CHAPTER IV

VARIOUS APPROACHES TO THE POLARON EFFECTIVE MASS

In the preceding chapter the polaron effective mass has been estimated according to the definition proposed by Feynman in analogous to that of a free particle. Viewing from different points, there are still other possible definitions which lead to somewhat different but related resulting expressions for the effective mass. As it is our aim to provide a complete review of the polaron effective mass investigated using the similar mathematical technique as that of Feynman, in this chapter we shall discuss qualitatively four alternative approaches basing on different definitions to the quantity. The first two will be that of the polaron at 0 K and the remaining of the generalized problem at finite temperatures. We are therefore required to give the statement of the problem at finite temperature. In addition, we shall introduce the polaron action at this general state in the intermediate section.

IV.1 Schultz's Approximation

Schultz[15] has developed a first order polaron effective mass

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15 See Reference (2) Appendix A.

approximation to be utilized in his calculation of polaron mobility. His procedure leads to the concept of virtual quasi-phonons and to the usual set of Feynman diagrams in describing the polaron propagator.

From the foregoing chapter, we have already seen that the polaron ground-state propagator is exactly

$$K(\vec{r}''t''; \vec{r}'t') \equiv \langle \vec{r}'' vac t' | \vec{r}' vac t' \rangle = \int \mathcal{D}\vec{r}(t)\, e^{i/2 \int \dot{\vec{r}}^2 dt}\, G_{00}[\vec{r}(t)]$$

$$= \int \mathcal{D}\vec{r}(t)\, e^{iS} \qquad (4.1)$$

The Feynman approximation is essentially to replace S by the trial action S_0. To get the ultimately correct result, the contribution of $\langle S - S_0 \rangle$ has to be included. In real time this implies

$$S_0 = \frac{1}{2}\int \dot{\vec{r}}^2 dt - \frac{i}{2} C \iint_{t'}^{t''} [\vec{r}(t) - \vec{r}(s)]^2 e^{-i\omega|t-s|} dt ds + \int_{t'}^{t''} \langle S - S_0 \rangle dt \qquad (4.2)$$

Obviously, the replacement of S by S_0 alone means that we just make the zeroth-order approximation in the exact expansion

$$e^{iS} = e^{iS_0} e^{i(S-S_0)} = e^{iS_0}\left[1 + i(S - S_0) + \frac{i^2}{2!}(S - S_0)^2 + \ldots\ldots\right] \qquad (4.3)$$

Physically, such a zeroth-order approximation describes the polaron as a two particle system composed of an electron of mass $m_{eff}=1$, connected to a fictitious second particle of mass M by a spring of force constant $\mathcal{K}$ with the following relations:

$$M = \left(\frac{\nu^2}{\omega^2} - 1\right) \quad ; \quad \mathcal{K} = \frac{4c}{\omega} = \nu^2 - \omega^2$$

and

$$\nu = \frac{1.M}{1+M} = \frac{\nu^2 - \omega^2}{\nu^2} \tag{4.4}$$

The static properties of this system are obtained implicitly in the corresponding zeroth-order propagator, $\int e^{S_0} \mathcal{D}\vec{r}(t)$ with imaginary time $t = it$. It is clear from the sec. III.2 that the zeroth-order approximation of the ground- state energy is readily

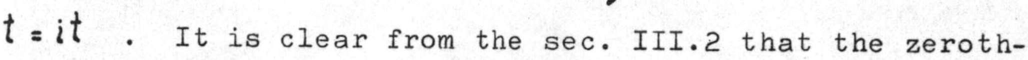
$$E \simeq E_1 = \frac{3}{2}(\nu - \omega) \tag{4.5}$$

and the consistent zeroth-order effective mass is merely

$$m_0 = 1 + \frac{4c}{\omega^3} = 1 + \left(\frac{\nu^2 - \omega^2}{\omega^2}\right) = \frac{\nu^2}{\omega^2} = 1 + M \tag{4.6}$$

the total mass of the two-particle system.

Now going back to the expansion given by (4.3), if we manipulate the sum corresponding to the Feynman diagrams



where the dashed line represent the quasi-phonons or specific contributions of each power of $(S - S_0)$ we shall obtain the corrections to the zeroth-order effective mass. Higher order approximation can be achieved by summing over the diagrams containing one, two, etc., virtual quasi-phonons. Consequently, the transformation function of interest turns to

$$\langle \vec{r}t'' | \vec{r}t' \rangle = \int \mathcal{D}\vec{r}(t)\, e^{i\left[\int_{t'}^{t''} \frac{\dot{\vec{r}}^2}{2} dt + S_0\right]} \left[1 + i(S - S_0) + \frac{i^2}{2!}(S - S_0)^2 + \ldots\ldots\right] \tag{4.7}$$

where we exclude the free electron action $\int_{t'}^{t''} \frac{\dot{\vec{r}}^2}{2} dt$ in the expression for S and S_o. Notice that because of the quadratic S_o any of the path integrals appear in (4.7) can be reduced to the evaluation of ordinary Riemann integrals. Since we have experienced that

$$\frac{1}{|\vec{r}|} = \frac{1}{2\pi^2}\int d^3k\, \frac{e^{i\vec{k}.\vec{r}}}{k^2}$$

and

$$r^2 = -\left[\nabla_{\vec{k}}^2 e^{i\vec{k}.\vec{r}}\right]_{\vec{k}=0} = -\int d^3k\,(\nabla_{\vec{k}}^2\delta(\vec{k})e^{i\vec{k}.\vec{r}}) ,$$

then the calculation of(4 .7) should concern with integral like :

$$\begin{aligned}
&\int \mathcal{D}\vec{r}(t)\, e^{i\left[\int_{t'}^{t''}\frac{\dot{\vec{r}}^2}{2}dt + S_o\right]}(S-S_o) \\
&= \frac{i\alpha}{2^{3/2}}\int\frac{d^3\vec{k}}{2\pi^3k^2}\iint_{t'}^{t''} d\tau d\sigma\, e^{-i|\tau-\sigma|}\int \mathcal{D}\vec{r}(t)\, e^{i\left[\int_{t'}^{t''}(\frac{\dot{\vec{r}}^2}{2} - \vec{f}_k\cdot\vec{r})dt + S_o\right]} \\
&- \frac{ic}{2}\int d^3k\,\nabla_k^2\delta(\vec{k})\iint_{t'}^{t''} d\tau d\sigma\, e^{-i\omega|\tau-\sigma|}\int \mathcal{D}\vec{r}(t)\, e^{i\left[\int_{t'}^{t''}(\frac{\dot{\vec{r}}^2}{2} - \vec{f}_k\cdot\vec{r})dt + S_o\right]} \\
&- \langle S-S_o\rangle T.\int \mathcal{D}\vec{r}(t)\, e^{i\left[\int_{t'}^{t''}\frac{\dot{\vec{r}}^2}{2}dt + S_o\right]}
\end{aligned} \tag{4.8}$$

where

$$\vec{f}_{\vec{k}} = -\vec{k}(\delta(t-\tau) - \delta(t-\sigma)) \tag{4.9}$$

Similar expressions can be verified for higher powers of $(S-S_o)$. To accomplish the optimal results one must sum over to.an infinite set of diagrams. As a result the path integrals come out to be very laborious to deal with. Schultz made all calculations simpler by working in a Hamiltonian operator formalism instead of in the path integralformalism. He has set up an extended Hamiltonian $\mathbb{R}$ which, if treated by path integrals, would lead to an expansion such as (4.7). It is clear from the two particle model system that S_o corresponds to a Hamiltonian

$$\mathbb{R}_{part} = \left(\frac{\mathbb{P}^2}{2m_o}\right) + \left(\frac{\pi^2}{2M}\right) + \frac{1}{2}\mu\nu\rho^2 - \left(\langle S - S_o\rangle + \frac{3}{2}\omega\right) \qquad (4.10)$$

here $\mathbb{P}$ is the momentum operator canonically conjugate to the center-of-mass coordinate

$$\vec{R} = (1.\vec{r} + M\vec{Y})/(m_{eff} + M) \quad ;$$

$\vec{\pi}$ is canonically conjugate to the interparticle separation $\vec{\rho} = \vec{r} - \vec{Y}$; $m_o = m_{eff} + M$ is the polaron mass in zeroth-approximation ; $\mu = 1.\frac{M}{m_o}$ and $\nu = \sqrt{\frac{K}{\mu}}$. One should recall that in the calculation of all transformation functions the initial and final states should be the ground harmonic oscillation state in their dependence on the internal coordinate $\vec{\rho}$.

Schultz has evaluated the first-order polaron effective mass to estimate the accuracy of m_o or m_p^* obtained by Feynman. Studying the contributions of the three terms given in (4.8) he was then led to introduce the extended Hamiltonian to be applied in his approximation as

$$\mathbb{R} = \mathbb{R}_o + \mathbb{R}_1 \qquad (4.11)$$

in which the unperturbed part $\mathbb{R}_o$ is

$$\mathbb{R}_o = \frac{\mathbb{P}^2}{2m_o} + \frac{\vec{\pi}}{2\mu} + \frac{1}{2}\mu\nu^2\vec{\rho}^2 - \left(\langle S - S_o\rangle + \frac{3}{2}\omega\right) + \sum_{\vec{k}} \tau_{\vec{k}}\, \tau_{\vec{k}} + \sum_{\vec{K}} \omega\, b^+_{\vec{K}} b_{\vec{K}}$$

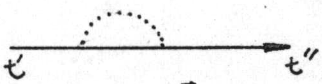
and the perturbed part $\mathbb{R}_1$ takes the form

$$\mathbb{R}_1 = \left(\frac{4\pi\alpha}{V\, 2^{1/2}}\right)^{1/2} \sum_{\vec{k}} \frac{1}{k}\left(\tau_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} + \tau^+_{\vec{k}}\, e^{-i\vec{k}\cdot\vec{r}}\right) - i\left(\frac{4\pi^3 C}{V}\right)^{1/2} \sum_{\vec{K}} \left(\nabla^2_{\vec{K}}\, \delta(\vec{K})\right)^{1/2} \left[b_{\vec{K}}\, e^{i\vec{K}\cdot\vec{r}} + b^+_{K}\, e^{-i\vec{K}\cdot\vec{r}}\right] + \langle S - S_o\rangle \qquad (4.12)$$

and where the conditions that initially and finally in any transformation function the relative coordinate $\vec{\rho}$ and the field $\mathbb{b}_{\vec{k}}$, $\mathbb{b}_{\vec{k}}^{+}$ shall be in their ground state and the $\tau_{\vec{k}}$, $\tau_{\vec{k}}^{+}$ field shall be in the vacuum state have to be imposed.

In principle, the ground energy of the polaron is the lowest eigenvalue of the extended Hamiltonian $\mathbb{R}$, or equivalently, the lowest pole of the Green function $(E-R+i\epsilon)^{-1}$ when $\epsilon \to 0^{+}$. Within Schultz's approximation the transformation function or the matrix element under consideration is $\langle \vec{P}''0;00|E-R+i\epsilon|\vec{P}'0;00\rangle$. Letting $\phi' = |\vec{P}'0\,;00\rangle$ and similarly $\phi'' = |\vec{P}''0;00\rangle$ the transformation from a state ϕ' at time t' to the state ϕ'' at time t'' for the system described by $\mathbb{R}$ becomes $(\phi'', \frac{1}{E-R+i\epsilon}\phi')$.

Now making an approximation corresponding to the diagram



writing $\quad R_1 = \bar{R}_1 + \langle S - S_0 \rangle = \bar{R}_1 + D$,

and $\quad G_E = (E - R_0 + i\epsilon)^{-1}$,

after some mathematical detailed working in operator formalism, it is found that

$$\left(\phi'', \frac{1}{E-R+i\epsilon}\phi'\right) \simeq \left(\phi'', \frac{1}{G_E^{-1}-V(E,\vec{P}')}\phi'\right) \simeq \left(\phi_0(\vec{P}), \frac{1}{E-R_0(\vec{P}')-V(E,\vec{P}')+i\epsilon}\phi_0(\vec{P})\right)\delta(\vec{P}',\vec{P}'') \quad (4.14)$$

in which, generally

$$V(E,\vec{P}) = \langle \phi'' | \bar{R}_1 G_E \bar{R}_1 + D | \phi' \rangle \quad (4.15)$$

has been introduced. Since the effect of V is (expected to be) small and since the excited states of two-particle system lie above the ground state, for most values of α , these states considerably above theenergies of first excited states of the field, all but the ground state of the $\vec{\rho}$-oscillation can be neglected in performing (4.14). In other words this has the effect of replacing $V(E;\vec{P}')$ by

$$\langle 0|V(E,\vec{P}')|0\rangle \equiv V_{00}(E,P')$$, which is spherical in $\vec{P}'$ (4.16)

and similarly for $R_0(\vec{P}')$. Thus (4.14) is now

$$\left(\Phi'', \frac{i}{E-R+i\epsilon}\Phi'\right) \simeq \frac{i}{\langle \hat{P}'0;00|E-R_0+i\epsilon|\hat{P}'0;00\rangle - V_{00}(E-P')} . \tag{4.17}$$

And it follows that the first-order polaron self-energy $E_1(P)$ is determined from the pole of (4.17) when $\epsilon \to 0$:

$$E_1 = E_0(P) + V_{00}(E_1,P) \tag{4.18}$$

where the zeroth-order self energy $E_0(P)$ is defined as

$$E_0(P) \equiv \langle \vec{P}0;00|R_0|\vec{P}0;00\rangle = E_p + \frac{P^2}{2m_0} \tag{4.19}$$

The explicit expression of $V_{00}(E,P)$ is verified to be

$$V_{00}(E,P) = \langle S-S_0\rangle - i\int_0^\infty dt\, e^{-\epsilon t}\int d^3\vec{k}\left[\frac{\alpha}{2\pi^2}\frac{e^{-it}}{k^2} - \frac{c}{2}e^{-i\omega t}\delta(\vec{k})\nabla_{\vec{k}}^2\right]\times$$
$$\times\left[e^{-\left(\frac{M}{m_0}\right)^2\frac{k^2}{2\mu\nu}(1-e^{-i\nu t})} \times e^{i\left(E-\frac{(\vec{P}-\vec{k})^2}{2m_0}-E_g\right)t}\right] \tag{4.20}$$

Defining the first order correction to the polaron energy

$$\Delta E = E_1(P) - E_0(P) = V_{00}(E_1,P), \tag{4.21}$$

and letting $it=\tau$, in terms of ΔE ,

$$V_{00}(E_1,P) = \langle S\rangle - \langle S_0\rangle - \mathcal{S}(\Delta E,P) - \mathcal{S}_0(\Delta E,P) \tag{4.22}$$

where

$$\mathcal{S}(\Delta E,P) \equiv \frac{\alpha}{2\pi^2}\int_0^\infty d\tau\, e^{-(1-\Delta E)\tau}\int d^3\vec{k}\, e^{-\frac{k^2\tau}{2m_0}-\left(\frac{M}{m_0}\right)^2\frac{K}{2\mu\nu}(1-e^{-\nu\tau})} \times e^{-\frac{\vec{P}\cdot\vec{K}\tau}{m_0}} \tag{4.23}$$

and

$$\mathcal{S}_0(\Delta E,P) \equiv -\frac{c}{2}\int_0^\infty d\tau\, e^{(\omega-\Delta E)\tau}\int d^3K\,\delta(\vec{K})\nabla_K^2 e^{-\frac{K^2\tau}{2m_0}-\left(\frac{M}{m_0}\right)^2\frac{K}{2\mu\nu}(1-e^{-\nu\tau})} \times e^{-\frac{\vec{P}\cdot\vec{K}\tau}{m_0}} \tag{4.24}$$

The notation $\mathcal{S}(\Delta E,P)$ and $\mathcal{S}_0(\Delta E,P)$ is reasonable as one can show from (4.23), (4.24) and definitions of $\langle S\rangle$ and $\langle S_0\rangle$ given in (3.28b) and (3.28c) that

$$\mathcal{S}(0,0) = \langle S\rangle \text{ and } \mathcal{S}_0(0,0) = \langle S_0\rangle \tag{4.25}$$

The transcendental equation (4.21) for ΔE or $E_1(P)$ canbe rewritten

$$\Delta E(P) = [\mathcal{S}(0,0) - \mathcal{S}(\Delta E,P)] + [\mathcal{S}_0(0,0) - \mathcal{S}_0(\Delta E,P)] \tag{4.26}$$

Clearly for $P=0$, the solution of (4.26) is $\Delta E=0$, or $V_{00}(E_0,0)=0$, i.e. there is no correction to the Feynman energy at $P=0$, since the term $\langle S-S_0\rangle$ was purposely included in $\mathbb{R}$ to produce first this result.

To calculate the first-order effective mass m_1 it is necessary to expand (4.26) in powers of P^2, noting that ΔE is also a function of P^2, then differentiating with respect to P^2 at $\vec{P}=0$, $\Delta E(P)=0$ gives

$$\left(\frac{\partial \Delta E}{\partial P^2}\right)_{\vec{P}=0} = -\left[\frac{\partial(\mathcal{S}+\mathcal{S}_0)}{\partial \Delta E}\right]_{0,0}\left(\frac{d\Delta E}{dP^2}\right)_{P=0} - \left[\frac{\partial(\mathcal{S}+\mathcal{S}_0)}{\partial P^2}\right]_{0,0}$$

or

$$\left(\frac{\partial \Delta E}{\partial P^2}\right)_{P=0} = \frac{-\left[\dfrac{\partial(\mathcal{S}+\mathcal{S}_0)}{\partial P^2}\right]_{00}}{1+\left[\dfrac{\partial(\mathcal{S}+\mathcal{S}_0)}{\partial \Delta E}\right]_{0,0}} \tag{4.27}$$

Finally, the operation

$$\frac{1}{m_1} = 2\left(\frac{\partial E_1}{\partial P^2}\right) = \frac{1}{m_0} + 2\left(\frac{\partial(\Delta E)}{\partial P^2}\right)_{P=0} \tag{4.28}$$

is readily performed to obtain the first-order effective mass m_1. It is encouraging to compare this result with Feynman expression for the effective mass given by eq. (3.90). In terms of m_0, $\mathcal{S}$ and $\mathcal{S}_0$

$$m^* \equiv m_f = m_0\left[1+2m_0\left(\frac{\partial}{\partial P^2}(\mathcal{S}+\mathcal{S}_0)\right)\right]_{0,0} \tag{4.29}$$

Combination of (4.29), (4.30) and (4.31) yields the relation:

$$m_1 = m_0\left\{1-\left[\frac{m_F}{m_0}-1\right]\left[1+\frac{\partial(\mathcal{S}+\mathcal{S}_0)}{\partial(\Delta E)}\right]^{-1}\right\}. \tag{4.30}$$

For small α

$$\left[\frac{\partial\langle S-S_0\rangle}{\partial(\Delta E)}\right]_{0,0} = O(\alpha)$$

and

$$\frac{m_F}{m_0} - 1 \quad = O(\alpha)$$

so that $\quad m_1 = m_F[1+O(\alpha^2)]$

$$(4.31)$$

which gives the improvement over m_0. Though in this case m_1 never differs from $\overset{*}{m}_F$ by more than 10% it does not agree with $\overset{*}{m}_F$ to first order in α.

For large α, since $\left[\frac{\partial\langle S-S_0\rangle}{\partial(\Delta E)}\right]_{0,0}$ increases from zero rapidly as α increases and $\frac{m_f}{m_0} > 1$ for all α, the inequalities

$$m_0 \leq m_1 \simeq m_0\left[1+\frac{\frac{m_f}{m_0}-1}{1+\left(\frac{\partial(\delta+\delta_0)}{\partial\Delta E}\right)_{0,0}}\right] < m_0\left[1+\left(\frac{m_f}{m_0}-1\right)\right] = m_F$$

are justified. Therefore the correction made by m_1 to m_0 is less than that made by $\overset{*}{m}_F$. Schultz argued that since the difference between m_0 and m_1 is very small one can consider the free propagation of a slow polaron with sufficient accuracy by neglecting quasi-phonon corrections.

IV.2 Marshall-Chawla Method

Considering a polaron in a weak magnetic field, Marshall and Chawla have also computed the ground-state energy and effective mass of the polaron following exactly the same technique used by Feynman in Chapter III. Their calculation (of the effective mass) is based upon still another definition which is equivalent to the free polaron effective mass as defined by Fröhlich. In this section we shall outline the major steps of this approach and present only the final results so obtained.

Marshall and Roberts (unpublished) have pointed out that the exact ground state energy of a polaron in a weak magnetic field $\vec{H}$ can be expanded in powers of a magnetic field strength H as

$$E_g(\alpha,H) = E(\alpha) + \frac{1}{2}\overset{*}{m}_{MS}(\alpha)^{-1}H + O(H^2) \,. \qquad (4.33)$$

The zeroth-order term gives exactly the polaron self-energy while the first-order term determines the inverse of the polaron effective mass. To obtain both quantities one must evaluate $E_g(\alpha,H)$ which is, according to Feynman's path-integral formalism,

$$E_g(\alpha,H) = -\lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \ln\left[\int e^{S}\mathcal{D}\vec{r}(t)\right]. \qquad (4.34)$$

all paths $\vec{r}(t)$ satisfying the boundary conditions $\vec{r}(0)=\vec{r}(\mathcal{T})=0$. If the uniform magnetic field (applied in $\hat{z}$-direction) is defined by the vector potential

$$\vec{A} = \vec{H}\wedge\hat{x} \qquad (4.35)$$

the polaron action in this case is then

$$S = \int_0^{\mathcal{T}}\left(-\frac{\dot{\vec{r}}^2}{2}+iHy\dot{x}\right)dt + 2^{-\frac{3}{2}}\alpha\int_0^{\mathcal{T}}\int_0^{\mathcal{T}} e^{-|t-s|}\left[\vec{r}(t)-\vec{r}(s)\right]^{-1}dt\,ds. \qquad (4.36)$$

including the additional term due to the magnetic field. Following Feynman method, the imaginary term in S need to be reconsidered by replacing the time variable t by $-it$

The corresponding trial action turns to

$$S_o = \int_0^{\mathcal{T}}\left(-\frac{\dot{\vec{r}}}{2}+iHy\dot{x}\right)dt - \frac{C}{2}\int_0^{\mathcal{T}}\int e^{-\omega|t-s|}\left[\vec{r}(t)-\vec{r}(s)\right]^2 dt\,ds \qquad (4.37)$$

Similarly to Chapter III

$$E(\alpha,H) = E_o(\alpha,H) - \lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}\langle S-S_o\rangle_{S_o} = E_o(\alpha,H) - \langle S\rangle + \langle S_o\rangle \qquad (4.38)$$

where $E_0(\alpha, H)$, $\langle S \rangle$ and $\langle S_0 \rangle$

take the same form as given in sec. III.2.

The real advantage of this approach arises from the fact that for a sufficiently weak magnetic field, the inequality

$$E_0(\alpha, H) \leq E(\alpha, H) \qquad (4.39)$$

still holds[16] and this indicates that an extension of Feynman's variational principle for this case is still applicable.

Evaluation of the key quantity $\langle e^{i\vec{k}(\vec{r}_\tau - \vec{r}_\sigma)} \rangle$, which in turn renders $\langle S \rangle$, $\langle S_0 \rangle$ and $E_0(\alpha, H)$, is then proceeded in the same manner as that of Feynman except that the three rectangular components $\bar{x}(t)$, $\bar{y}(t)$ and $\bar{z}(t)$ of the classical path $\bar{\vec{r}}(t)$ involved have to be solved separately. The resulting integrodifferential equations for these components are found to be

$$\ddot{\bar{x}}(t) = 2C\int_0^{\mathcal{T}} e^{-\omega|t-s|}[\bar{x}(t) - \bar{x}(s)]ds + iH\dot{\bar{y}} - f_x, \qquad (4.40a)$$

$$\ddot{\bar{y}}(t) = 2C\int_0^{\mathcal{T}} e^{-\omega|t-s|}[\bar{y}(t) - \bar{y}(s)]ds - iH\dot{\bar{x}} - f_y, \qquad (4.40b)$$

$$\ddot{\bar{z}}(t) = 2C\int_0^{\mathcal{T}} e^{-\omega|t-s|}[\bar{z}(t) - \bar{z}(s)]ds - f_z. \qquad (4.40c)$$

In the limit $\mathcal{T} \to \infty$, the above equations may be solved by the Fourier transform method. Substitution of $\bar{x}$, $\bar{y}$, $\bar{z}$ thus obtained finally yields

$$\langle e^{i\vec{k}\cdot(\vec{r}_\tau - \vec{r}_\sigma)} \rangle = e^{\frac{1}{2}\int_0^{\mathcal{T}} \vec{f}\cdot\bar{\vec{r}}(t)dt}$$

$$= \exp.[(k_x^2 + k_y^2)G_{xx}(|\tau-\sigma|) + k_z^2 G_{zz}(|\tau-\sigma|) \qquad (4.41)$$

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16 See Reference (6) Appendix.

in which

$$G_{xx}(|\tau-\sigma|) = G_{zz}(|\tau-\sigma|) + \frac{1}{4} H(\tau-\sigma)^2 \omega^4 \nu^{-4} + O(H^2) \tag{4.42a}$$

and

$$G_{zz}(|\tau-\sigma|) = -\frac{1}{2}\nu^{-2}\left[\nu^{-1}(\nu^2-\omega^2)(1-e^{-\nu|\tau-\sigma|}) + \omega^2|\tau-\sigma|\right]. \tag{4.42b}$$

Making use of (4.41) leads to all other required quantities

$$\langle S\rangle = \lim_{T\to\infty} \alpha T^{-1} 2^{-\frac{3}{2}} \int_0^{\mathcal{T}}\int_0^{\mathcal{T}} e^{-|\tau-\sigma|} \int (2\pi^2 k^2)^{-1} \langle e^{i\vec{k}.(\vec{r}_\tau-\vec{r}_\sigma)}\rangle d^3\vec{k}\, d\tau\, d\sigma$$

$$= \alpha \pi^{-\frac{1}{2}} \nu \int_0^\infty [F(\tau)]^{-\frac{1}{2}} e^{-\tau} d\tau + \frac{1}{6} H \alpha \pi^{-\frac{1}{2}} \frac{\omega^4}{\nu} \int_0^\infty [F(\tau)]^{-3/2} \tau^2 e^{-\tau} d\tau + O(\alpha^2) \tag{4.43}$$

$$\langle S_0\rangle = \lim_{T\to\infty} \frac{c}{2} \mathcal{T}^{-1} \int_0^{\mathcal{T}}\int_0^{\mathcal{T}} e^{-\omega|\tau-\sigma|} \left[-\nabla_{\vec{k}}^2 \langle e^{i\vec{k}.(\vec{r}_\tau-\vec{r}_\sigma)}\rangle\right]_{\vec{k}=0} d\tau\, d\sigma$$

$$= \frac{3}{4}\nu^{-1}(\nu^2-\omega^2) - \frac{1}{2} H\omega^2\nu^{-4}(\nu^2-\omega^2) + O(H^2) \tag{4.44}$$

and

$$E_0(\alpha,H) = \frac{1}{2}H + \int_0^c c^{-1}\langle S_0\rangle\, dc$$

$$= \frac{3}{2}(\nu-\omega) + \frac{1}{2} H\omega^2\nu^{-2} + O(H^2) \tag{4.45}$$

where

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

$$\nu^2 = \omega^2 + \frac{4c}{\omega}$$

Recalling (4.38) & (4.39) the equations (4.43), (4.44) together with (4.45) give precisely the upper-bound energy $E(\alpha,H)$. Equating this $E(\alpha,H)$ to $E(\alpha)+\frac{1}{2}\mu(\alpha)^{-1}H+O(H^2)$ one obtains the self-energy

$$E(\alpha) \equiv E_F(\alpha) = \frac{3}{4\nu}(\nu-\omega)^2 - \pi^{-\frac{1}{2}}\alpha\nu\int_0^\infty \left[\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu\tau})+\omega\tau\right]^{-\frac{1}{2}} e^{-\tau}d\tau \tag{4.47}$$

and the effective mass

$$\overset{*}{m}_{MS}(\alpha) = \left[1-(1-\frac{\omega^2}{\nu^2})^2-\frac{1}{3}\alpha\pi^{-\frac{1}{2}}\frac{\omega^4}{\nu}\int_0^\infty [F(\tau)]^{-\frac{3}{2}}\tau^2 e^{-\tau}d\tau\right]^{-1} \tag{4.48}$$

where the optional values of parameters ν and ω to be employed are just those which minimize $E_F(\alpha)$

For small α

$$\overset{*}{m}_{MS} = 1+\frac{1}{6}\alpha+\frac{73}{2916}\alpha^2+O(\alpha^3). \tag{4.49}$$

Comparing with

$$\overset{*}{m}_F(\alpha) = 1+\frac{1}{6}\alpha+\frac{72}{2916}\alpha^2+O(\alpha^3),$$

the difference is extremely small.

For large α,

$$\nu = \frac{4}{9\pi}\alpha^2+O(\alpha^0)\,; \quad \omega = 1+O(\alpha^{-2}) \,,$$

$$\overset{*}{m}_{MS}(\alpha) \sim m_F(\alpha) = \frac{16\alpha^4}{81\pi^2}+O(\alpha^2) \tag{4.50}$$

IV.3 The Polaron Action at Finite Temperatures

We now extend our study to the polaron problem in general state, i.e., we intend to examine the behavior of the electron-lattice system at arbitrary temperatures through the corresponding action. In this situation effects of the thermodynamic properties of the system arise from the interaction between a large number of electrons and the phonon system.

Assuming that there are no direct interactions of electrons with one another and the interaction of each electron with its surrounding lattice is independent of the presence and interaction of other electrons with the lattice, the partition function for this system has been obtained by Krivoglaz-Pekar[17] and independently by Osaka[18] by means of ordered-operation method. This can also be done simply by making use of Feynman's path integrations provided in sec. III.1.

We have realized from sec. II.3 that giving a transformation $\langle \vec{r}''t'' | \vec{r}'t' \rangle$ for any system the density matrix of the system $\rho(\vec{r}''\vec{r}';\beta)$ for the canonical ensemble at temperature $T = \frac{1}{k_B \beta}$ is easily obtained by the relation

$$\rho(\vec{r}''\vec{r}';\beta) \equiv \langle \vec{r}'' | \rho | \vec{r}' \rangle = \langle \vec{r}'', t' - i\beta | \vec{r}' t' \rangle , \qquad (4.51)$$

and the partition function

$$Z = \int d\vec{r} \langle \vec{r}, -i\beta | \vec{r}\, 0 \rangle \qquad (4.52)$$

where we have set $t' = 0$.

For our electron-lattice system, dealing with the imaginary time $\tau = it$ etc. Z becomes separable as

$$Z_{tot} = \int d^3\vec{r}' \int_{\vec{r}' \to \vec{r}'} \mathcal{D}\vec{r}(\tau)\, e^{-\frac{1}{2}\int_0^\beta \left(\frac{d\vec{r}}{d\tau}\right)^2 d\tau} \prod_{\vec{k}} \int dQ_{\vec{k}} \langle Q_{\vec{k}} \beta | Q_{\vec{k}} 0 \rangle_{\gamma_{\vec{k}}(\tau)} , \qquad (4.53)$$

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17 See Reference (7) P. 21

18 Yukio Ōsaka, "Polaron State at a Finite Temperature.", Progress of Theoretical Physics, 22 (1959) 437.

$$Z_{tot} = \int d^3\vec{r}' \int_{\vec{r}' \to \vec{r}'} \mathcal{D}\vec{r}(\tau) e^{-\frac{1}{2}\int_0^\beta \left(\frac{d\vec{r}}{d\tau}\right)^2 d\tau} \prod_{\vec{k}} \int dQ_{\vec{k}} \langle Q_{\vec{k}}\beta | Q_{\vec{k}} 0\rangle_{\gamma_{\vec{k}}(\tau)} , \tag{4.53}$$

Making use of the expression for the propagator of the forced harmonic oscillator derived in sec. II.2

$$\langle Q_{\vec{k}}\beta / Q_{\vec{k}} 0\rangle_{\gamma_{\vec{k}}(\tau)} = \left(\frac{M_f\omega_L}{2\pi \sinh\beta\omega_L}\right)^{\frac{1}{2}} \exp\left\{-\frac{M_f\omega_L}{2\sinh\beta\omega_L}\left[2(\cosh\beta\omega_L - 1)Q_{\vec{k}}^2 - \right.\right.$$

$$- \frac{2Q_{\vec{k}}}{M_f\omega_L}\int_0^\beta d\tau\, \gamma_{\vec{k}}(\tau)\left(\sinh\omega_L\tau + \sinh\omega_L(\beta-\tau)\right) -$$

$$\left.\left. - \frac{2}{(M_f\omega_L)^2}\int_0^\beta d\tau \int_0^\tau d\sigma\, \gamma_{\vec{k}}(\tau)\gamma_{\vec{k}}(\sigma)\sinh\omega_L\tau \sinh\omega_L(\beta-\sigma)\right]\right\}. \tag{4.54}$$

Performing the Gaussian integral on $\vec{k}$ the trace of the $\vec{k}$ th oscillator is finally

$$\int dQ_{\vec{k}} \langle Q_{\vec{k}}\beta / Q_{\vec{k}} 0\rangle_{\gamma_{\vec{k}}(t)} = \left(2\sinh\frac{\beta\omega_L}{2}\right)^{-1} \exp\left\{\frac{1}{2M_f\omega_L}\int_0^\beta\int_0^\tau \gamma_{\vec{k}}(\tau)\gamma_{\vec{k}}(\sigma) \times \right.$$

$$\left. \times\left[\bar{n}\, e^{\omega_L(\tau-\sigma)} + (\bar{n}+1)\, e^{-\omega_L(\tau-\sigma)} d\tau d\sigma\right]\right\} , \tag{4.55}$$

where the definition for the average number of phonons in $\vec{k}$ th mode

$$\bar{n} = \frac{1}{e^{\omega_L\beta} - 1}$$

has been employed. Clearly, if we set $\bar{n} = 0$ the propagator is reduced to the transformation function from ground state to ground state. Substituting (4.55) into (4.53), performing the integration over $\vec{r}'$, since the path integral is independent of $\vec{r}'$, the integration yields first the volume V, and we have

$$Z_{tot} = Z_{ph} \cdot V \int \mathcal{D}\vec{r}(\tau)\, e^{-\frac{1}{2}\int_0^\beta \left(\frac{d\vec{r}}{d\tau}\right)^2 d\tau} \exp\left\{\frac{1}{2M_f\omega_L} \int\int^{\beta\ \tau} \sum_{\vec{k}} \gamma_{\vec{k}}(\tau)\gamma'_{\vec{k}}(\sigma) \times \right.$$
$$\times \left[\bar{n}e^{\omega_L(\tau-\sigma)} + (\bar{n}+1)e^{-\omega_L(\tau-\sigma)}\right] \quad (4.56)$$

where $Z_{ph} = \left(2\sinh\frac{\beta\omega}{2}\right)^{-N}$ is merely the partition function for the system of phonons alone.

Recalling the definition of α and the result of $\sum_{\vec{k}} \gamma_{\vec{k}}(\tau)\gamma_{\vec{k}}(\sigma)$, Z_{tot} is finally

$$Z_{tot} = Z_{ph} V \int \mathcal{D}\vec{r}(t) \exp\left\{-\frac{1}{2}\int_0^\beta \left(\frac{d\vec{r}}{d\tau}\right)^2 d\tau + \frac{\alpha}{2^{3/2}} \int_0^\beta\int_0^\beta d\tau\, d\sigma \times \right.$$
$$\left. \times \frac{\left[\bar{n}e^{|\tau-\sigma|} + (\bar{n}+1)e^{-|\tau-\sigma|}\right]}{|\vec{r}(\tau)-\vec{r}(\sigma)|}\right\}, \quad (4.57)$$

where again we have set $\omega_L = 1$.

Consequently, the polaron action at finite temperatures is explicitly,

$$S = -\frac{1}{2}\int_0^\beta \left(\frac{d\vec{r}}{dt}\right)^2 dt + \frac{\alpha}{2^{3/2}}\left\{\frac{e^\beta}{e^\beta - 1}\int_0^\beta\int_0^\beta dt\,ds\, \frac{e^{-|t-s|}}{|\vec{r}(t)-\vec{r}(s)|} + \frac{1}{e^\beta - 1}\int_0^\beta\int_0^\beta \frac{e^{|t-s|}}{|\vec{r}(t)-\vec{r}(s)|}\, dt\,ds\right\},$$
$$(4.58)$$

in which the phonon variable is no longer appear. In terms of electron's position S manifests the electron in the coulomb potential with the energy depending upon the average number of phonons.

IV.4 Krivoglaz-Pekar Approach

Krivoglaz and Pekar have proposed another effective approach to the polaron at finite temperatures. Instead of dealing with wave functions or other characteristic functionals of the polaron, they worked the results out in operator formalism by means of a so-called "method of traces" accompanied with an ordered-operator calcution introduced earlier by Feynman. However, trying not to go beyond the path-integral formalism, we shall present here principal ideas of this method and concentrate on the various limiting results of the polaron effective mass.

Krivoglaz and Pekar generally considered a system consisting of a crystal and a conduction electron described by the Hamiltonian, in operator form,

$$\mathbb{H} = -\frac{\hbar^2}{2m_{eff}}\vec{\nabla} + \sum_{\vec{k}} \hbar\omega_{\vec{k}} a^{+}_{\vec{k}} a_{\vec{k}} + \sum_{\vec{k}} \left(V_{\vec{k}} a_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + V^{*}_{\vec{k}} a^{+}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \right) \qquad (4.59)$$

To obtain the self-energy and the effective mass of the system in principle, it is necessary to evaluate precisely the trace of the operator $e^{-\beta\mathbb{H}}$. After the elimination of vibrational degree of freedom of the system by ordering the operators involved in $\mathbb{H}$, this quantity is left with the operator depending on the electron's position $\vec{r}$ only and is denoted by

$$Z \equiv \mathrm{sp.}\, e^{-\beta\mathbb{H}} = \mathrm{sp.}\, \mathbb{L}(\vec{r}) \qquad (4.60)$$

The difficulty in calculating $sp.\mathbb{L}(\vec{r})$ comes from the fact that it is not "disentangled" without restriction of the coupling constant to be weak. To avoid this the approximation is then made to $\mathbb{H}$ and the appropriate variational principle has to be imposed.

Krivoglaz and Pekar have proved a theorem stating that:

If

$$I = sp.e^{\int_0^{\lambda} A_{\lambda_1} d\lambda_1 + s\int_0^{\lambda} B_{\lambda_1} d\lambda_1} \equiv sp.e^{P} e^{sQ}, \qquad (4.61)$$

where A and B are self-conjugate operators, λ_1 is an ordering index and s is an arbitrary parameter, introducing a certain average, defined by

$$\lambda\bar{B} = \frac{sp.\{e^P Q\}}{sp.\ e^P} \equiv \bar{Q}$$

and letting

$$I_1 = sp.e^{P} e^{s\bar{Q}},$$

then

$$I \geqslant I_1 .$$

In according with this theorem

$$Z \geqslant Z_1 = Z' e^{\bar{\mathcal{G}}-\bar{\mathcal{G}}_0}$$

where
$$Z' \equiv e^{-\beta \mathbb{H}'} = sp\,\mathbb{L}'(\vec{r})$$

Here the effect of atomic vibrations on the electron is approximated by the attraction of a second particle whose system is represented by the Hamiltonian

$$\mathbb{H}' = -\frac{\hbar^2}{2m_{eff}}\vec{\nabla} - \frac{\hbar^2}{2M}\vec{\nabla}_2 + \frac{\mathcal{K}}{2}(\vec{r}-\vec{r}_2)^2, \qquad (4.64)$$

and the average $\bar{\mathcal{G}}$ and $\bar{\mathcal{G}}_0$ in (4.62) are derived to be:

$$\bar{\mathcal{G}}_{\vec{k}} = \frac{|V_{\vec{k}}|^2}{Z'}\left(\frac{dZ''}{d|V_{\vec{k}}|^2}\right)_{|V_{\vec{k}}|^2=0}$$

$$\bar{\mathcal{G}} = -3\ln\left(2\sinh\frac{\beta}{2}\hbar\omega\right)+\frac{\varkappa}{Z'}\left(\frac{\partial Z'}{\partial\varkappa}\right)_{\omega=\text{constant}}.$$

To reduce the complexity in computing $\bar{\mathcal{G}}$, the additional Hamiltonian $\mathbb{H}''$ has been constructed and this gives rise to Z'' as can be visualized in (4.65). It is just

$$\mathbb{H}'' = \mathbb{H}' - \frac{\hbar^2}{2m_{eff}}\frac{\partial^2}{\partial x_3^2} + m_{eff}\frac{\omega^2_{\vec{k}}}{2}x_3^2 + V_{\vec{k}}\,d_3 e^{i\vec{k}\cdot\vec{r}} + V^*_{\vec{k}}\,d_3^+ e^{-i\vec{k}\cdot\vec{r}} \qquad (4.67)$$

a transition of $\mathbb{H}'$ given by (4.64). This can be thought of as equivalent to the addition of a third particle undergoing one-dimensional harmonic oscillations of frequency $\omega_{\vec{k}}$ about a fixed equilibrium position and having an infinitesimally weak interaction with the first particle. Here d_3 and d_3^+ are annihilation and creation operators for the oscillation quanta of this third particle.

The problem is thus turned to the mathematical manipulation of Z', $\bar{\mathcal{G}}$ and $\bar{\mathcal{G}}_0$. The final results comes out as

$$Z \geqslant Z_1 = Z^{(0)}\left(\frac{\nu}{\omega}\right)^3\left(\frac{\sinh\frac{\beta\hbar\omega}{2}}{\sinh\frac{\beta\hbar\nu}{2}}\right)\times\exp\left\{\frac{3}{4}\beta\hbar\omega\,\frac{\nu^2-\omega^2}{\omega\nu}\coth\frac{\beta\hbar\nu}{2}-\frac{3}{2}\frac{\nu^2-\omega^2}{\nu^2}+\bar{\mathcal{G}}\right\} \qquad (4.68)$$

in which

$$\bar{\mathcal{G}} = \frac{\beta^2}{2}\sum_{\vec{k}}|V_{\vec{k}}|^2\int_0^1 d\left(1-\frac{2}{\beta}\tau\right)e^{-\frac{\beta\hbar\varkappa^2}{8m_0}\left(1-\left(1-\frac{2}{\beta}\tau\right)^2\right)}\frac{\cosh\frac{\beta\hbar\omega}{2}\vec{k}\left(1-\frac{2}{\beta}\tau\right)}{\sinh\frac{\beta\hbar\omega}{2}\vec{k}}\times$$

$$\times\exp\left\{-\frac{1}{2}\frac{M\hbar\varkappa^2}{m_0 m_{eff}\nu}\left(\frac{\coth\frac{\beta\hbar\nu}{2}-\cosh\frac{\beta\hbar\nu}{2}\left(1-\frac{2}{\beta}\tau\right)}{\sinh\frac{\beta\hbar\nu}{2}}\right)\right\} \qquad (4.69)$$

and

$$Z^{(0)} = 2V\prod_{\vec{k}}\left(1-e^{-\beta\hbar\omega_{\vec{k}}}\right)^{-1}. \qquad (4.70)$$

Specially, for the Fröhich polaron

$$\omega_{\vec{k}} = \omega_L \quad ; \quad V_{\vec{k}} = \frac{i}{|\vec{k}|}\left(\frac{\sqrt{2}\,\pi\alpha}{V}\right)^{\frac{1}{2}}$$

setting as before:

$$\omega_L = \hbar = m_{eff} = 1 ,$$

one easily deduces from (4.68)

$$\ln Z_1 = \ln Z^{(0)} + 3\ln\frac{\nu}{\omega} - 3\ln\sinh\frac{\beta\nu}{2} + 3\ln\sinh\frac{\beta\omega}{2} - \frac{3}{2} + \frac{3\omega^2}{2\nu^2} + \frac{3}{2}\,\frac{\nu^2-\omega^2}{\omega\nu}\,\frac{\beta\omega}{2}\coth\frac{\beta\nu}{2} +$$

$$+ \frac{\beta^{3/2}}{\pi^{\frac{1}{2}}\sinh\frac{\beta}{2}}\,\alpha\,\frac{\nu}{\omega}\int_0^1 \frac{\cosh\frac{\beta}{2}\left(1-\frac{2}{\beta}\tau\right)d\left(1-\frac{2}{\beta}\tau\right)}{\sqrt{1-\left(1-\frac{2\tau}{\beta}\right)^2 + \frac{2(\nu^2-\omega^2)}{\frac{\beta\omega^2\nu}{2}}\left[\coth\frac{\beta\nu}{2} - \frac{\cosh 3\nu\left(1-\frac{2}{\beta}\tau\right)}{\sinh\frac{\beta\nu}{2}}\right]}} \qquad (4.71)$$

for arbitrary coupling constants α and temperatures $\frac{1}{k_B\beta}$, where the parameters ν and ω have to be varied so as to maximize $\ln Z_1$

At low temperature i.e. $T \to 0$, $\beta \to \infty$ eq. (4.71) reduces to

$$\ln Z_1 = \ln Z^{(0)} + 3\ln\frac{\nu}{\omega} - \frac{3}{4}\beta\frac{\omega^2}{\nu}\left(\frac{\nu}{\omega}-1\right)^2 - \frac{3}{2} + \frac{3}{2}\frac{\omega^2}{\nu^2} +$$

$$+ \frac{2}{\pi^{1/2}}\cdot\frac{\beta}{2}\,\alpha\,\frac{\nu}{\omega}\int_0^\infty e^{-\tau}d\tau\left[\frac{\nu^2-\omega^2}{\nu^2}\left(1-e^{-\nu\tau}\right) + \tau\left(1-\frac{\tau}{\beta}\right)\right]^{-\frac{1}{2}} \qquad (4.72)$$

for arbitrary coupling constants α .

The states accessible to the polaron at very low temperatures are those with small momenta in which any internal degrees of freedom are not excited. If the energy distribution of the system is of the form

$$E = \varepsilon_0 + \varepsilon_2 P^2 + \varepsilon_4 P^4 + \cdots\cdots \tag{4.73}$$

where P is the total momentum of the system, then the polaron effective mass

$$m^*_{KP} = \frac{1}{2\varepsilon_2}$$

is introduced. Expression of $\ln Z$ in powers of β, gives

$$\ln Z = \ln Z^{(0)} - \beta(\varepsilon_0 - E^{(0)}) + \frac{3}{2}\ln m^*_{KP} - \frac{15\, m^*_{KP}}{\beta}\varepsilon_4 + \cdots\cdots, \tag{4.74}$$

where $Z^{(0)}$ is the partition function for the entire non-interacting electron-phonon system and $E^{(0)}$ is the non-interacting ground state energy. Noting that in this way the polaron effective mass is defined implicitly in the β-independent term. Therefore if one expands $\ln Z_1$ in powers of $\frac{1}{\beta}$ and identifies various powers of β with the corresponding terms in (4.74), the effective mass is then determined. Expanding $\ln Z_1$ in powers of $\frac{1}{\beta}$ one finds that

$$\ln Z_1 = \ln Z^{(0)} + \beta\left(f_0 + \frac{f_1}{\beta} + \frac{f_2}{\beta} + \cdots\cdots\right), \tag{4.75}$$

and

$$f_1 = 3\ln\frac{\nu}{\omega} - \frac{3}{2} + \frac{3}{2}\frac{\omega^2}{\nu^2} + \frac{\alpha}{2\pi^{1/2}}\left(\frac{\nu}{\omega}\right)\int_0^\infty \tau^2 e^{-\tau}\left[\frac{\nu^2-\omega^2}{\nu^2}(1-e^{-\nu\tau}) + \tau\right]^{-\frac{3}{2}} d\tau. \tag{4.76}$$

Comparing (4.75) with (4.75) one obtains

$$m^*_{KP} = e^{\frac{2}{3}f_1}$$

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

$$\frac{m^*_{KP}}{\frac{\nu^2}{\omega^2}} = \exp\left\{\frac{\omega^2}{\nu^2}\left[1 + \frac{\alpha}{3\pi^{1/2}}\nu^3\int_0^\infty \tau^2 e^{-\tau}\left[\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu\tau}) + \omega^2\tau\right]^{-3/2} d\tau\right] - 1\right\}. \tag{4.77}$$

Recalling (3.90), rearranging of (4.77) reveals

$$\frac{\overset{*}{m}_{KP}}{\nu^2/\omega^2} = \exp\left\{\frac{\overset{*}{m}_F}{\nu^2/\omega^2} - 1\right\} \geqslant \overset{*}{m}_F ,$$

the relation between the Feynman's effective mass and

At low temperatures and weak coupling, basing on the two equations $\frac{\partial \ln Z_1}{\partial \nu}=0$ and $\frac{\partial \ln Z_1}{\partial \omega}=0$, the appropriate value of ν and ω are estimated in the same manner as proceeded by Feynman in chapter III. The asymptotic expression for $\ln Z_1$: is then

$$\ln Z_1 = \ln Z^{(0)} + \beta\alpha\left[1+\frac{1}{4\beta}+\frac{9}{32\beta^2}\right] + \frac{\beta\alpha^2}{81}\left[1+\frac{4}{3\beta}+\frac{2034}{\beta^2}\right] , \qquad (4.79)$$

which renders

$$\overset{*}{m}_{KP} = 1+\frac{\alpha}{6}+0.0249\alpha^2 , \quad \omega = 3 . \qquad (4.80)$$

At low temperatures and strong coupling, $\beta\nu \gg 1$ and $\frac{\nu}{\omega} \gg 1$, one can approximate

$$\ln \sinh\frac{\beta\nu}{2} \simeq \frac{\beta\nu}{2} - \ln 2 ,$$

$$\coth\frac{\beta\nu}{2} = 1 , \quad \frac{\coth\frac{\beta\nu}{2}\left(1-\frac{2}{\beta}\tau\right)}{\sinh\frac{\beta\nu}{2}} \simeq e^{-\nu\tau} ,$$

and expand the integral term of (4.71) in power of first expression under the radical sign to obtain

$$\ln Z_1 = \ln Z^{(0)} + 3\ln\frac{\nu}{\omega} - \frac{3}{2}\cdot\frac{\beta}{2}\omega\left(\frac{\nu}{\omega}+\frac{\omega}{\nu}\right) + 3\ln 2 + 3\ln\sinh\frac{\beta\omega}{2} - \frac{3}{2} + \frac{3\omega^2}{2\nu^2} +$$
$$+ \frac{2}{\pi^{1/2}}\frac{\beta}{2}(\nu)^{\frac{1}{2}}\left[1+\frac{2\ln 2\coth\frac{\beta}{2}}{\nu} - \frac{\omega^2}{\beta\nu}\left(\frac{\beta}{2}\coth\frac{\beta}{2}-1\right)\right]\alpha . \quad (4.81)$$

The extremum of $\ln Z_1$ occurs when

$$\omega = 1+\ldots\ldots\ldots , \quad \frac{\nu}{\omega} = \frac{4}{9\pi}\alpha^2+\ldots\ldots\ldots \qquad (4.82)$$

On substitution of (4.82) into (4.81), one has

$$\ln Z_1 = \ln Z^{(0)} + 3\ln\frac{4\alpha^2}{9\pi} + \frac{\alpha^2}{3\pi}\beta + 3\beta\left(\ln 2+\frac{1}{4}\right) + \varphi(\beta) \quad (4.83)$$

and this in turn gives

$$\overset{*}{m}_{KP} = \overset{*}{m}_F = \left(\frac{\nu}{\omega}\right)^2 = \left(\frac{4\alpha^2}{9\pi}\right)^2 = \frac{16}{81\pi^2}\alpha^4 = 200\times10^{-4}\alpha^4 \qquad (4.84)$$

IV.5 Hellwarth-Platzman Method.

An extension of Feynman's path integral variational calculation of the polaron problem has been employed by Hellwarth and Platzman[19] to investigate the polaron properties at arbitrary temperatures under an applied uniform magnetic field $\vec{H}$. This approach concerns with an attempt to find an approximate expression for the free energy of the polaron in a static magnetic field. The explicit form of the result is given in terms of a model system with a two-parameter action functional S_0 instead of the actual action S , then the variational method is imposed to achieve the optimal result obtained by this approach can be derived for any values of the field, temperature and coupling constant. Practically, however, various limiting cases have been worked out.

Now let us go through some important steps of this method. Studying of sec. IV.2 and V.3 manifests that the appropriate action of the polaron at arbitrary temperature $\frac{1}{k_0\beta}$ in a magnetic field $\vec{H}$ applied in $\hat{z}$ -direction should take the form

$$S = -\int_0^\beta \left[\frac{1}{2}\left(\frac{d\vec{r}(t)}{dt}\right)^2 + iHy(t)\dot{x}(t)\right] + \frac{\alpha}{2^{3/2}}\int\frac{d^3k}{2\pi^2k^2}\int_0^\beta dt\int_0^\beta ds \times$$

$$\times\, e^{i\vec{k}\cdot[\vec{r}_t-\vec{r}_s]}\left[(\bar{n}+1)e^{-\omega_{\vec{k}}|t-s|} + \bar{n}e^{\omega_{\vec{k}}|t-s|}\right] \qquad (4.85)$$

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19 See Reference (8)

where $\bar{n} = \frac{1}{e^{\beta\omega_{\vec{k}}}-1}$.

If we let $H=0$, $\beta=\infty$, $\omega_{\vec{k}}=0$ eq. (4.86) reduces to the action of the polaron at ground state in absence of a magnetic field as used by Feynman. The approximate free energy F of the problem is given by

$$e^{-\beta F} = \int \mathcal{D}\vec{r}(t)\, e^{S[\vec{r}(t)]}$$

$$\simeq e^{\langle S-S_o\rangle}\int \mathcal{D}\vec{r}(t)\, e^{S_o[\vec{r}(t)]} \qquad (4.86)$$

where we have defined the average of $\langle A\rangle$ to be taken with the weighing function S_o

$$\langle A\rangle = \int \mathcal{D}\vec{r}(t)\, A[\vec{r}(t)]\, e^{S_o} \Big/ \int \mathcal{D}\vec{r}(t)\, e^{S_o}. \qquad (4.87)$$

Hellwarth and Platzman introduced a somewhat general trial action S_o to be employed in (4.86) as

$$S_o = -\int_0^\beta \left[\frac{1}{2}\left(\frac{d\vec{r}}{dt}\right)^2 + iHy(t)\dot{x}(t)\right]dt - \frac{1}{2}\gamma\int_0^\infty \delta W\, C(W)\int_0^\beta dt\int_0^\beta ds[\vec{r}(t)-\vec{r}(s)]\times$$

$$\times\left[(\bar{W}+1)\, e^{-W|t-s|} + \bar{N}\, e^{W|t-s|}\right], \qquad (4.88)$$

in which $\bar{N} = \frac{1}{e^{\beta W}-1}$ and γ and W are adjustable parameters

It follows from (4.86)

$$F \simeq F_o - \langle S_o\rangle - \langle S\rangle \qquad (4.89a)$$

where we have defined

$$F_o = -\frac{1}{2\beta}\ln\int \mathcal{D}\vec{r}(t)\, e^{S_o} \qquad (4.89b)$$

$$\langle S_o\rangle = \frac{1}{2\beta}\gamma\int_0^\beta dt\int_0^\beta ds\, C(W)\, dW\left[(\bar{N}+1)e^{-W|t-s|} + \bar{N}e^{W|t-s|}\right]\times$$

$$\times\langle(\vec{r}_t - \vec{r}_s)^2\rangle \qquad (4.89c)$$

$$\langle S \rangle = \frac{1}{\beta}\frac{\alpha}{2^{3/2}}\int \frac{d^3\vec{k}}{2\pi^2 k^2}\int_0^\beta ds\left[(\bar{n}+1)\, e^{-w_{\vec{k}}|t-s|} + \bar{n}\, e^{w_{\vec{k}}|t-s|}\right] \langle e^{i\vec{k}\cdot(\vec{r}_t-\vec{r}_s)} \tag{4.89 d}$$

Making use of the formula

$$\int \mathcal{D}\bar{x}(t) \exp\left[i\int_0^\beta x(t) f(t)\, dt - \frac{1}{2}\int_0^\beta dt \int_0^\beta ds\, a(t-s)\right.$$
$$= N \exp\left[-\frac{1}{2}\int_0^\beta dt \int_0^\beta ds\, f(t) f(s)\, a^{-1}(t-s)\right) \tag{4.90}$$

which is valid for $x(0)=x(\beta)$, $a(0)=a(\beta)$ and where $a(t-s)$ is an operator with positive nonzero eigenvalues with a well-defined inverse $a^{-1}(t-s)$, the resulting expression for F_0 is found to be

$$\beta F_0 = \frac{3}{2}\sum_{n=-\infty}^{+\infty} \ln(b_n) + \frac{1}{2}\sum_{n=-\infty}^{+\infty} \ln\left(1+W_n^2 H^2/b_n^2\right), \tag{4.91}$$

where

$$b_n = W_n^2 + 4\gamma\int_0^\infty dW \cdot c(W)\, W^{-1}\left[\frac{W_n^2}{(W_n^2+W)}\right]. \tag{4.92}$$

Once F_0 is calculated, $\langle S_0\rangle$ is easily obtained by the relation:

$$\langle S_0 \rangle = \gamma \frac{\partial F_0}{\partial \gamma}, \tag{4.93}$$

as can be verified from (4.89b), (4.89c) and (4.87)

Performing the differentiation of F_0, eq. (4.93) shows

$$\langle S_0 \rangle = \frac{3}{2}\gamma\beta^{-1}\sum_n\left[\frac{c_n}{b_n} - \frac{3}{2}\gamma W_n^2 H^2 c_n/(b_n^3 + W_n^2 H^2 b_n)\right], \tag{4.94}$$

here

$$\gamma C_n \equiv b_n - W_n^2 . \qquad (4.95)$$

Again the formula (4.90) is applied in computing the average $\langle e^{i\vec{k}.(\vec{r}_t-\vec{r}_s)} \rangle$ within A and this yields

$$\langle e^{i\vec{k}.(\vec{r}_t-\vec{r}_s)} \rangle = e^{-k^2 D + H^2(k_x^2+k_y^2)G} , \qquad (4.96)$$

where

$$D(t-s) = \beta^{-1} \sum_n (1 - \cos W_n(t-s)/b_n , \qquad (4.97)$$

and

$$G(t-S) = \beta^{-1} \sum_n W_n^2 (1 - \cos W_n(t-S)) / (b_n^3 + W_n^2 H^2 b_n) . \qquad (4.98)$$

Therefore equations (4.91), (4.94), (4.96), (4.97) and (4.99) together give the general approximation to the free energy F at any temperature, magnetic field and coupling constant. The most accurate F would be attained by considering H to be pure imaginary so that $F_0 - \langle S_0 \rangle - \langle S \rangle$ is an upper bound to F and then minimizing the result by varying the function C(W), however to obtain the solution of the full variation problem a digital computer has to be employed. To be consistent with Feynman's approximation, in their work Hellwarth and Platzman considered a simpler two parameter function for C(W). They chose

$$\gamma = 1 \quad \text{and} \quad C(W) = C\delta(W-\omega) . \qquad (4.99)$$

This choice corresponds to S_0 in the form

$$S_0 = -\frac{1}{2}\int_0^\beta \left(\frac{d\vec{r}}{dt}\right)^2 dt - \frac{C}{2}\int_0^\beta\int dt\, ds \left[(\bar{N}+1)e^{-\omega|t-s|} + \bar{N} e^{\omega|t-s|}\right](\vec{r}_t - \vec{r}_s)^2 \qquad (4.100)$$

which is solely the Feynman polaron trial action at finite temperature. From (4.92) b_n , for this model becomes

$$b_n = W_n^2(W_n^2 + \nu^2)/(W_n^2 + \omega^2) , \tag{4.101}$$

where $$\nu^2 \equiv \omega^2 + \frac{4C}{\omega} \tag{4.102}$$

and all sums over n can be done using a formula

$$\beta^{-1} \sum_{n=-\infty}^{+\infty} \frac{\cos W_n q}{W_n^2 + a^2} = \left[e^{-a|q|} + \frac{2\cosh aq}{(e^{\beta a} - 1)} \right] \Big/ 2a . \tag{4.103}$$

For small magnetic fields H and finite coupling constants, the sums containing in F_0 , $\langle S_0 \rangle$and $\langle S \rangle$ can be expanded in a power series to order H^2 . Limiting to the case of low temperatures i.e.,$\beta \to \infty$, the term proportional to H^2 in $\langle S \rangle$ can be further expanded in powers of $\frac{1}{\beta}$. Considering only contributions from the resulting terms which are proportional to β to the free energy F(H) one thus obtains the magnetic contribution F(H)

$$\delta F = \beta H^2 \left(\frac{\omega}{\nu}\right)^6 \left(\frac{3\nu^2}{\omega^2} - 2 m_F^*\right) \Big/ 24 . \tag{4.104}$$

It is well-known that for a free electron viz., for $\alpha = 0$, at finite temperatures in a weak magnetic field the free energy is

$$F_0 = \frac{\beta H^2}{24} \left(\frac{1}{m_e}\right)^2 . \tag{4.105}$$

Furthermore, Blount[20] has shown that the complete effect of electron-lattice interactions can be taken into account by replacing the free mass by the exact effective mass .
This leads Hellwarth and Platzman to

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20 E.I. Blout, "Bloch Electrons in a Magnetic Field.", Physical Review, 126, (1962) 1636.

define the polaron effective mass by

$$\delta F = \frac{\beta H^2}{24}\left(\frac{1}{\overset{*}{m}_{HP}}\right)^2 \tag{4.106}$$

It follows immediately from (4.104) that the approximate polaron effective mass in this approach is

$$\left(\frac{1}{\overset{*}{m}_{HP}}\right)^2 = \left(\frac{\omega}{\nu}\right)^6\left(\frac{3\nu^2}{\omega^2} - 2\overset{*}{m}_F\right). \tag{4.107}$$

Recalling that

$\frac{\nu^2}{\omega^2} = m_0$, the zero-order polaron effective mass on the total mass of two-particle model system, eq.(4.107) can be rewritten as

$$(\overset{*}{m}_{HP})^{-2} = (3m_0 - 2m_F)/m_0^3 \tag{4.108}$$

Hellwarth and Platzman concluded that if the best model S_0 can be maintained by fully optimized the infinite set of parameters b_n from (4.108),

$$m_H \longrightarrow m_F \longrightarrow m_0 .$$

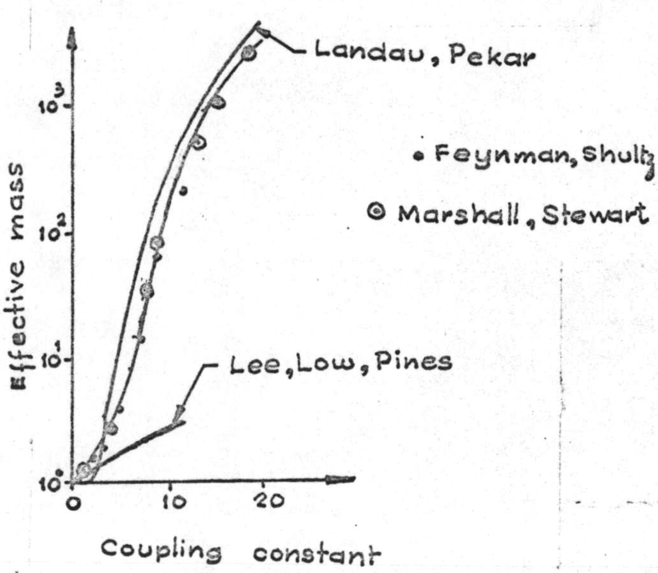

Fig. III Comparison of the Polaron Effective Mass as a Function of the Coupling Constant Approached by Various Methods.