher order than $\frac{1}{\nu}$.

Nevertheless, this $\omega=0$ case contains a discontinuity at $\alpha = 6$ and Feynman avoided the disadvantage by choosing another corresponding ω .

For large ν , $\omega \neq 0$ the integral $\langle\delta\rangle$ comes out as

$$\langle S\rangle = \alpha\left(\frac{\nu}{\pi}\right)^{\frac{1}{2}}\int_0^\infty \left\{\frac{\nu^2-\omega^2}{\nu^2}(1-e^{-\nu\tau})\right\}^{-\frac{1}{2}}\left[1+\frac{\omega^2\tau}{\nu(1-e^{-\nu\tau})}\right]^{-\frac{1}{2}} e^{-\tau} d\tau$$

$$\frac{\omega}{\nu} \ll 1, \quad \langle S\rangle \simeq \alpha\left(\frac{\nu}{\pi}\right)^{\frac{1}{2}}\int_0^\infty (1-e^{-\nu\tau})^{-\frac{1}{2}}\left[1-\frac{1}{2}\frac{\omega^2\tau}{\nu}(1-e^{-\nu\tau})\right] e^{-\tau} d\tau$$

$$= \alpha\left(\frac{\nu}{\pi}\right)^{\frac{1}{2}}\left[1+\frac{2\ln 2}{\nu}-\frac{\omega^2}{2\nu}\int_0^\infty \tau e^{-\tau} d\tau\right]$$

$$= \alpha\left(\frac{\nu}{\pi}\right)^{\frac{1}{2}}\left[1+\frac{2\ln 2}{\nu}-\frac{1}{2}\frac{\omega^2}{\nu}\right]$$

(3.57)

in which we have used the asymptotic form (3.16) and taken $e^{-\nu\tau} \longrightarrow 0$.
Within this approximation the expression for E is

$$E = \frac{3}{4}(\nu - 2\omega) - \frac{\alpha}{\pi^{1/2}}\left(\nu^{\frac{1}{2}} + \frac{4\ln 2 - \omega^2}{2\,\nu^{1/2}}\right) \tag{3.58}$$

which is readily to be minimized with respect to both ν and ω independently. Operating $\frac{\delta E}{\delta \nu} = 0$ gives

$$\frac{3}{4}\nu^{3/2} - \frac{\alpha\nu}{2\pi^{1/2}} + \frac{\alpha}{4\pi^{1/2}}(4\ln 2 - \omega^2) = 0\,, \tag{3.59}$$

which is easily solved by the iteration method.
As $\nu \to \infty$, (3.59) simplifies to

$$\frac{3}{4} - \frac{\alpha}{2\pi^{1/2}}\nu^{-\frac{1}{2}} = 0\,,$$

giving the asymptotic solution for (3.59) as

$$\nu^{1/2} = \frac{2\alpha}{3\pi^{1/2}} \quad \text{or} \quad \nu = \frac{4}{9}\frac{\alpha^2}{\pi}\,. \tag{3.60}$$

Applying this to (3.59) yields the general solution

$$\nu = \frac{4}{9}\frac{\alpha^2}{\pi} - (4\ln 2 - \omega^2) \tag{3.61}$$

Our next step is to work out the corresponding numerical value of ω so as to get explicit ν or the minimum E. Differentiating (3.58) with respect to ω and equating the result to zero i.e., $\frac{\delta E}{\delta \omega} = 0$, one has

$$\frac{\alpha\omega}{(\pi\nu)^{1/2}} = \frac{3}{2} \tag{3.62}$$

As an approximation we may replace $\nu^{\frac{1}{2}}$ by its asymptotic value given by (3.60) and this gives

$$\omega \simeq 1 \tag{3.63}$$

Recalling (3.61) the resulting ν is then

$$\nu \simeq \frac{4}{9}\frac{\alpha^2}{\pi} - (4\ln 2 - 1) \tag{3.64}$$

Thus in case of large α , the minimum E is approximately (3.58) with ω and ν given by (3.63) and (3.64) successively, i.e.,

$$E \simeq -\frac{\alpha^2}{3\pi} - 3\ln 2 - \frac{3}{4} = -0.106\,\alpha^2 - 2.83 \tag{3.65}$$

For small α, if we extremely take $\alpha=0$, it is evident from (3.53) that the minimum will occur when $\nu=\omega$. Therefore for $\alpha \sim 0$ it is reasonable to set

$$\nu = (1+\epsilon)\omega \ ; \quad \epsilon << 1, \tag{3.66}$$

and we notice that ϵ is of order of α .

Consider $\langle S \rangle$ in this limit, substituting ν in terms of ϵ and ω and treating ϵ small yield

$$\langle S \rangle = \pi^{-\frac{1}{2}} \alpha \nu \int_0^{\infty} [\omega^2 \tau + 2\epsilon\omega(1 - e^{-\omega\tau})]^{-\frac{1}{2}} e^{-\tau} d\tau \tag{3.67}$$

Expanding the radical term in the integral in powers of ϵ leads to

$$\langle S \rangle = \pi^{-\frac{1}{2}} \alpha \frac{\nu}{\omega} \int_0^{\infty} [\tau^{-\frac{1}{2}} - \frac{\epsilon}{\omega} \tau^{-\frac{3}{2}} (1 - e^{-\omega\tau}) + \ldots] e^{-\tau} d\tau$$

$$= \alpha\left(\frac{\nu}{\omega}\right)\left[1-\frac{\epsilon}{\omega\pi^{1/2}}\int_0^\infty \tau^{-3/2}e^{-\tau}(1-e^{-\omega\tau})\,d\tau\right]$$

$$= \alpha\left(\frac{\nu}{\omega}\right)\left[1-\epsilon\left(\frac{2}{\omega}\left\{(1+\omega)^{1/2}-1\right\}\right)\right]$$

$$= \alpha + \alpha\epsilon(1-P)\,, \tag{3.68}$$

where $\quad P \equiv \frac{2}{\omega}\left[(1+\omega)^{1/2}-1\right]$ (3.69)

and in which we have kept only terms up to order ϵ^2. Now the expression of E turns out to be

$$E = \frac{3}{4}\omega\epsilon^2 - \alpha - \alpha\epsilon(1-P) \tag{3.70}$$

concerning two parameters ϵ and ω. Our objective is then to search for the appropriate ϵ and ω so that E can attain minimum. We first minimize (3.70) with respect to ϵ, that is

$$\frac{\delta E}{\delta\epsilon} = 0$$

which gives at once

$$\epsilon = \frac{2\alpha}{3\omega}(1-P)\,. \tag{3.71}$$

Since ϵ is small this equation is valid for small α only. Elimination of ϵ in (3.70) results

$$E = -\alpha - \frac{\alpha^2}{3\omega}\left\{1-\frac{2}{\omega}\left[(1+\omega)^{1/2}-1\right]\right\} \tag{3.72}$$

Next we perform $\frac{\delta E}{\delta\omega} = 0$ and readily find an equation for ω as

$$-\frac{1}{2}+\frac{2}{2+\omega p}(P-1)+2P-\frac{3}{2}P^2=0. \tag{3.73}$$

It happens that the equation (3.73) is satisfied when we put $\omega = 3$. It follows from (3.71) that in this limit the minimized energy takes the form

$$E = -\alpha - \frac{\alpha^2}{81} = -\alpha - 1.23\left(\frac{\alpha}{10}\right)^2 \tag{3.74}$$

And the appropriate ν to be chosen in this case is

$$\nu = 3 + 2.22\left(\frac{\alpha}{10}\right)$$

after inserting ϵ and ω in (3.66) .

It is an advantage to notice that the resulting energy E is not sensitive to the choice of ω. This can be shown easily if we take $\omega=1$ instead of $\omega=3$, the factor 1.23 in (3.74) changes only to 0.98 . For this reason we can fix $\omega=1$ for all α with sufficient accuracy and our further numerical work reduces to a minimization with respect to only a single parameter ν .

Physically, $\omega=1$ implies that the trial action S_1 has the same time exponential in the interaction term as does the actual S .

Once ω is set to equal to 1 , the situation for small α is slightly modified as :

$\alpha \to 0$; $\omega=1$, $\nu=(1+\epsilon)$ or $\epsilon=(\nu-1)$

Consider ϵ small, the integral is now expanded in powers of $(\nu-1)$. The resulting energy becomes $(\omega=1)$

$$E = -\alpha - 0.98\left(\frac{\alpha}{10}\right)^2 - 0.60\left(\frac{\alpha}{10}\right)^3 - \cdots\cdots . \tag{3.75}$$

and the corresponding ν ,

$$\nu = 1 + 1.14\left(\frac{\alpha}{10}\right) + 1.35\left(\frac{\alpha}{10}\right)^2 + \cdots\cdots$$

III.3 Evaluation of the Effective Mass

In principle, the determination of a particle effective mass can be proceeded in the following way: As we have observed that for a free particle of mass m whose initial coordinate is 0 and final coordinate is $\vec{r}_{\mathcal{T}}$, with the Lagrangian $\mathcal{L} = \frac{1}{2}m\dot{\vec{r}}^2$, the propagator of this system possesses the form

$$e^{-\frac{m\vec{r}_{\mathcal{T}}^{\,2}}{2\mathcal{T}}}$$

Hence, in analogy to this, we are able to estimate the effective mass for our polaron system by studying the asymptotic form of the path integral $\int e^{S}\mathcal{D}\vec{r}(t)$, which is essentially similar to the previous case of finding ground state energy, but now with $\vec{r}(\mathcal{T}) \neq 0$. This means that an end point is allowed to move as the limit $\mathcal{T} \to \infty$ is taken. As a result the asymptotic decay rate of the propagator may no longer by dominated by the ground state energy but it would rather vary as

$$e^{-E_g\mathcal{T} - \frac{\overset{*}{m}\vec{r}^{\,2}(\mathcal{T})}{2\mathcal{T}}} \quad ; \text{ for small } \vec{r}(\mathcal{T}), \tag{3.76}$$

the additional term depending on $\vec{r}(\mathcal{T})$ determines the effective mass $\overset{*}{m}$. Consequently we have to solve (3.33) under the boundary conditions $\bar{x}(t=0)=0$ and $\bar{x}(t=\mathcal{T})=x_{\mathcal{T}}$. However there are some confusing difficulties at the end points. Feynman removed these complications by assuming the final point :

$$\vec{r}(\mathcal{T}) = \vec{U}\mathcal{T}, \tag{3.77}$$

in which $\vec{U}$ is an imaginary average velocity. With $\vec{r}$ given by (3.76) the asymptotic decay rate (3.75) turns out to be, for small U ,

$$\int e^{S} \mathcal{D}\vec{r}(t) \sim e^{-E_g\mathcal{T} - \frac{1}{2} \overset{*}{m}_F U^2 \mathcal{T}}$$

or to be consistent with the preceding section

$$e^{-E_0(U) - S(U) - S_0(U)\mathcal{T}} = e^{-(E_g + \frac{1}{2}\overset{*}{m}_F U^2)\mathcal{T}} \equiv e^{-E(U)\mathcal{T}}. \tag{3.78}$$

To obtain $\overset{*}{m}$ we are required to evaluate the total energy $E(U)$ and equate it to $E_g + \frac{1}{2}\overset{*}{m} U^2$; now the dependence on U yields $\overset{*}{m}_F$. The mathematical detailed calculation of $E(U)$ is analogous to that of E except that there are extra terms arising from such new boundary conditions.

Now we reconsider the key quantity $\langle e^{i\vec{k}\cdot(\vec{r}(\tau)-\vec{r}(\sigma))}\rangle$, replacing $\bar{x}(t)$ with $\bar{x}+ut$ in (3.37a) gives

$$\langle e^{ik_x(x_\tau - x_\sigma)}\rangle = \exp\Big[-\frac{1}{2}\int \dot{\bar{x}}^2(t)dt - \frac{c}{2}\iint(\bar{x}_t-\bar{x}_s)^2 e^{-\omega|t-s|}dtds$$
$$+ \int f_x(t)\bar{x}_t dt + \int t u_x f(t)dt\Big]. \tag{3.79}$$

Again this can be simplified by the virtue of (3.38) to be

$$\langle e^{ik_x(x_\tau - x_\sigma)} \rangle = \exp\left[\frac{1}{2}\iint f(t)\bar{x}_t dt + \int t u_x f(t) dt\right]. \qquad (3.80)$$

For $f(t)$ given by (3.31), recalling (3.40) and (3.46) expression (3.80) is completely

$$\langle e^{i\vec{k}.(\vec{r}_\tau - \vec{r}_\sigma)} \rangle = \exp\left[-\frac{k^2}{2\nu^2}F(|\tau-\sigma|) + i\vec{k}.\vec{u}(\tau-\sigma)\right], \qquad (3.81)$$

where

$$F(\tau) = \left[\omega^2\tau + \frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu\tau})\right]. \qquad (3.82)$$

Substitution of (3.81) into (3.30) and (3.29b) given for $\langle S(u)\rangle$ the extended value

$$\langle S(u)\rangle = 2^{-\frac{3}{2}}\alpha \iint_0^\infty (2\pi^2k^2)^{-1} e^{-\tau} \exp\left[-\frac{k^2}{2\nu^2}F(\tau) + i\vec{k}.\vec{u}\tau\right] d^3k\, d\tau . \qquad (3.83)$$

Restrict to the case of a slow electron i.e., $\vec{u} \ll 1$, expansion of $\langle S(u)\rangle$ to order u^2 yields

$$\langle S(u)\rangle = 2^{-\frac{3}{2}}\alpha \iint_0^\infty (2\pi^2k^2)^{-1} e^{-\tau} \times e^{-\frac{k^2}{2\nu^2}F(\tau)}\left[1 + i\vec{k}.\vec{u}\tau - \frac{(\vec{k}.\vec{u}\tau)^2}{2}\right] d^3k\, d\tau$$

Concentrate on the term that contribute factor u^2 to $\langle S(u)\rangle$, for simplicity or as an average for isotropic medium we treat

$$(\vec{k}.\vec{u})^2 \simeq \frac{1}{3}k^2u^2,$$

then

$$\langle S(u)\rangle = 2^{-\frac{3}{2}}\alpha \iint_0^\infty (2\pi^2k^2)^{-1} e^{-\tau} \times e^{-\frac{k^2}{2\nu^2}F(\tau)}\left[1 + i\vec{k}.\vec{u}\tau\right] d^3k\, d\tau -$$

$$- 2^{3/2}\alpha \cdot \frac{u^2}{6} \iint_0^\infty (2\pi^2k^2)^{-1} e^{-\frac{k^2}{2\nu^2}} k^2 d^3k\, d\tau \qquad (3.84)$$

Integration over $\vec{k}$ is now readily performed and the u^2-term comes out as

$$-\frac{u^2}{6}\frac{\alpha}{\pi^{1/2}}\nu^3\int_0^\infty [F(\tau)]^{-3/2} e^{-\tau}\tau^2\, d\tau \qquad (3.85)$$

Differentiating (3.80) with respect to $\vec{k}$ twice, then taking $\vec{k} \longrightarrow 0$, we obtain

$$\tfrac{1}{3}\langle(\vec{r}_t-\vec{r}_s)^2\rangle = F(t-s)\,\nu^{-2}+\tfrac{1}{3}u^2(t-s)^2 \qquad (3.86)$$

The modified value of $\langle S_0(u)\rangle$ is therefore

$$\langle S_0(u)\rangle = \frac{C}{2}\int_0^\infty \left[\frac{3F}{\nu^2}(t-s)+u^2(t-s)^2\right]e^{-\omega|t-s|}ds,$$

making use of the identity $\int_0^\infty e^{-\omega|t-s|}ds=\frac{2}{\omega}$, $\langle S_0(u)\rangle$ is now explicitly

$$\langle S_0(u)\rangle = \frac{3C}{\nu\omega}+\frac{2C}{\omega^3}u^2 \qquad (3.87)$$

Again we solve for $E_0(u)$ from the relation: $\left(\frac{\delta E_0}{\delta C}\right)_\omega = \frac{\langle S_0(u)\rangle}{C}$, but now with the boundary condition $E_0 = \frac{1}{2}u^2$ for $C=0$.

Hence

$$E_0(u) = \tfrac{3}{2}(\nu-\omega)+\tfrac{1}{2}u^2\left(1+\frac{4C}{\omega^3}\right). \qquad (3.88)$$

and the total energy expression reads

$$E(u) = E_0(u)-\langle S(u)\rangle-\langle S_0'(u)\rangle$$

$$= \tfrac{1}{2}u^2+\frac{3}{4\nu}(\nu-\omega)^2-\langle S(u)\rangle,$$

where $\langle S(u)\rangle$ is given in (3.84) and (3.85). The definition $E(u) \equiv E_g+\frac{1}{2}\overset{*}{m}_F u^2$ then gives for $\overset{*}{m}_F$ the value

$$m_F^* = 1 + \frac{\pi^{-\frac{1}{2}}}{3} \alpha \nu^3 \int_0^\infty [F(\tau)]^{-\frac{3}{2}} e^{-\tau} \tau^2 d\tau ,$$

(3.90)

the appropriate parameters ν and ω to be employed are those which were previously obtained in minimizing $E(u)$ when $U = 0$.

The two limiting case : weak and strong couplings, for m_F^* are easily found under the same detailed approximations made earlier.

For large α, which implies large ν, taking $\frac{\nu}{\omega} << 1$ and $e^{-\nu\tau} \rightarrow 0$, m_F^* reduces to

$$m_F^* \simeq 1 + \frac{2}{3} \pi^{-\frac{1}{2}} \alpha \nu^{\frac{3}{2}} , \tag{3.91}$$

with $\nu = \frac{4\alpha^2}{9\pi} - (4 \ln 2 - 1)$, m_F^* is found to be dominated by α^4 term as

$$m_F^* \simeq \frac{16\alpha^4}{81\pi^2} = 200 \left(\frac{\alpha}{10}\right)^4$$

(3.92)

For small α , $\nu = (1+\epsilon)\omega; \epsilon << 1$, m_F^* in this case

$$m^* \simeq 1 + \frac{1}{3} \pi^{-\frac{1}{2}} \alpha (1+3\epsilon) \omega^3 \int_0^\infty (\omega^2 \tau)^{-3/2} [1 - \frac{3}{2} \cdot \frac{2}{\omega\tau} \epsilon (1 - e^{-\omega\tau})] e^{-\tau} \tau^2 d\tau$$

$$= 1 + \frac{1}{3} \alpha \left[\frac{1}{2} + \frac{3}{2}\epsilon - \frac{3}{\omega}\epsilon + \frac{3\epsilon}{\omega(1+\omega)^{1/2}} \right] ,$$

providing

$$\epsilon = \frac{2\alpha}{3\omega} [1 - P] ; \quad P = \frac{2}{\omega} [(1+\omega)^{\frac{1}{2}} - 1]$$

gives

$$m_F^* \simeq 1 + \frac{1}{6} \alpha + 0.025 \alpha^2 ; \text{ for } \omega = 3$$

and

$$m_F^* \simeq 1 + \frac{1}{6} \alpha + 0.023 \alpha^2 ; \text{ for } \omega = 1 .$$