CHAPTER VI

DISCUSSION

In the previous chapter, we have attempted to find the polaron effective mass at considerably low temperatures by means of a density matrix method. Basing on the definition modified from that of a free particle, we have worked out the general expression of the effective mass for all α and the two limiting analytical cases of the effective mass for large and small α. In this chapter, the consistency of these results with those obtained by other methods will be inspected. Finally, possible improvements of the results and suggestive lines for future investigations will be discussed.

VI. Comparison of Results

According to Chapter V, we have proceeded to evaluate the polaron effective mass $\overset{*}{m}$ under the boundary conditions $\vec{r}(0)=\vec{r}\,'$; $\vec{r}(\beta)=\vec{r}\,''$ and with the definition

$$\rho_1(\vec{r}\,''\vec{r}\,';\beta) \underset{\substack{|\vec{r}\,''-\vec{r}\,'|\to 0 \\ \beta\to\infty}}{\sim} e^{-E\beta-\overset{*}{m}\frac{|\vec{r}\,''-\vec{r}\,'|}{2\beta}}, \tag{6.1}$$

which is just an extension of the definition of mass for a free particle.

Our approach renders the key quantity $\langle e^{i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))}\rangle$ as

$$\langle e^{i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))}\rangle_{ours} = e^{-\frac{\vec{k}}{2\nu^2}[(\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu s})+\omega^2 s]+i\vec{k}\cdot[\frac{1}{2}(1-\frac{\omega^2}{\nu^2})(1+e^{-\nu s})+\frac{\omega^2}{\nu^2}(1-\frac{s}{\beta})]\times(\vec{r}-\vec{r}')} \tag{6.2}$$

and the general expression of $\overset{*}{m}$ for all α as

$$\begin{aligned}\overset{*}{m} = 1-\left(1-\frac{\omega^2}{\nu^2}\right)^2+\frac{1}{3}\cdot 2^{-\frac{3}{2}}\pi^{-\frac{1}{2}}\alpha\frac{\omega^4}{\nu^4}\int_0^\infty ds\, e^{-s}\Big\{s^2\Big[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)(1-e^{-\nu s})+\frac{1}{2}\frac{\omega^2}{\nu^2}s\Big]^{-\frac{3}{2}}\\ -\frac{3}{2}s^3\Big[\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)(1+e^{-\nu s})+\frac{\omega^2}{\nu^2}\Big]\Big[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)(1-e^{-\nu s})+\frac{1}{2}\frac{\omega^2}{\nu^2}s\Big]^{-\frac{5}{2}}\\ +\frac{3\times 5}{16}s^4\Big[\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)(1+e^{-\nu s})+\frac{\omega^2}{\nu^2}\Big]\Big[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)(1-e^{-\nu s})+\frac{1}{2}\frac{\omega^2}{\nu^2}s\Big]^{-\frac{7}{2}}\Big\}\end{aligned} \tag{6.3}$$

In the meantime, we consider Feynman's method in which the specified paths $\vec{r}(t)=\vec{U}t$ have been assumed and the modified boundary conditions: $\vec{r}(0)=0$; $\vec{r}(\mathcal{T})=\vec{U}\mathcal{T}$ have been imposed in obtaining the key quantity

$$\langle e^{i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))}\rangle = e^{-\frac{k^2}{2\nu}[\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu t})+\omega^2 t]+i\vec{k}\cdot\vec{U}(t-s)} \tag{6.4}$$

Using the modified definition:

$$K(\vec{r}_{\mathcal{T}}\mathcal{T};00)\underset{\mathcal{T}\to\infty}{\sim} e^{-[E+\frac{1}{2}\overset{*}{m}_F U^2]\mathcal{T}} \tag{6.5}$$

Feynman's polaron effective mass $\overset{*}{m}_F$ can be expressed as

$$\overset{*}{m}_F = 1+\frac{1}{3}\pi^{-\frac{1}{2}}\alpha\,\nu^3\int_0^\infty dt\, e^{-t}t^2\Big[\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu t})+\omega^2 t\Big]^{-\frac{3}{2}} \tag{6.6}$$

Noting that if we neglect all other terms in (6.3) except for the unity and the leading term of the integral, i.e., we examine just

$$1+\frac{1}{3}\pi^{-\frac{1}{2}}\alpha\frac{\omega^4}{\nu^4}\int_0^\infty ds\, e^{-s}s^2\Big[\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu s})+\omega^2 s\Big]^{-\frac{3}{2}}$$

our m^* looks quite the same as the m_F^* in (6.6) apart from a multiplying factor $\left(\frac{\omega}{\nu}\right)^4$.

However it is evident from Chap. III and V that the two limiting values of the polaron effercțive mass deduced from (6.6) and (6.3) can be written in comparison as:

	m_F^*	m^*	
Weak Coupling $\alpha \simeq 0$ $\omega = 3$; $\nu \simeq 3 + 2.22\left(\frac{\alpha}{10}\right)$	$1 + \frac{1}{6}\alpha + O(\alpha^2)$	$1 + \frac{7}{24}\alpha + O(\alpha^2)$	(6.7)
Strong Coupling $\alpha \simeq \infty$ $\omega = 1$; $\nu \simeq \frac{4\alpha^2}{9\pi}$	$\frac{16\alpha^4}{81\pi^4}$	$O(\alpha^{-4}) - O(\alpha^{-2}) + \frac{45}{4}$	(6.8)

As it is expected, for weak coupling; $\alpha \simeq 0$, m^* is slightly larger than m_F^* and this due to the positive resulting first-order α contribution from the following terms of the integral in (6.3). Since the difference is insignificant, we may approve that in this limit our result agrees with Feynman's. Consequently, this implies that our result is also comparable with Schultz's, Krivoglaz-Pekar's and Marshall-Chawla's.

Here we note that as $\alpha \simeq 0$; $\frac{\omega}{\nu} \simeq 1 + \epsilon$; $\epsilon \ll 1$, the factor $\left(\frac{\omega}{\nu}\right)^4$ does not have marked effect on m^*.

In case of large α , the situation taking place in our approach becomes peculiar because now the multiplying factor $\left(\frac{\omega}{\nu}\right)^4$ plays an important role in reducing the α -dependent contributions to m^*. Recalling (5.60), if we keep only the first term inside the integral sign of the approximate m^*, viz.,

$$m^* \simeq \frac{1}{3} \cdot 2^{-\frac{3}{2}} \pi^{-\frac{1}{2}} \alpha \left(\frac{\omega}{\nu}\right)^4 \int_0^\infty ds\, e^{-s} \left(\frac{1}{2\nu}\right)^{-\frac{3}{2}} s^2 \quad ; \qquad (6.9)$$

furthermore, if we exclude the multiplying factor $\left(\frac{\omega}{\nu}\right)^4$, our resulting m^* will be exactly the same as m^*_F. On the contrary, when the factor is taken into account it damps m^* rapidly by the power of α^{-4}. As a result, for large α our m^* tends to zero whereas m^*_F being proportional to α^4, reaches infinite value.

The effective damping factor $\left(\frac{\omega}{\nu}\right)^4$ in strong coupling limit originates from the off-diagonal part of the key quantity (recall eq. (5.36b)) or the average of arbitrary path difference.

$$\langle (\vec{r}(t) - \vec{r}(s)) \rangle = \left[\left(1 - \frac{\omega^2}{\nu^2}\right) \frac{\sinh \nu\left(\frac{t-s}{2}\right) \cosh \nu\left(\frac{\beta - (t+s)}{2}\right)}{\sinh \frac{\nu\beta}{2}} + \frac{\omega^2}{\nu^2} \left(\frac{t-s}{\beta}\right) \right] (\vec{r}'' - \vec{r}') \qquad (6.10)$$

If we set $\nu = \sqrt{\frac{K}{\mu}} \Rightarrow 0$; since μ is fixed, this causes $K \to 0$ i.e., the force that couples an electron to a second fictitious particle is then removed and a polaron reduces to a free electron. It follows that as $\nu \to 0$,

$$\frac{\sinh \nu\left(\frac{t-s}{2}\right) \cosh \nu\left(\frac{\beta - (t+s)}{2}\right)}{\sinh \frac{\nu\beta}{2}} \approx \left(\frac{t-s}{\beta}\right) \qquad (6.11)$$

and the average path travelled by the polaron turns out to be

$$\langle(\vec{r}(t)-\vec{r}(s))\rangle \underset{\nu\to 0}{\approx} (t-s)\left(\frac{\vec{r}''-\vec{r}'}{\beta}\right) , \tag{6.12}$$

which is classically the time interval multiplied by the average velocity. Recalling (6.4), eq. (6.12) is equivalent to the off-diagonal contribution of the Feynman's key quantity. Therefore, we have shown that for large α , our result will be in agreement with Feynman's and other authors' only if $\nu \approx 0$. For $\nu \neq 0$, the electron is now joined to the second fictitious particle by a forced harmonic oscillator to represent a polaron system; the reduced mass μ of this two-particle model system executes vibration with frequency ν . Moreover if $\frac{\omega}{\nu} \ll 1$ which corresponds to small α , eq. (6.10) becomes

$$\langle(\vec{r}(t)-\vec{r}(s))\rangle \underset{\nu\neq 0}{\simeq} \frac{\omega^2}{\nu^2}(t-s)\left(\frac{\vec{r}''-\vec{r}'}{\beta}\right) \lesssim (t-s)\left(\frac{\vec{r}''-\vec{r}'}{\beta}\right) \tag{6.13}$$

This manifests that, in average and for any time intervals, a polaron can cover, travel smaller distance than a free electron. Comparing this with Feynman's result in which this quantity makes no difference for all ν , ours seems to be more reasonable. But why does Feynman's approach yield polaron effective mass consistent with those obtained by other theories such as the perturbation theory? Why does our m^*, for large α , appear opposite to m_F^* ? The contradiction encourages us to interpret the physical meaning underlying our particular result from another view. We accomplish this through further investigation of the definitions concerned.

Let us try an alternative definition for our 'density matrix' approach. Starting with the general expression of the approximate density matrix

$$\rho_1(\vec{r}''\vec{r}';\beta) = \left(\frac{1}{2\pi\beta}\right)\left(\frac{\nu}{\omega}\frac{\sinh\frac{\omega\beta}{2}}{\sinh\frac{\nu\beta}{2}}\exp\left\{\frac{3}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\left(\frac{\nu\beta}{2}\coth\frac{\nu\beta}{2}-1\right)\right.\right.$$
$$+\,2^{-\frac{3}{2}}\alpha\int_0^\beta\!\!\int_0^\beta dt\,ds\left[(\bar{n}+1)e^{-|t-s|}+\bar{n}e^{|t-s|}\right]\int\frac{d^3\vec{k}}{2\pi^2k^2}e^{i\vec{k}\cdot\vec{B}-k^2A}$$
$$\left.+\,\frac{|\vec{r}''-\vec{r}'|}{2\beta}\left[-\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)^2\left(\frac{\nu\beta}{2}\operatorname{cosech}\frac{\nu\beta}{2}\right)^2-\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)^2\frac{\nu\beta}{2}-\left(1-\left(1-\frac{\omega^2}{\nu^2}\right)^2\right)\right]\right\}$$

(6.14)

If we mean to be parallel to Krivoglaz and Pekar principle, we assume that: for a slow electron, $|\vec{r}''-\vec{r}'|\to 0$, at very low temperatures, $\beta\to\infty$, $\rho_1(\vec{r}''\vec{r}';\beta)$ can be expanded in powers of $\frac{1}{\beta}$ as

$$\rho_1(\vec{r}''\vec{r}';\beta)\underset{\substack{|\vec{r}''-\vec{r}'|\to 0\\ \beta\to\infty}}{\sim}\rho^{(0)}e^{\beta f_0+f_1+\frac{f_2}{\beta}+\cdots\cdots}, \qquad (6.15)$$

where $\rho^{(0)}$ is the density matrix for the non-interacting electron-phonon system. Making use of the definition introduced by Krivoglaz and Pekar, we argue that the polaron effective mass is $\overset{*}{m} \equiv e^{\frac{2}{3}f_1}$ (6.16)

As $|\vec{r}''-\vec{r}'|\to 0$ and $\beta\to\infty$, we find that

$$\vec{B}\equiv\vec{B}(\vec{r}''-\vec{r}';\beta,t,s;\nu,\omega)\simeq 0 \qquad (6.17a)$$

$$\left(\frac{\sinh\frac{\omega\beta}{2}}{\sinh\frac{\nu\beta}{2}}\right)^3\approx e^{-\frac{3}{2}\beta(\nu-\omega)} \qquad (6.17b)$$

and

$$2^{-\frac{3}{2}}\alpha \int_0^\beta\int_0^\beta dt\, ds \left[(\bar{n}+1)e^{-|t-s|} + \bar{n}\, e^{|t-s|}\right] \int \frac{d^3\vec{k}}{2\pi^2 k^2}\, e^{-\vec{k}^2 A(\beta, t-s; \nu, \omega)}$$

$$\simeq 2^{-\frac{3}{2}}\alpha\, \pi^{-\frac{1}{2}} \cdot 2\beta \int_0^\beta e^{-s} A^{-\frac{1}{2}}(\beta, \beta-s; \nu, \omega) \qquad (6.17c)$$

where

$$A^{-\frac{1}{2}}(\beta, \beta-s; \nu, \omega) = \left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right) + \frac{\omega^2}{2\nu^2} s\left(1-\frac{s}{\beta}\right)\right]^{-\frac{1}{2}}$$

If we retain only the first two terms in $\frac{1}{\beta}$ -expansion of $A^{-\frac{1}{2}}$ in (6.17c), substitution of (6.17a), (6.17b) and of the resulting (6.17c) into (6.14) shows

$$\begin{aligned}
\rho_1(\vec{r}'', \vec{r}'; \beta) \underset{|\vec{r}''-\vec{r}'|\to 0}{\sim} \left(\frac{1}{2\pi\beta}\right)^{\frac{3}{2}} \exp.\Big\{ &\frac{3}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\frac{\nu\beta}{2} - \frac{3}{2}\beta(\nu-\omega) \\
&+ 2\beta\pi^{-\frac{1}{2}}\alpha\,\nu^3 \int_0^\infty ds\, e^{-s}\left[\left(\frac{\nu^2-\omega^2}{\nu}\right)\left(1-e^{-\nu s}\right) + \omega^2 s\right]^{-\frac{1}{2}} \\
&+ 3\ln\frac{\nu}{\omega} - \frac{3}{2}\left(1-\frac{\omega^2}{\nu^2}\right) + \left(\frac{\omega^2}{\nu^2}\right)\cdot \pi^{-\frac{1}{2}}\alpha\,\nu^3 \int_0^\infty ds\, e^{-s} s^2 \times \\
&\times \left[\left(\frac{\nu^2-\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right) + \omega^2 s\right]^{-\frac{3}{2}} \Big\} \qquad (6.18)
\end{aligned}$$

Therefore our $\overset{*}{m}$, within the definition (6.16), reads

$$\overset{*}{m} = \left(\frac{\nu}{\omega}\right)^2 e^{\frac{\omega^2}{\nu^2} - 1 + \frac{\omega^2}{\nu^2}\frac{\pi^{-\frac{1}{2}}}{3}\alpha\,\nu^3 \int_0^\infty ds\, e^{-s} s^2 \left[\left(\frac{\nu^2-\omega^2}{\nu}\right)\left(1-e^{-\nu s}\right) + \omega^2 s\right]^{-\frac{3}{2}}} \qquad (6.19)$$

or

$$\overset{*}{m} = e^{\left\{\frac{\overset{*}{m}_F}{(\nu/\omega)^2} - 1\right\}} \equiv \overset{*}{m}_{KP} \qquad (6.20)$$

is identical with that of Krivoglaz-Pekar and this also indicates that the two limiting values of $\overset{*}{m}$ corresponding to small and large α are in excellent agreement with Feynman's results.

We are now convinced that different difinitions may lead to different forms of results. We also notice that for a simplest case of a free particle whose density matrix is well-known to be

$$\rho^{(0)}(\vec{r}\,''\vec{r}\,';\beta) = \left(\frac{m}{2\pi\beta}\right)^{\frac{3}{2}} e^{-\frac{m|\vec{r}\,''-\vec{r}\,'|^2}{2\beta}}, \tag{6.21}$$

the free particle's mass appears in both the first multiplicative function and in the other exponential function as a coefficient of $-\frac{|\vec{r}\,''-\vec{r}\,'|^2}{2\beta}$. In accordance with this case, the effective mass of Krivoglaz-Pekar seems to be extracted from the first function while ours from the latter and Feynman's from a special form of the latter. For clarity we analyze (6.21) in terms of its corresponding kernel which is readily found to be

$$K^{(0)}(\vec{r}\,t;\vec{r}\,'0) = \left(\frac{m}{2\pi i t}\right)^{\frac{3}{2}} e^{\frac{im|\vec{r}\,''-\vec{r}\,'|^2}{2t}} \tag{6.22}$$

If $|\vec{r}\,''-\vec{r}\,'|$ is fixed, the exponential function oscillates as a function of time t. Physically, this describes the extended or free state of the particle. In some systems whose potential energies are strong enough to entirely bind the particles their kernels cannot be expressed in the form like eq. (6.22). We say that no extended states are available for these systems. As an example, we look at the kernel of a harmonic oscillator with potential energy $\frac{m\omega^2\vec{r}^{\,2}}{2}$:

$$\bar{K}^{(HO)}(\vec{r}''t;\vec{r}',0) = \left(\frac{m\omega'}{2\pi i \sin\omega' t}\right)^{3/2} e^{\frac{im\omega'}{2\sin\omega' t}\left[(\vec{r}''+\vec{r}')^2\cos\omega' t - 2\vec{r}''\vec{r}'\right]} \tag{6.23}$$

as $t \to \infty$, the asymptotic from of the exponential function behaves in different manner from that of a free particle. Consequently, we cannot deduce another expression of 'mass' corresponding to the coefficient of $\frac{|\vec{r}''-\vec{r}'|^2}{2t}$ in the exponent or We say that equivalently the probability that a harmonic oscillator will be in extended states goes to zero.

Accordingly, we can now interpret the physical arguments underneath our resulting polaron effective mass. Referring to our approach a general expression of the density matrix is firstly evaluated; within the exponential function obtained, all terms except those containing $\frac{|\vec{r}''-\vec{r}'|^2}{2\beta}$ are discarded, further detailed considerations are made solely upon particular part of the exponential function. Such a part, as we have discussed, describes only the extended state of the polaron.

Keeping in mind a two-particle model approximation of the polaron, we can physically intepret our two limiting results of m^* as follows :

For weak coupling, $\alpha \approx 0$, the polaron behaves closely to a free electron. The major contribution to the total mass comes from the extended state, therefore our definition still gives the total effective mass comparable with those obtained by other approaches.

For strong coupling, as α increases, the electron is harmonically bound by the second fictitious particle. The reduced mass vibrates with extremely high frequency ν and this in turn induces a polarization. The electron is trapped in a deep potential well due to this polarization. In this case, the localized states contribute significantly to the total effective mass with the magnitude strongly depending on the coupling constant α, whereas the extended states contribute only irrelevant amount. In other words, in this limit the electron has to move along carrying a large distortion of the lattice; the total polaron effective mass becomes very large. It constitutes mainly inertia due to the localized states and negligibly one associated with the kinetic energy of the translational motion.

It is now clear that our definition of effectivemass gives quite reasonable result of the effective mass corresponding to the extended states. This may be counted as an advantage of our approach for it yields additional information about the polaron extended states in terms of the extended effective mass apart from the total effective mass which can also be drawn from the β-independent part of our general expression of the density matrix as we have pointed out in this section.

VI.2 Conclusions.

Our main purposes in carrying out the present research are: to analyze in detail both the physical and the mathematical features of the Feynman path integral theory and to apply this powerful device to the Fröhlich polaron problem, particularly to estimate the polaron effective mass.

The polaron model under our consideration consists of a slow electron dressed by a cloud of virtual phonons due to the distortion of the lattice induced by the electric field of the electron. This electron-phonon interaction strength is characterized by a coupling constant α. The Fröhlich's polaron Lagrangian has been established basing on various simplifying assumptions whose origins and physical meanings have been already summarized in sec. I.2. In short, all approximations are well justified provided the electron moves with a low speed so that the effective electron cloud dimension is far larger than the lattice spacing.

Feynman's path integral approach to the polaron problem at 0 K has been motivated when the classical Lagrangian

$$\mathcal{L} = 1 \cdot \frac{\dot{\vec{r}}^2}{2} - e \int \nabla_{\vec{r}'} \left(\frac{1}{|\vec{r}' - \vec{r}|} \right) \cdot \vec{P}(\vec{r}') \, d^3\vec{r}' + \frac{M_f}{2} \int \frac{\dot{\vec{P}}^2(\vec{r}') - \omega_L^2 \vec{P}^2(\vec{r}')}{2} \, d^3\vec{r}' \qquad (6.24)$$

derived in sec. I.2 is transformed into the quantum-mechanical form as

$$\mathcal{L} = \frac{\dot{\vec{r}}^2}{2} - 4\pi e \sqrt{\frac{2}{V}} \sum_{\vec{k}} \frac{q_{\vec{k}}}{k} \begin{Bmatrix} \cos \vec{k}\cdot\vec{r} \\ \sin \vec{k}\cdot\vec{r} \end{Bmatrix} + \frac{M_f}{2} \sum_{\vec{k}} \left(\dot{Q}_{\vec{k}}^2 - \omega^2 Q_{\vec{k}}^2 \right),$$

since then the path integral formalism makes it possible to eliminate the coordinates of the phonons $Q_{\vec{k}}$ from the problem.

At 0 K, the phonons are initially and finally in the ground state; the polaron action describing the motion of the electron in the effect of the phonon field is explicitly

$$S = -\frac{1}{2}\int\left(\frac{d\vec{r}}{dt}\right)^2 dt + \frac{\alpha}{2^{\frac{3}{2}}}\iint dt\,ds\,\frac{e^{-|t-s|}}{|\vec{r}(t)-\vec{r}(s)|} \quad . \qquad (6.26)$$

The electron produces a field which acts back on itself as it is evident from the retarded nonlocal Coulomb potential involved in the second part of S . Furthermore, the time decaying factor $e^{-|t-s|}$ arises from the fact that the electron still "feels" the past-time disturbance during the relaxation period of the lattice distortion.

To determine the ground state energy E_g , the exponential decay of the propagator $K_{oo}(\vec{r}''t'';\vec{r}'t') \equiv \int e^{S}\mathcal{D}\vec{r}(t)$ with $T = (t''-t') \rightarrow \infty$ has to be considered. Realizing that S is not quadratic, an approximate quadratic trial action

$$S_o = -\frac{1}{2}\int\left(\frac{d\vec{r}}{dt}\right)^2 dt + \frac{C}{2}\iint dt\,ds\,e^{-\omega|t-s|}(\vec{r}(t)-\vec{r}(s))^2 \qquad (6.27)$$

with two adjustable parameters C and ω is introduced to imitate the effect of actual S . The optimal choice for C and ω can be maintained by the Feynman variational principle for the ground state energy. Physically, Feynman's approximation is to represent the polaron by a simple two-particle model system in which the electron is in harmonic interaction with a second fictitious particle. The Lagrangian of such a model system is

$$\mathcal{L}_o = \frac{1}{2}\dot{\vec{r}}^2 + \frac{1}{2}M\dot{\vec{Y}}^2 - K(\vec{r}-\vec{Y})^2. \qquad (6.28)$$

Consequently, the two parameters can be physically viewed through the relations: $M = \frac{4C}{\omega^3} = \left(\frac{\nu^2}{\omega^2}-1\right)$ and $K = \frac{4C}{\omega} = \nu^2 - \omega^2$.

We have experienced that all complexity in attacking the polaron problem by path integral approach emerges mainly from an attempt to carry out the average $\langle S \rangle_{S_0}$, or strictly speaking, the key quantity $\langle e^{i\vec{K}\cdot(\vec{r}(t)-\vec{r}(s))} \rangle_{S_0}$ which comes out to require the precise expression of the classical paths $\vec{r}(t)$. The principle of least action renders the integro-differential equation for $\vec{r}(t)$. This equation can be transformed into the ordinary fourth-order differential equation which is readily solved under the boundary conditions $\vec{r}(0) = \vec{r}(\mathcal{T}) = 0$ and by ignoring transient terms in the subsequent consideration.

The Feynman approach obtains the upper bound to the ground state energy as

$$E = \frac{3(\nu^2-\omega^2)}{4\nu} - \pi^{-\frac{1}{2}}\alpha\nu\int_0^\infty \left[\frac{\nu^2-\omega^2}{\nu}(1-e^{-\nu t}) + \omega^2 t\right]^{-\frac{1}{2}} e^{-t}\,dt \quad (6.29)$$

Merely two limiting cases can be determined analytically. For weak coupling, $\alpha \simeq 0$, the optimal choices for ω and ν which give the minimum E are $\omega \simeq 3$, $\nu \simeq 3 + 2.22\left(\frac{\alpha}{10}\right)$. For strong coupling, $\alpha \simeq \infty$, the appropriate values of ν and ω is found to be $\omega \simeq 1$, $\nu \simeq \frac{4\alpha^2}{9\pi} - (4\ln 2 - 1)$.

Feynman has intuitively extended his procedure to yield the polaron effective mass at 0 K. His indirect approximate way, though seemingly ad hoc in the sense that it cannot prove the conservation of the momentum, happens to give the effective mass in agreement with those deduced by other theories. The polaron is ascribed to move with an average 'velocity' $\vec{U}$. With the boundary conditions $\vec{r}(0)=0,\ \vec{r}(\mathcal{T})=\vec{U}\mathcal{T}$, Feynman argued that as $\mathcal{T}\to\alpha$, for small $\vec{U}$, the polaron propagator should take the asymptotic form

$$K \sim e^{-E(U)\mathcal{T}} \equiv e^{-[E_{\cdot}+\frac{1}{2}\overset{*}{m}_F U^2]\mathcal{T}} . \qquad (6.30)$$

The total energy is no longer dominated by the ground state energy, it also includes the kinetic energy part from which the polaron effective mass $\overset{*}{m}_F$ can be drawn. It should be remarked that as a consequence of the energy determination the effective mass thus obtained is still the approximate expression in terms of the parameter ν and ω , but there is not another variational principle to give an upper limit to the total energy for each value of $\vec{U}$. Feynman proceeded by retaining those values of ω and ν which were previously found to minimize E when $\vec{U}=0$. Feynman got: $\overset{*}{m}_F = 1+\frac{1}{6}\alpha+0.025\alpha^2$ for small α and $\overset{*}{m}_F = \frac{16\alpha^4}{81\pi^2} = 200\left(\frac{\alpha}{10}\right)^4$ for large α .

At finite temperatures, the electron is now surrounded by a number of real phonons in the $\vec{k}$ th mode. This consequently affects the strength of the electron potential energy. The polaron's properties are thermodynamically investigated through the characteristic functional i.e., the partition function or generally, the density matrix $\rho(\vec{r}''\vec{r}';\beta)$ which specifies temperature development of the polaron. Fortunately, this temperature development is in close connection with the time development of the system as it has been shown that the parameter β in the density matrix is just $\beta \equiv \frac{1}{k_B T} = i(t''-t')$, the imaginary time interval in the propagator. Moreover, if we generally considered the system at arbitrary temperatures T and then on a slowly cooling process, $\beta \to \infty$ or $i(t''-t') \to \infty$, the polaron attains ground state; we also gain the information of the polaron at absolute zero temperature.

At finite temperatures the polaron is described by the action

$$S = -\frac{1}{2}\int_0^\beta \left(\frac{d\bar{r}}{dt}\right)^2 dt + \frac{\alpha}{2^{3/2}} \int_0^\beta \int_0^\beta dt\,ds \left[(\bar{n}+1)e^{-|t-s|} + \bar{n}\,e^{|t-s|}\right] \times \frac{1}{|\vec{r}(t) - \vec{r}(s)|} \qquad (6.31)$$

recalling that we have always set $m_{eff} = \hbar = \omega_L = 1$. The electron-phonon interaction term is now modified by $\bar{n} = \frac{1}{e^\beta - 1}$, the average number of phonons. And the trial action, in this case, β becomes

$$S_0 = -\frac{1}{2}\int_0^\beta \left(\frac{d\vec{r}}{dt}\right)^2 dt + \frac{c}{2}\int_0^\beta \int_0^\beta dt\,ds \left[(\bar{n}+1)e^{-\omega|t-s|} + \bar{n}\,e^{\omega|t-s|}\right] \times (\vec{r}(t) - \vec{r}(s))^2. \qquad (6.32)$$

Within Feynman approximation, the self-energy of the polaron in this general state has widely been examined[22] and has turned out to yield satisfactory results. Up to now the method has been extended to improve the self-energy by introducing two additional parameters to the original trial action

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22 See Reference (7), (8) and (18).

(6.27) and (6.33)[23-24]. In the meantime, several authors have attempted to evaluate the polaron effective mass at this state. Among these authors are Krivoglaz and Pekar, Ōsaka and Hellwarth and Platzman using path-integral calculations. Besides these, other attempts are made by Fulton[25] and Yokota[26] using different theories. Only a few of them have succeeded in deducing an explicit expression describing the temperature-dependent behavior of the polaron effective mass. Furthermore the resulting temperature dependent effective mass comes out to vary in opposite directions. In fact, the underlied physical argument of these results are still in doubt.

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[23] R. Abe, and K. Okamoto, "An Improvement of Feynman Action in the Theory of Polaron I.", Journal of the Physical Society of Japan, 31 (1971) 1337.

[24] M. Natenapit, "Path Integral Theory of Polarons", Unpublished M.Sc. Thesis, Department of Physics, Chulalongkorn University, Bangkok, (1973).

[25] T. Fulton, "Self-Energy of the Polaron for Intermediate Temperatures.", Physical Review, 103 (1956) 1712.

[26] T. Yokota, "Interaction in the Electron-Lattice System (I) Correspondence Principle.", Busseiron-Kenkyu, 69 (1953) 137.

Schultz[27] has remarked for this failure that at finite temperatures, a description of the polaron between collisions with phonons or the concept of a polaron as an entity distinct from the field is required to give the effective mass. In his philosophy, this entity of the polaron itself is temperature independent.

In Chapter V, we have intended to find the polaron effective mass at considerably low temperature by looking into a general functional i.e., the density matrix, which includes the kinetic diagonal contribution. Our definition of the effective mass is closely parallel to that of Feynman, viz.,

$$\rho_1(\vec{r}''\vec{r}';\beta) \underset{\substack{|\vec{r}''-\vec{r}'|\to 0 \\ \beta\to\infty}}{\sim} F(\beta)\, e^{-E\beta - \frac{m^*|\vec{r}''-\vec{r}'|}{2\beta}}$$

thus we expect the result to be consistent at least with Feynman's. In obtaining the approximate $\rho_1(\vec{r}''\vec{r}';\beta)$ with the boundary conditions: $\vec{r}(0)=\vec{r}'$ and $\vec{r}(\beta)=\vec{r}''$, we have avoided the situation in which the complicated integro-differential equation had to be solved in determining the key quantity $\langle e^{i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))}\rangle_{S_0}$ with respect to S_0 given by (6.32), by making use of the simple model Lagrangian of the form:

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27 T.D. Schultz, Tech. Report No. 9, "Electron-Lattice Interactions in Polar Crystals.", Molecular Physics Group M.I.T. Cambridge, Mass. (1956) 189.

$$\mathcal{L}_0' = \frac{1}{2}\left[\dot{\vec{r}}^2(t) + M\dot{\vec{Y}}^2(t) - \kappa\left(\vec{r}(t) - \vec{Y}(t)\right)^2\right] + \vec{f}(t)\cdot\vec{r}(t) \qquad (6.32)$$

The boundary conditions imposed on the variable $\vec{Y}(t)$ are $\vec{Y}(0) = \vec{Y}'$ and $\vec{Y}(\beta) = \vec{Y}''$. The action resulted from $\mathcal{L}_0'$ still involved $\vec{Y}'$ and $\vec{Y}''$ which could be integrated out, given $\vec{R}' = \vec{R}''$.

We have noticed that from the general expression $\rho_1(\vec{r}'',\vec{r}';\beta)$ if we have extracted the polaron effective mass according to the definition defined by Krivoglaz and Pekar, our $\overset{*}{m}$ should have taken the same form as $\overset{*}{m}_{KP}$ and could also be related to Feynman's as

$$\frac{\overset{*}{m}}{(\frac{v}{\omega})^2} = e^{\left\{ \frac{\overset{*}{m}_F}{(\frac{v}{\omega})^2} - 1 \right\}} \qquad (6.33)$$

But when the definition (6.31) has been utilized, the effective mass obtained gives consistent result only for weak coupling. Strikingly, for strong coupling, our result contradicts with Feynman's. The subsequent detailed study of the physical ideas lying beyond each definition leads us to the interpretation that our definition, defined as it is in (6.35), contributes the effective mass corresponding to the extended states of the polaron whereas others' yield the total effective mass of the system.

The success of Feynman method in obtaining the superior results for the whole range of α in spite of his seemingly ad hoc effective mass definition can be viewed quantitatively as arising from the following reasons: since the two-particle model system or the harmonic approximation has been accepted to describe the polaron, he needs only consider the relative motion of the electron with respect to the polaron center in translation. He intuitively excludes the translational motion of the system by choosing the center of mass of the two-particle model system as the center of the polaron. Moreover, in his definition; the average "velocity $\vec{v}$ " can be thought of as being "the group velocity" associated with such a relative motion of the electron. Incidentally, these arguments turn out to be an accurate account of the polaron motion for both limiting cases, since for weak coupling, $m_{eff} \gg M$, the polaron center is nearly coincident with the electron's position; for weak coupling, $m_{eff} \ll M$, the polaron center may be taken at rest.

VI.3 Recommendations

As far as the path integral technique is concerned in dealing with the polaron problem, a quadratic approximation of the polaron exact action is inevitable. Throughout this research, the Feynman's approximation of two-particle model system, in which the electron and the second fictitious particle are in harmonic interaction, has been applied to replace the polaron model depicting the electron and the lattice in Coulomb interaction. In fact, only a harmonic oscillator is inadequate to take care of the deep bound state allowable within the exact Coulomb potential. Naturally, Feynman's principle and the consequent result can be improved if one approximates the action

$$S_o = -\frac{1}{2}\int_0^{\mathcal{T}}\left(\frac{d\vec{r}}{dt}\right)^2 dt - \frac{1}{2}\sum_{n=1}^{N} C_n \int_0^{\mathcal{T}}\int_0^{\mathcal{T}} dt\,ds\, e^{-\omega_n|t-s|}\,(\vec{r}(t)-\vec{r}(s))^2 \qquad (6.34)$$

to the polaron in the ground state and

$$S_o = -\frac{1}{2}\int_0^{\beta}\left(\frac{d\vec{r}}{dt}\right) dt - \frac{1}{2}\sum_{n=1}^{N} C_n \int_0^{\beta}\int_0^{\beta} dt\,ds\left[\frac{e^{\omega|t-s|}}{e^{\omega\beta}-1} + \frac{e^{\omega\beta}}{e^{\omega\beta}-1}\cdot e^{-\omega|t-s|}\right]\times$$
$$\times\,(\vec{r}(t)-\vec{r}(s))^2 \qquad (6,35)$$

to the polaron at arbitrary temperatures. Such S_o represents the many coupled particle model system.

Abe and Okamoto have calculated the improvement of the upper bound of the ground state energy and the effective mass of the polaron using S_0 with $N=2$. The corresponding physical picture is the three-coupled particle model in which the electron is joined to two fictitious particles, each by a harmonic force (See Fig.V). The strength and frequency of the harmonic oscillation can be varied by four parameters viz., C_1, C_2 , ω_1 , and ω_2 . Their extension gives only 0.1% correction to Feynman's ground state energy and 0.4% larger for the polaron effective mass in comparison with Feynman's. As it is recognized that the optimal effective mass is required in the mobility analysis, the improved trial action for the polaron is expected to offer better understanding of the polaron mobility. Moreover, it has recently been evident from cyclotron resonance experiments in some polar crystals and semiconductors that the polaron effect give rise to a shift in the measured cyclotron frequency.

Cyclotron resonance measurements on such materials do not measure the rigid lattice conduction band mass but rather the magnetic levels of the polaron consisting of the electron and its accompanying lattice distortion. Therefore, one could deduce the precise band masses which take into account the polaron effect from the measured polaron effective masses with the aid of the theoretical interpolation formula giving the ratio $\frac{m^*_{polaron}}{m_{eff}}$.

We are thus led to remark that for a theoretical treatment, the future research into higher order corrections to the polaron effective mass using S_o given by (6.34) or more generally by (6.35) with $N > 2$ is a challenge.

Staying within the framework of path integrals, a few over-simplifying basic assumptions that have been made in studying the polaron properties could be removed or at least refined to attain a more realistic polaron picture. A so-called continuum approximation, as we have discussed in Sec. I.2, is well justified only for the polaron having a dimension far larger than the lattice spacing, but that in most ionic crystals, this is not the case. Thus, it is interesting to investigate how the introduction of a finite cut off $\vec{k}_o$ would affect the polaron features concluded by Feynman's former theory with infinite cut off $\vec{k}_o$. The only change in mathematical treatment of the effective mass is that the integral over $\vec{k}$ in evaluation of the key quantity $\langle e^{i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))}\rangle$ is now limited to range over a sphere of radius k_o instead of over all space.

Other approximations such as the band mass approximation and the Born and Huang theory which is responsible for the electron-phonon interaction should also be re-examined according to the more detailed phonon dispersion characteristics evidenced by the recent investigations[28].

We heartily hope to see in the near future the complete dissertation including a full account of the polaron effective mass for all coupling strength α and at arbitrary temperature $\frac{1}{k_B \beta}$.

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28 Kittel Charles, Introduction to Solid State Physics, 4th Ed., New York: John Wiley & Sons, Inc. (1971) 166-193.