CHAPTER V

THE POLARON EFFECTIVE MASS AT LOW TEMPERATURES,

DENSITY-MATRIX APPROACH

So far, we have seen that all approaches to the polaron effective mass at finite temperatures have dealt with the evaluation of the partition function or the diagonal part of the density matrix of the polaron system. In this chapter we shall extend the calculation of this quantity to a more general one i.e., we shall directly investigate the polaron effective mass through the density matrix of the system.

We shall set out by giving briefly the statement of our problem. Next we shall present quantitatively the equivalence of the Feynman's approximate model of S_0 and the two-particle model system. The successive section will be due to a calculation of the quantities $\langle \vec{r}(\tau)\rangle$ and $\langle \vec{r}(\tau)\cdot\vec{r}(\sigma)\rangle$ required to obtain the key quantity $\langle e^{i\vec{k}\cdot(\vec{r}(\tau)-\vec{r}(\sigma))}\rangle$. Such a calculation enable us to carry out the polaron effective mass in the last section.

V.1. The Statement of the Problem.

We consider the density matrix of the polaron system expressed in path integral form as

$$\rho(\vec{r}''\vec{r}';\beta) = \int e^{S}\mathcal{D}\left(\vec{r}(t): \begin{matrix}\vec{r}(\beta)=\vec{r}''\\ \vec{r}(0)=\vec{r}'\end{matrix}\right), \tag{5.1}$$

where symbolically $\mathcal{D}\left(\vec{r}(t): \begin{matrix}\vec{r}(\beta)=\vec{r}''\\ \vec{r}(0)=\vec{r}'\end{matrix}\right)$ denotes the path performance under the boundary conditions $\vec{r}(0)=\vec{r}'$ and $\vec{r}(\beta)=\vec{r}''$. Recalling sec. IV.3, after averaging the lattice vibrational part the action of the polaron at finite temperatures reads

$$S = -\frac{1}{2}\int_0^\beta (\dot{\vec{r}}(t))^2 dt + 2^{-\frac{3}{2}}\alpha\left\{\frac{e^{\beta}}{e^{\beta}-1}\int_0^\beta\int_0^\beta |\vec{r}(t)-\vec{r}(s)|^{-1} e^{-|t-s|}dt\,ds + \right.$$
$$\left. + \frac{1}{e^{\beta}-1}\int_0^\beta\int_0^\beta |\vec{r}(t)-\vec{r}(s)|^{-1} e^{|t-s|} dt\,ds\right\} \tag{5.2}$$

Feynman trial action at 0 K to finite temperatures is found by Abe and Ōsaka to be

$$S_0 = -\frac{1}{2}\int_0^\beta (\dot{\vec{r}})^2 dt - \frac{C}{2}\int_0^\beta\int_0^\beta dt\,ds\,|\vec{r}(t)-\vec{r}(s)|^2 \frac{\cosh\omega(\frac{\beta}{2}-|t-s|)}{\sinh\frac{\omega\beta}{2}}$$

or

$$S_0 = -\frac{1}{2}\int_0^\beta (\dot{\vec{r}})^2 dt - \frac{C}{2}\left\{\frac{e^{\beta\omega}}{e^{\beta\omega}-1}\int_0^\beta\int_0^\beta (\vec{r}(t)-\vec{r}(s))^2 e^{-\omega|t-s|} + \right.$$
$$\left. + \frac{1}{e^{\beta\omega}-1}\int_0^\beta\int_0^\beta (\vec{r}(t)-\vec{r}(s))^2 e^{\omega|t-s|} dt\,ds\right\}, \tag{5.3}$$

The physical picture underlying this approximation will be pointed out in sec. II.2. Making use of the Feynman variational method given in detail in sec. III.2, we arrive at

$$\rho(\vec{r}''\vec{r}';\beta) \geq \rho_{S_0} e^{\langle S-S_0\rangle_{S_0}}, \tag{5.4}$$

where we have defined the average of any functional f to be performed with respect to S_o viz.,

$$\langle f \rangle_{S_o} \equiv \int f e^{S_o} \mathcal{D}\left(\vec{r}(t): \begin{array}{l} \vec{r}(\beta) = \vec{r}'' \\ \vec{r}(0) = \vec{r}' \end{array}\right) \Big/ \rho_{S_o} \tag{5.4a}$$

and

$$\rho_{S_o} \equiv \int e^{S_o} \mathcal{D}\left(\vec{r}(t): \begin{array}{l} \vec{r}(\beta) = \vec{r}'' \\ \vec{r}(0) = \vec{r}' \end{array}\right). \tag{5.4b}$$

Precisely,

$$\langle S - S_o \rangle = \langle S \rangle_{S_o} - \langle S_o \rangle_{S_o} \tag{5.5}$$

where

$$\langle S - S_o \rangle_{S_o} = 2^{-\frac{3}{2}} \alpha \int_0^\beta \int_0^\beta \left[\frac{e^\beta}{e^\beta - 1} \cdot e^{-|t-s|} + \frac{1}{e^\beta - 1} \cdot e^{|t-s|} \right] \langle |\vec{r}(t) - \vec{r}(s)|^{-1} \rangle_{S_o} dt\,ds$$

$$= 2^{-\frac{3}{2}} \alpha \int_0^\beta \int_0^\beta dt\,ds \left[\frac{e^\beta}{e^\beta - 1} e^{-|t-s|} + \frac{1}{e^\beta - 1} \cdot e^{|t-s|} \right] \int d^3\vec{k} \frac{1}{2\pi^2 k^2} \langle e^{i\vec{k}\cdot(\vec{r}(t) - \vec{r}(s))} \rangle \tag{5.5a}$$

and

$$\langle S_o \rangle_{S_o} = \frac{C}{2} \int_0^\beta \int_0^\beta dt\,ds \left[\frac{e^{\omega\beta}}{e^{\omega\beta} - 1} e^{-\omega|t-s|} + \frac{1}{e^{\omega\beta} - 1} e^{\omega|t-s|} \right] \langle (\vec{r}(t) - \vec{r}(s))^2 \rangle \tag{5.5b}$$

Since S_o is quadratic, the cumulant expansion of the average $\langle e^{i\vec{k}\cdot(\vec{r}(t) - \vec{r}(s))} \rangle$ retains only the first two cumulants[21]

$$\langle e^{i\vec{k}\cdot(\vec{r}(t) - \vec{r}(s))} \rangle_{S_o} = e^{i\vec{k}\cdot\langle(\vec{r}(t) - \vec{r}(s))\rangle_{S_o} - \frac{1}{2} k^2 \left[\frac{1}{3} \langle (\vec{r}(t) - \vec{r}(s))^2 \rangle_{S_o} - \langle X(t) - X(s) \rangle_{S_o}^2 \right]} \tag{5.6}$$

Furthermore, the path-integral method permits us to separate ρ_{S_o} into:

$$\rho_{S_o} = F(\beta; C, \omega) e^{\bar{S}_o}, \tag{5.7}$$

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21 See Reference (1) P. 184

two factors in which $F(\beta;C,\omega)$ is a multiplicative factor independent of paths $\vec{r}(t)$ and the other is the exponential of the action corresponding to the classical path .

Thus the density matrix of our interest becomes

$$\rho(\vec{r}''\vec{r}';\beta) \geq F(\beta;C,\omega)e^{\bar{S}_0 + \langle S\rangle - \langle S_0\rangle} \qquad (5.8)$$

With $F(\beta)$, $\bar{S}_0$, $\langle S\rangle$ and $\langle S_0\rangle$ to be evaluated explicitly.

Following Feyman suggestion of the direct way in defining an effective mass as we have mentioned in sec. III.3, we argue that for a slow electron in the limits $|\vec{r}''-\vec{r}'|\to 0$ and $\beta\to\infty$, the asymptotic form of (5.1) should vary as

$$\rho(\vec{r}''\vec{r}';\beta) \underset{\substack{|\vec{r}''-\vec{r}'|\to 0 \\ \beta\to\infty}}{\sim} e^{-E\beta - \frac{\overset{*}{m}|\vec{r}''-\vec{r}'|^2}{2\beta}}, \qquad (5.9)$$

the exponential term that depends on $|\vec{r}''-\vec{r}'|^2$ determines the polaron effective mass $\overset{*}{m}$.

V.2 The Two-Particle Model Lagrangian.

The trial action S_0 has been introduced initially by Feynman in order to imitate the effects of the real action S and to render a performable path integral. The physical picture of the polaron corresponding to this approximation is made clearer when it is recognized that the system giving rise to S_0 can be equivalently represented by a simple two-particle model system in which the electron is coupled by a harmonic force to a fictitious second particle (See Fig.IV). Let us justify this quantitatively as follow.

Consider such a two-particle model Lagrangian

$$\mathcal{L}_0 = \frac{1}{2}\dot{\vec{r}}^2 + \frac{1}{2}M\dot{\vec{Y}}^2 - K(\vec{r}-\vec{Y})^2, \tag{5.10}$$

where M and $\vec{Y}$ refer to the mass and position of the fictitious second particle. If we replace $K\vec{r}$ by $\vec{\gamma}(t)$ and rearrange (5.10), we get

$$\mathcal{L}_0 = \left(\frac{1}{2}\dot{\vec{r}}^2 - \frac{1}{2}K\vec{r}^2\right) + \left(\frac{1}{2}M\dot{\vec{Y}}^2 - \frac{1}{2}K\vec{Y}^2 + \vec{\gamma}(t)\vec{Y}\right). \tag{5.11}$$

Clearly, the second part is just the forced harmonic oscillator Lagrangian whose corresponding propagator has been given in sec. II.2. Then going into imaginary time and defining $\omega' = \sqrt{\frac{K}{M}}$, the density matrix of $\mathcal{L}_0$ is readily

$$\rho_{\mathcal{L}_0}(\vec{r}''\vec{r}';\beta) = \int \mathcal{D}\vec{r}(\tau)\, e^{-\frac{1}{2}\int_0^\beta\left[\left(\frac{d\vec{r}(\tau)}{d\tau}\right)^2 + K\vec{r}^2\right]d\tau} \int d\vec{Y}(\tau) \langle \vec{Y}\beta | \vec{Y}0 \rangle_{\vec{\gamma}(\tau)}$$

$$\rho_{\mathcal{L}_0}(\vec{r}''\vec{r}';\beta) = \left(2\sinh\frac{\beta\omega'}{2}\right)^{-3} \int \mathcal{D}\vec{r}(\tau)\, e^{-\frac{1}{2}\int_0^\beta\left(\frac{d\vec{r}}{d\tau}\right)^2 d\tau}\, e^{-\frac{M\omega'^3}{8}\int_0^\beta\int_0^\beta\left[\frac{e^{\beta\omega'}e^{-\omega|\tau-\sigma|}}{e^{\beta\omega'}-1} + \frac{1}{e^{\beta\omega}-1}e^{\omega'|\tau-\sigma|}\right](\vec{r}(\tau)-\vec{r}(\sigma))^2 d\tau\, d\sigma} . \tag{5.12}$$

If we set:

$$\omega' = \omega \qquad \text{and} \qquad M = \frac{4C}{\omega^3} \tag{5.13}$$

besides the factor $\left(2\sinh\frac{\beta\omega}{2}\right)^{-3}$, the action resulted by (5.12) is in the same form as S_0 given by (5.3). Therefore this implies that practically, the two-particle model described by the Lagragian (5.11) can be used instead of S_0.

We note from (5.11) that the two-particle model system can be viewed to be consisting of two independent kinds of motion, one is free translation in three dimensions with mass

$M+1$ and the other is free vibration in three dimensions of the reduced mass $\mu = \frac{1\cdot M}{1+M}$ with frequency $\nu = \sqrt{\frac{\varkappa}{\mu}}$.

V.3. Evaluation of the Quantities $\langle \vec{r}(\tau) \rangle$ and $\langle \vec{r}(\tau)\vec{r}(\sigma) \rangle$

We have seen from sec. V.1 that to obtain the final expression of the density matrix ρ we again encounter the key quantity $\langle e^{i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))} \rangle_{S_0'}$. If we proved in the same manner as that given by Feynman in Chap. III, the form of S_0' in this case will give rise to the more complicated integro-differential equation which is difficult to handle. To remedy this we choose another effective method introduced by Feynman and Hibbs.

Recalling (5.6), we have expressed the key quantity as

$$\langle e^{i\vec{k}\cdot(\vec{r}(t)-\vec{r}(s))} \rangle_{S_0} = e^{i\vec{k}\cdot\langle\vec{r}(t)-\vec{r}(s)\rangle_{S_0} - \frac{1}{2}k^2[\frac{1}{3}\langle(\vec{r}(t)-\vec{r}(s))^2\rangle - \langle x(t)-x(s)\rangle^2} . \quad (5.14)$$

Therefore a precise expression of (5.14) implies calculations of $\langle\vec{r}(t)\rangle$ and $\langle\vec{r}(t)\cdot\vec{r}(s)\rangle$. To achieve this let us consider a functional

$$\langle e^{\int_0^\beta dt\,\vec{f}(t)\cdot\vec{r}(t)} \rangle_{S_0'} \equiv \frac{\int \mathcal{D}\left(\vec{r}(t): \begin{matrix}\vec{r}(\beta)=\vec{r}''\\ \vec{r}(0)=\vec{r}'\end{matrix}\right) e^{S_0+\int_0^\beta dt\,\vec{f}(t)\cdot\vec{r}(t)}}{\int \mathcal{D}\left(\vec{r}(t): \begin{matrix}\vec{r}(\beta)=\vec{r}''\\ \vec{r}(0)=\vec{r}'\end{matrix}\right) e^{S_0}} \quad (5.15)$$

where $\vec{f}(t)$ is an arbitrary function of time.

Substituting

$$S_0' = S_0 + \int_0^\beta dt\,\vec{f}(t)\cdot\vec{r}(t) \quad (5.16)$$

and typically performing the path integrations in (5.15), the multiplying factors in the numerator and the denominator cancel each other out, (5.15) reduces to

$$\left\langle e^{\int_0^\beta dt\, \vec{f}(t)\cdot\vec{r}(t)} \right\rangle_{S_0} = e^{\bar{S}_0' - \bar{S}_0} \tag{5.17}$$

where $\bar{S}_0'$ and $\bar{S}_0$ stand for the corresponding classical actions of the actions S_0' and S_0 respectively.

Eq. (5.17) formally gives the characteristic functional needed in computing $\langle\vec{r}(t)\rangle$ and $\langle\vec{r}(\tau)\cdot\vec{r}(\sigma)\rangle$ which are to be employed in (5.14).

Differentiating (5.17) with respect to $\vec{f}(t)$ and evaluating both sides when $\vec{f}(t) = 0$, one easily find

$$\left\langle \vec{r}(t)\, e^{\int_0^\beta \vec{f}(t)\cdot\vec{\gamma}(t)dt} \right\rangle_{S_0} = \frac{\delta\bar{S}_0'}{\delta\vec{f}(t)} e^{\bar{S}_0' - \bar{S}_0}, \quad \langle\vec{r}(t)\rangle_{S_0} = \left.\frac{\delta\bar{S}_0'}{\delta\vec{f}(t)}\right|_{\vec{f}\equiv 0} \tag{5.18}$$

Repeating the process to obtain the second derivative, this yields

$$\langle\vec{r}(t)\cdot\vec{r}(s)\rangle_{S_0} = \left.\frac{\delta^2}{\delta\vec{f}(t)\,\delta\vec{f}(s)} e^{\bar{S}_0' - \bar{S}_0}\right|_{f\equiv 0} = \left[\frac{\delta^2\bar{S}_0'}{\delta\vec{f}(t)\,\delta\vec{f}(s)} + \frac{\delta\bar{S}_0'}{\delta\vec{f}(t)}\cdot\frac{\delta\bar{S}_0'}{\delta\vec{f}(t)}\right]_{\vec{f}\equiv 0}. \tag{5.19}$$

It is now clear that our problem turns to an evaluation of $\bar{S}_0'$. As we have discussed in sec. V.2 that the action S_0 can be equivalently represented by a two-particle model Lagrangian given by (5.10). Under the similar circumstance and with the definition of S_0' the action S_0' or the classical action $\bar{S}_0'$ is derivable from a model Lagrangian,

$$\mathcal{L}_0' = \frac{1}{2}\left[\dot{\vec{r}}^2(t) + M\dot{\vec{Y}}^2(t) - \kappa\left(\vec{r}(t) - \vec{Y}(t)\right)^2\right] + \vec{f}(t)\cdot\vec{r}(t), \tag{5.20}$$

which is just the two-particle model system joined by an external force $\vec{f}$.

Introducing the relations

$$\vec{\rho} = \vec{r} - \vec{Y}, \quad \vec{R} = \frac{1\cdot\vec{r} + M\vec{Y}}{1+M}, \quad m_0 = 1+M$$

$$\mu = \frac{1\cdot M}{1+M}, \quad \nu^2 = \frac{K}{\mu} \quad \text{and} \quad \omega^2 = \frac{K}{M} \tag{5.21}$$

the Lagrangian $\mathcal{L}_0'$ can be rewritten, going to imaginary time, as

$$\mathcal{L}_0' = \left[\tfrac{1}{2}(\mu\dot{\vec{\rho}}^2(t) - K\vec{\rho}^2(t)) + \tfrac{\mu}{1}\vec{f}(t)\cdot\vec{\rho}(t)\right] + \left[\tfrac{1}{2}m_0\dot{\vec{R}}^2(t) + \vec{f}(t)\cdot\vec{R}(t)\right]. \tag{5.22}$$

Formally, $\mathcal{L}_0'$ is merely composed of two forced harmonic oscillators, one with the reduced mass μ , frequency ν coupled to the force $\frac{\mu}{1}\vec{f}(t)$ and the other with total mass m_0 , zero frequency, coupled to the force $\vec{f}(t)$. This enables us to determine the contribution from each oscillator to $\bar{S}_0'$ independently.

Now we determine

$$\int_0^\beta dt\,\bar{\mathcal{L}}_0' = \int_0^\beta dt\left[-\tfrac{1}{2}(\mu\dot{\bar{\vec{\rho}}}^2 + K\bar{\vec{\rho}}^2(t)) + \mu\vec{f}(t)\cdot\bar{\vec{\rho}}(t)\right] + \int_0^\beta dt\left[-\tfrac{1}{2}m_0\dot{\bar{\vec{R}}}^2 + \vec{f}(t)\cdot\bar{\vec{R}}(t)\right]. \tag{5.23}$$

Principle of least action then gives the equations of motion for the classical paths $\bar{\vec{\rho}}(t)$ and $\bar{\vec{R}}(t)$ as

$$\ddot{\bar{\vec{\rho}}}(t) - \nu^2\bar{\vec{\rho}} = -\vec{f}(t) \tag{5.24}$$

and

$$\ddot{\bar{\vec{R}}}(t) - 0 = -\vec{f}(t)/m_0 \tag{5.25}$$

Eq. (5.24) may be solved conveniently by using the Green function method; the solution is

$$\bar{\vec{\rho}}(t) = (\vec{\rho}'\sinh\nu(\beta-t) + \vec{\rho}''\sinh\nu t)/\sinh\nu\beta - \int_0^\beta ds\,\vec{f}(s)G(s,t), \tag{5.26a}$$

where

$$G(s,t) = -\frac{\sinh\nu t}{\nu}(\coth\nu t - \coth\nu\beta)\sinh\nu s\,H(t-s) - \frac{\sinh\nu t}{\nu}(\coth\nu\beta - \coth\nu\beta\sinh\nu s)H(s-t), \tag{5.26b}$$

and in which the boundary conditions

$\bar{\vec{\rho}}(0) = \vec{\rho}'$ and $\bar{\vec{\rho}}(\beta) = \vec{\rho}''$ have been imposed.

Consider first part of (5.23)

$$\int_0^\beta dt\left[-\tfrac{1}{2}\mu\dot{\vec{\bar\rho}}^2(t)-\tfrac{\gamma}{2}\vec{\bar\rho}(t)+\mu\vec{f}(t)\vec{\bar\rho}(t)\right]=\tfrac{\mu}{2}\left(-\vec{\rho}''\cdot\dot{\vec{\bar\rho}}(\beta)-\vec{\rho}'\cdot\dot{\vec{\bar\rho}}(0)\right)+\tfrac{\mu}{2}\int_0^\beta \vec{f}(t)\cdot\vec{\bar\rho}(t)\,dt. \quad (5.27)$$

Deducing $\dot{\vec{\bar\rho}}(\beta$, $\dot{\vec{\bar\rho}}(0)$ from (5.26a) and substituting these into (5.27) we get

$$\int_0^\beta dt\left[-\tfrac{1}{2}\mu\dot{\vec{\bar\rho}}^2(t)-\tfrac{\gamma}{2}\vec{\bar\rho}(t)+\mu\vec{f}(t)\cdot\vec{\bar\rho}(t)\right]=\frac{\mu\nu}{2\sinh\nu\beta}\left[-(\vec{\rho}''^2+\vec{\rho}'^2)\cosh\nu\beta+2\vec{\rho}''\vec{\rho}'\right]+$$

$$+\frac{2\vec{\rho}''}{\nu}\int_0^\beta dt f(t)\sinh\nu t+\frac{2\vec{\rho}'}{\nu}\int_0^\beta dt f(t)\sinh\nu(\beta-t)$$

$$+\frac{2}{\nu^2}\int_0^\beta\int_0^t dt\,ds\,f(s)f(t)\sinh\nu(\beta-t)\sinh\nu s. \quad (5.28a)$$

Similarly we readily find, for the other part of $\bar{S}_0'$

$$\int_0^\beta dt\left[-\tfrac{1}{2}m_0\dot{\vec{\bar R}}^2+\vec{f}(t)\cdot\vec{\bar R}(t)\right]=-\frac{m_0}{2}\frac{(\vec{R}''-\vec{R}')^2}{\beta}+\vec{R}''\int_0^\beta dt f(t)\frac{t}{\beta}+\vec{R}'\int_0^\beta dt f(t)\frac{(\beta-t)}{\beta}$$

$$+\frac{1}{m_0^2}\int_0^\beta\int_0^t dt\,ds\,f(t)f(s)(\beta-t)\frac{s}{\beta}, \quad (5.28b)$$

Under the boundary conditions

$$\vec{\bar R}(0)=\vec{R}' \quad \text{and} \quad \vec{\bar R}(\beta)=\vec{R}''.$$

Therefore combination of (5.28a) and (5.28b) gives time dependent expression of $\bar{S}_0'$ but still in terms of $\vec{\rho}''$, $\vec{\rho}'$, $\vec{R}''$ and $\vec{R}'$.

Transform the result into the original coordinates $\vec{r}''$, $\vec{r}'$, $\vec{Y}''$ and $\vec{Y}'$ and set $\vec{Y}''=\vec{Y}'$, we come out with

$$\int_0^t dt\,\bar{\mathcal{L}}_0'=\frac{\mu\nu}{2\sinh\nu\beta}\left[-(\vec{r}''^2+\vec{r}'^2)\cosh\nu\beta+2\vec{r}''\vec{r}'\right]-\frac{1}{2}\frac{1}{m_0\beta}(\vec{r}''-\vec{r}')^2$$

$$+\vec{r}''\left[\int_0^\beta dt\vec{f}(t)\left(\frac{\mu}{1}\cdot\frac{\sinh\nu t}{\sinh\nu\beta}+\frac{1}{m_0}\cdot\frac{t}{\beta}\right)\right]$$

$$+\vec{r}'\left[\int_0^\beta dt\vec{f}(t)\left(\frac{\mu}{1}\cdot\frac{\sinh\nu(\beta-t)}{\sinh\nu\beta}+\frac{1}{m_0}\frac{(\beta-t)}{\beta}\right]\right.$$

$$+\int_0^\beta\int_0^t dt\,ds\,\vec{f}(t)\vec{f}(s)\left(\frac{\mu}{1^2}\frac{\sinh\nu(\beta-t)\sinh\nu s}{\nu\sinh\nu\beta}+\frac{1}{m_0^2}\frac{(\beta-t)s}{\beta}\right)$$

$$+\mu\nu\tanh\frac{\nu\beta}{2}\vec{Y}''^2$$

$$+\left[-\mu\nu\tanh\frac{\nu\beta}{2}(\vec{r}''+\vec{r}')-\int_0^\beta dt\,\vec{f}(t)\left\{\frac{\mu}{1}\left(\frac{\sinh\nu t+\sinh\nu(\beta-t)}{\sinh\nu\beta}\right)+\frac{\mu}{1}\right\}\right]\vec{Y}'' \tag{5.29}$$

To eliminate the second particle coordinate $\vec{Y}''$ out we perform the integration

$$\int_{-\infty}^{\infty}d\vec{Y}''e^{\int_0^\beta dt\bar{\mathcal{L}}_0'}=\int_{-\infty}^{\infty}d\vec{Y}''e^{D(\vec{r}'',\vec{r}')}e^{E\vec{Y}''^2+F\vec{Y}''}$$

$$=\sqrt{\frac{\pi}{E}}\cdot e^{D-\frac{F^2}{4E}} \tag{5.30a}$$

where a formula

$$\int_{-\infty}^{\infty}e^{ax^2+bx}dx=\sqrt{-\frac{\pi}{a}}\,e^{-\frac{b^2}{4a}}$$

is used, and where

$$D=\frac{\mu\nu}{2\sinh\nu\beta}\left[-(\vec{r}''^2+\vec{r}'^2)\cosh\nu\beta+2\vec{r}''\vec{r}'\right]-\frac{1}{2m_0\beta}(\vec{r}''-\vec{r}')^2+\vec{r}''\left[\int_0^\beta dt\,\vec{f}(t)\left\{\frac{\mu}{1}\frac{\sinh\nu t}{\sinh\nu\beta}+\right.\right.$$
$$\left.\left.+\frac{1}{m_0}\frac{t}{\beta}\right)\right]+\vec{r}'\left[\int_0^\beta dt\,\vec{f}(t)\left(\frac{\mu}{1}\frac{\sinh\nu(\beta-t)}{\sinh\nu\beta}+\frac{1}{m_0}\cdot\frac{(\beta-t)}{\beta}\right)\right]+\int_0^\beta\int_0^t dt\,ds\,\vec{f}(t)f(s)\left(\frac{\mu}{1^2}\times\right.$$
$$\left.\times\frac{\sinh\nu(\beta-t)\sinh\nu s}{\nu\sinh\nu\beta}+\frac{1}{m_0^2}\frac{(\beta-t)s}{\beta}\right) \tag{5.30b}$$

$$E=\mu\nu\tan\frac{\nu\beta}{2} \tag{5.30c}$$

and
$$F=\left[-\mu\nu\tanh\frac{\nu\beta}{2}(\vec{r}''+\vec{r}')-\int_0^\beta dt\,\vec{f}(t)\left\{\frac{\mu}{1}\left(\frac{\sinh\nu t+\sinh\nu(\beta-t)}{\sinh\nu\beta}\right)-\frac{\mu}{1}\right\}\right] \tag{5.30d}$$

Once (5.30a) is carried out the action of one interest $\bar{S}_0'$ can be deduced immediately, since

$$\int_{-\infty}^{\infty}d\vec{Y}''e^{\int_0^\beta dt\bar{\mathcal{L}}_0'}$$

is directly proportional to $e^{\bar{S}_0'}$.

Further calculation gives finally,

$$\bar{S}_0' = D - \frac{F^2}{4E} = -\left[\frac{\mu\nu}{4}\coth\frac{\nu\beta}{2} + \frac{1}{2}\frac{\mu}{M\beta}\right]|\vec{r}\,'' - \vec{r}\,'|^2 + \vec{r}\,''\int_0^\beta dt f(t)\left\{\frac{\mu}{1}\left(\frac{\sinh\nu t}{\sinh\nu\beta} + \frac{\sinh\frac{\nu(\beta-t)}{2}\sinh\frac{\nu t}{2}}{\cosh\frac{\nu\beta}{2}}\right) + \right.$$
$$\left. + \frac{\mu t}{M\beta}\right\} + \vec{r}\,'\int_0^\beta dt f(t)\left\{\frac{\mu}{1}\left(\frac{\sinh\nu(\beta-t)}{\sinh\nu\beta} + \frac{\sinh\frac{\nu(\beta-t)}{2}\sinh\frac{\nu t}{2}}{\cosh\frac{\nu\beta}{2}}\right) + \frac{\mu}{M}\frac{(\beta-t)}{\beta}\right\}$$
$$+ \int_0^\beta\int_0^t dt\, ds\, f(t) f(s)\left\{\frac{\mu}{\nu\sinh\nu\beta}\left(\sinh\nu(\beta-t)\sinh\nu s - 4\sinh\frac{\nu(\beta-t)}{2}\sinh\frac{\nu t}{2}\times\right.\right.$$
$$\left.\left.\times\sinh\frac{\nu(\beta-t)}{2}\sinh\frac{\nu s}{2}\right) + \frac{\mu}{M}\frac{(\beta-t)}{\beta}s\right\} \qquad (5.31)$$

Recalling (5.16), if we set $\vec{f}(t)=0$, we easily obtain

$$\bar{S}_0 = -\left[\frac{\mu\nu}{4}\coth\frac{\nu\beta}{2} + \frac{1}{2}\frac{\mu}{M\beta}\right]|\vec{r}\,'' - \vec{r}\,'|^2. \qquad (5.32)$$

Using a full expression of $\vec{\bar{S}}_0'$ given by (5.31), calculations of the quantities $\langle \vec{r}(t)\rangle$ and $\langle \vec{r}(t)\vec{r}(s)\rangle$ or specially $\langle \vec{r}(s)\rangle$, $\langle r^2(t)\rangle$ and $\langle \vec{r}^{\,2}(s)\rangle$ are straight-forward.

V.4 Evaluation of the Polaron Effective Mass.

We have already stated in sec.V.1 that the approximation of the effective mass can be obtained, once the density matrix $\rho_1(\vec{r}\,''\vec{r}\,';\beta)$:

$$\rho_1(\vec{r}\,''\vec{r}\,';\beta) \simeq F(\beta;c,\omega)\, e^{\bar{S}_0 + \langle S\rangle_{S_0} - \langle S\rangle_{S_0}} \qquad (5.33)$$

is known. $\bar{S}_0$ has been expressed in (5.32) and from the definition of ρ_{S_0} and $\langle S\rangle_{S_0}$ one can easily verify that

$$\langle S_0\rangle_{S_0} = c\frac{\delta}{\delta c}\ln\rho_{S_0}(\vec{r}\,''\vec{r}\,';\beta)\Big|_{\omega = \text{constant}}$$
$$= c\frac{\delta}{\delta c}\ln\left(F(\beta;c,\omega)\, e^{\bar{S}_0}\right)\Big|_{\omega=\text{constant}} \qquad (5.34)$$

Therefore our task is to search the expressions of $\langle S\rangle_{S_0}$ and $F(\beta;c,\omega)$. First we consider

$$\langle S\rangle_{S_0} = 2^{-\frac{3}{2}}\alpha\int_0^\beta\int_0^\beta\left[(\bar{n}+1)e^{-|t-s|} + \bar{n}\, e^{|t-s|}\right]\int d^3\vec{k}\,\frac{1}{2\pi^2 k^2}\, e^{i\vec{k}\cdot\vec{B} - k^2 A} \qquad (5.35a)$$

in which

$$\bar{n} = \frac{1}{e^{\beta}-1} \quad , \quad A = \frac{1}{2}\left[\frac{1}{3}\langle(\vec{r}(t)-\vec{r}(s))^2\rangle_{S_0} - \frac{\vec{B}^2}{3}\right] \qquad (5.35b)$$

and

$$\vec{B} = \langle(\vec{r}(t)-\vec{r}(s))\rangle_{S_0} \qquad (5.35c)$$

To find $\vec{B}$, the formula (5.18) is employed. That is

$$\vec{B} = \langle\vec{r}(t)\rangle_{S_0} - \langle\vec{r}(s)\rangle_{S_0} = \left.\frac{\delta S_0'}{\delta \vec{f}(t)}\right|_{f(t)=0} - \left.\frac{\delta S_0'}{\delta \vec{f}(s)}\right|_{f(s)=0}$$

$$= \vec{r}''\left\{\frac{\mu}{1}\left(\frac{\sinh \nu t}{\sinh \nu\beta} + \frac{\sinh \nu\frac{(\beta-t)}{2}\sinh\frac{\nu t}{2}}{\cosh\frac{\nu\beta}{2}} - \frac{\sinh \nu s}{\sinh \nu\beta} - \frac{\sinh\frac{\nu(\beta-s)}{2}\sinh\frac{\nu s}{2}}{\cosh\frac{\nu\beta}{2}}\right) + \frac{\mu}{M}\frac{(t-s}{\beta}\right.$$

$$+ \vec{r}'\left\{\frac{\mu}{1}\left(\frac{\sinh \nu(\beta-t)}{\sinh \nu\beta} + \frac{\sinh\frac{\nu(\beta-t)}{2}\sinh\frac{\nu t}{2}}{\cosh\frac{\nu\beta}{2}} - \frac{\sinh\frac{\nu(\beta-s)}{2}\sinh\frac{\nu s}{2}}{\cosh\frac{\nu\beta}{2}} + \frac{\mu}{M}\left(\frac{s-t}{\beta}\right)\right)\right\}$$

$$= \vec{r}''\left\{\frac{\mu}{\sinh\nu\beta}\cosh\frac{\nu\beta}{2}\left[\sinh\nu\left(t-\frac{\beta}{2}\right)-\sinh\nu\left(s-\frac{\beta}{2}\right)\right] + \frac{\mu}{M}\left(\frac{t-s}{\beta}\right)\right\} + \vec{r}'\left\{\frac{\mu}{\sinh\nu\beta}\sinh\frac{\nu(s-t)}{2}\right.$$

$$\left.\times\left[\cosh\frac{\nu(t-s)}{2} + \cosh\nu\left(\beta-\left(\frac{t+s}{2}\right)\right) - \frac{\mu}{M}\left(\frac{t-s}{\beta}\right)\right]\right\}.$$

Given $t>s$, final expression of $\vec{\beta}$ is simply

$$\vec{B} = \vec{B}(\vec{r}''-\vec{r}'; \beta, t, s, \nu, \tfrac{\mu}{M}) = \mu\left[\frac{\sinh\nu\frac{(t-s)}{2}\cosh\nu\left(\frac{\beta-(t+s)}{2}\right)}{\sinh\frac{\nu\beta}{2}} + \frac{(t-s)}{M\beta}\right](\vec{r}''-\vec{r}') \qquad (5.36a)$$

The relations (5.14b) and (5.22) reveal that $\mu = 1-\frac{\omega^2}{\nu^2}$ and $\mu = 1-\frac{\omega^2}{\nu^2}$. Hence $\vec{B}$ becomes

$$\vec{B} = \vec{B}(\vec{r}''-\vec{r}'; \beta, t, s, \nu, \omega) = \left[\left(1-\frac{\omega^2}{\nu^2}\right)\frac{\sinh\nu\left(\frac{t-s}{2}\right)\cosh\nu\left(\frac{\beta-(t+s)}{2}\right)}{\sinh\frac{\nu\beta}{2}} + \frac{\omega^2}{\nu^2}\frac{(t-s)}{\beta}\right](\vec{r}''-\vec{r}') \qquad (5.36b)$$

Our next objective is to compute A in which the unknown quantity is $\langle(\vec{r}(t)-\vec{r}(s))^2\rangle_{S_0}$.

The expansion of $\langle(\vec{r}(t)-\vec{r}(s))^2\rangle_{S_0}$ is simply

$$\langle(\vec{r}(t)-\vec{r}(s))^2\rangle_{S_0} = \langle(\vec{r}(t))^2\rangle_{S_0} + \langle(\vec{r}(s))^2\rangle_{S_0} - 2\langle\vec{r}(t)\vec{r}(s)\rangle$$

Making use of the formula (5.20), this is

$$\langle(\vec r(t)-\vec r(s))^2\rangle_{S_0} = \Big[\frac{\delta^2 \bar S_0'}{\delta \vec f(t)\,\delta \vec f(s)}\Big|_{s=t} + \frac{\delta^2 \bar S_0'}{\delta \vec f(s)\,\delta \vec f(t)}\Big|_{t=s} - \frac{2\,\delta^2 \bar S'}{\delta \vec f(t)\,\delta\vec f(s)}\Big]_{I}\Big|_{f\equiv 0}$$

$$+\Big[\frac{\delta \bar S_0'}{\delta \vec f(t)}\cdot\frac{\delta\bar S_0'}{\delta\vec f(s)}\Big|_{s=t} + \frac{\delta(\bar S_0'}{\delta \vec f(s)}\cdot\frac{\delta \bar S_0'}{\delta\vec f(t)}\Big|_{t=s} - 2\,\frac{\delta\bar S_0'}{\delta\vec f(t)}\cdot\frac{\delta\bar S_0'}{\delta \vec f(s)}\Big]_{II}\Big|_{f\equiv 0}$$

$$(5.37)$$

Calculating one rectangular component of the first square bracket of (5.37), we find that (5.37)

$$\frac{1}{3}[\cdots\cdots]_{I} = \Big[-\mu\Big\{\frac{1}{\nu\sinh\nu\beta}\Big(\sinh\nu(\beta-t)\sinh\nu t + 4\sinh\nu\frac{(\beta-t)}{2}\sinh\frac{\nu t}{2}\sinh\nu\frac{(\beta-t)}{2}\sinh\frac{\nu}{2}$$

$$+\sinh\nu(\beta-s)\sin\nu s + 4\sinh\nu\frac{(\beta-s)}{2}\sinh\frac{\nu s}{2}\sinh\nu\frac{(\beta-s)}{2}\sinh\frac{\nu s}{2}$$

$$-2\sinh\nu(\beta-t)\sinh\nu s - 8\sinh\nu\frac{(\beta-t)}{2}\sinh\nu\frac{(\beta-s)}{2}\sinh\frac{\nu s}{2}\Big) + \frac{1}{2M}\Big(\frac{\beta-t}{\beta}\Big)t$$

$$+\frac{1}{2M}\frac{(\beta-s)}{\beta}\cdot s - 2\cdot\frac{1}{2M}\frac{(\beta-t)}{\beta}\cdot s\Big]$$

$$= \mu\Big\{\frac{1}{\nu\sinh\frac{\nu\beta}{2}}\sinh\nu\Big(\frac{t-s}{2}\Big)\sinh\nu\Big(\frac{\beta-(t-s)}{2}\Big) + \frac{1}{2M\beta}(\beta-(t-s))(t-s)\Big\} \qquad (5.38a)$$

The second square bracket results just for 1 rectangular component, and for $t>\sigma$, it is

$$\frac{1}{3}[\cdots\cdots]_{II} = (W(t)-W(s))^2(X''-X')^2$$

$$= \mu^2\Big[\frac{\sinh\frac{\nu(t-s)}{2}\cosh\nu\Big(\frac{\beta-(t+s)}{2}\Big)}{\sinh\frac{\nu\beta}{2}} + \frac{(t-s)}{M\beta}\Big]^2(X''-X')^2. \qquad (5.38b)$$

$$= \frac{\vec B^2}{3} \qquad (5.38c)$$

where

$$W(t) = \frac{\mu}{\sinh\nu\beta}\Big(\sinh\nu t + 2\sinh\frac{\nu\beta}{2}\sinh\nu\frac{(\beta-t)}{2}\sinh\frac{\nu t}{2}\Big) + \frac{\mu}{M}\frac{t}{\beta}.$$

and

$$W(s) = \frac{\mu}{\sinh\nu\beta}\Big(\sinh\nu s + 2\sinh\frac{\nu\beta}{2}\sinh\nu\frac{(\beta-s)}{2}\sinh\frac{\nu s}{2}\Big) + \frac{\mu}{M}\cdot\frac{s}{\beta}$$

Combination of (5.38a) and (5.38c) gives suddenly $\frac{1}{3}\langle(\vec r(t)-\vec r(s))^2\rangle$

and substitution of this into (5.35) shows

$$A = \left[\frac{\mu \sinh \nu\left(\frac{t-s}{2}\right) \sinh \nu\left(\frac{\beta-(t-s)}{2}\right)}{\nu \sinh \frac{\nu\beta}{2}} + \frac{\mu}{2M\beta}\left(\beta-(t-s)\right)(t-s)\right] \tag{5.39a}$$

or, in terms of ν and ω,

$$A(\beta,(t-s),\nu,\omega) = \left[\frac{1}{\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\frac{\sinh \nu\left(\frac{t-s}{2}\right)\sinh \nu\left(\frac{\beta-(t-s)}{2}\right)}{\sinh \frac{\nu\beta}{2}} + \frac{1}{2}\frac{\omega^2}{\nu^2}\frac{(\beta-(t-s))(t-s)}{\beta} \tag{5.39b}$$

The next quantity needed to be considered is the multiplicative factor $F(\beta;c,\omega)$ which corresponds to the trial action S_0. We can calculate this more easily by making use of the two-particle model Lagrangian. It is evident from sec. V.2 that the only effect of replacing S_0 by the one obtained from the model Lagrangian $\mathcal{L}_0$ is that the contributes a path-independent multiplying factor to the corresponding density matrix. Similarly, the partition function corresponding to the action S_0 should be different from the partition function resulting from the two-particle model system by a multiplying constant. Thus

$$\mathrm{sp.}\rho_{S_0}(\vec{r}''-\vec{r}';\beta) = \mathrm{Constant.sp.}\left[\int \mathcal{D}\left(\vec{r}(t): \begin{array}{l}\vec{r}(\beta)=\vec{r}''\\ \vec{r}(0)=\vec{r}'\end{array}\right) e^{-\int_0^\beta dt\,\frac{1}{2}[\dot{\vec{r}}^2+\varkappa\vec{r}^2]} \times \right.$$

$$\times \int \mathcal{D}\left(\vec{x}(t): \begin{array}{l}\vec{Y}(\beta)=\vec{Y}''\\ \vec{Y}(0)=\vec{Y}'\end{array}\right) e^{-\int_0^\beta dt\,\frac{1}{2}[M\dot{\vec{Y}}^2+\varkappa\vec{Y}^2-2M\varkappa\vec{r}\vec{Y}]}$$

$$V\,F(\beta;c,\omega) = \mathrm{Constant}.\,V\left(\frac{1+M}{2\pi\beta}\right)^{\frac{3}{2}}\left(2\sinh\frac{\nu\beta}{2}\right)^{-3}$$

$$F(\beta;c,\omega) = \mathrm{Constant}.\left(\frac{1+M}{2\pi\beta}\right)^{\frac{3}{2}}\left(2\sinh\frac{\nu\beta}{2}\right)^{-3} \tag{5.40}$$

Physically, the resulting partition function on the right of the above equation is simply a constant multiplied by two factors, one is the contribution from the center-of-mass motion with the total mass $(1+M)$, the other from a simple harmonic oscillator of reduced mass μ and frequency ν. The unknown 'constant' can be determined by imposing the boundary condition: For fixed ω and $\mathcal{K}=0$, $F(\beta;c,\omega)$ reduces to the value for a free electron viz., $\left(\frac{1}{2\pi\beta}\right)^{3/2}$. To accomplish this we rewrite (5.40) in terms of $\mathcal{K}$ and ω:

$$F(\beta;c,\omega) = \text{Constant}\cdot\left(\frac{1+\frac{\mathcal{K}}{\omega^2}}{2\pi\beta}\right)^{3/2}\left(2\sinh\frac{\beta}{2}\sqrt{\mathcal{K}+\omega^2}\right)^{-3} \tag{5.41}$$

Setting $\mathcal{K}=0$ and $F(\beta;c,\omega)=\left(\frac{1}{2\pi\beta}\right)^{3/2}$ yields

$$\text{Constant} = \left(2\sinh\frac{\beta\omega}{2}\right)^3 \tag{5.42}$$

Finally, recalling $(1+M)=\frac{\nu^2}{\omega^2}$, we have

$$F(\beta;c,\omega) = \left(\frac{1}{2\pi\beta}\right)^{3/2}\left(\frac{\nu\sinh\frac{\beta\omega}{2}}{\omega\sinh\frac{\nu\beta}{2}}\right)^3 \tag{5.43}$$

Substitution of $F(\beta;c,\omega)$ and $\bar{S}_0$ into (5.34) enables us to compute $\langle S_0\rangle_{S_0}$, viz.,

$$\langle S_0\rangle_{S_0} = 3c\frac{\delta}{\delta c}\ln\left(\frac{\nu}{\omega}\frac{\sinh\frac{\beta\omega}{2}}{\sinh\frac{\nu\beta}{2}}\right)\Bigg|_{\omega=\text{constant.}} - c\frac{\delta}{\delta c}\left[\frac{\mu\nu}{4}\coth\frac{\nu\beta}{2}+\frac{\mu}{2M\beta}\right]\Bigg|_{\omega=\text{constant.}}(\vec{r}''-\vec{r}')^2 \tag{5.44}$$

Knowing that

$$\mu = \left(1-\frac{\omega^2}{\nu^2}\right),\quad \frac{\mu}{M} = \frac{\omega^2}{\nu^2}\quad \text{and}\quad \nu^2 = \omega^2+\frac{4c}{\omega},$$

eq. (5.44a) can be performed directly to give

$$\langle S_0\rangle_{S_0} = -\frac{3}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\left(\frac{\nu\beta}{2}\coth\frac{\nu\beta}{2}-1\right) - \frac{(\vec{r}''-\vec{r}')^2}{2\beta}\Bigg\{-\left(1-\frac{\omega^2}{\nu^2}\right)^2\left(\frac{\nu\beta}{2}\operatorname{cosech}^2\frac{\nu\beta}{2}+\right.$$

$$\left.+\left(1-\frac{\omega^2}{\nu^2}\right)\frac{\nu\beta}{2}\cdot\coth\frac{\nu\beta}{2}-\frac{1}{2}\left(1-\frac{\nu^2}{\omega^2}\right)^2\frac{\nu\beta}{2}\coth\frac{\nu\beta}{2}-\frac{\omega^2}{\nu^2}\left(1-\frac{\omega^2}{\nu^2}\right)\right\} \tag{5.45}$$

Collecting all necessary results given explicitly by (5.43), (5.45), (5.32) and (5.35a), we obtain the general expression for the approximate density matrix

$$\rho_1(\vec{r}\,'',\vec{r}\,';\beta) = \left(\frac{1}{2\pi\beta}\right)^{\frac{3}{2}}\left(\frac{\nu}{\omega}\,\frac{\sinh\frac{\omega\beta}{2}}{\sinh\frac{\nu\beta}{2}}\right)^{3}\exp\Big\{\frac{3}{2}\Big(1-\frac{\omega^2}{\nu^2}\Big)\Big(\frac{\nu\beta}{2}\coth\frac{\nu\beta}{2}-1\Big)$$
$$+\,2^{-\frac{3}{2}}\alpha\int_0^{\beta}\!\!\int_0^{\beta} dt\,ds\left[(\bar{n}+1)e^{-|t-s|}+\bar{n}\,e^{|t-s|}\right]\int d^3\vec{k}\,\frac{1}{2\pi^2k^2}\,e^{i\vec{k}\cdot\vec{B}-k^2A}$$
$$+\,\frac{|\vec{r}\,''-\vec{r}\,'|^2}{2\beta}\Big[-\frac{1}{2}\Big(1-\frac{\omega^2}{\nu^2}\Big)^2\Big(\frac{\nu\beta}{2}\operatorname{cosech}\frac{\nu\beta}{2}\Big)^2-\frac{1}{2}\Big(1-\frac{\omega^2}{\nu^2}\Big)^2\frac{\nu\beta}{2}-\Big(1-\Big(1-\frac{\omega^2}{\nu^2}\Big)^2\Big)\Big]\Big\} \tag{5.46}$$

with the expression of A and B given by (5.39b) and (5.36b) respectively.

Restrict ourself to a case of a slow electron i.e., $|\vec{r}\,''-\vec{r}\,'|\to 0$, the integral in the exponent of (5.46) can be simplified by expanding $e^{i\vec{k}\cdot\vec{B}(\vec{r}\,'',\vec{r}\,';\beta,t,s,\nu,\omega)}$ in powers of $\vec{B}$. That is

$$e^{i\vec{k}\cdot\vec{B}} = 1+i\vec{k}\cdot\vec{B}-\Big(\frac{\vec{k}\cdot\vec{B}}{2}\Big)^2-\cdots\cdots \; . \tag{5.47}$$

According to our definition of mass we need only consider the terms that are proportional to $|\vec{r}\,''-\vec{r}\,'|^2$, therefore we pick up only the second-order term in (5.47). Assuming isotropic medium and choosing a direction of $\vec{B}$ along the wave vector $\vec{k}$, we have $-(\vec{k}\cdot\vec{B})^2 = -\frac{1}{3}\vec{k}B^2$. Consequently, the $\vec{k}$-integration is performable and the result is

$$\int d^3\vec{k}\,\frac{1}{2\pi^2k^2}\Big(-\frac{1}{3}\cdot\frac{k^2B^2}{2}\Big)e^{-k^2A} = -\frac{1}{3}\,\frac{B^2}{\pi^{1/2}}\cdot\frac{1}{4A^{3/2}}\,, \tag{5.48}$$

where

$$\int_0^\infty x^2 e^{-ax^2} dx = \frac{\pi^{\frac{1}{2}}}{4a^{3/2}}$$

have been applied.

Collecting all terms in the exponent of ρ_1 that involve $|\vec{r}'' - \vec{r}'|^2$, we come out with

$$\rho_1(\vec{r}''\vec{r}';\beta) \sim \exp\Big\{ -\frac{|\vec{r}''-\vec{r}'|^2}{2\beta}\Big[\cdot \frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)^2\left(\frac{\nu\beta}{2}\operatorname{Cosech}\frac{\nu\beta}{2}\right)^2 + \frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)^2\frac{\nu\beta}{2}$$
$$+ \left(1-\left(1-\frac{\omega^2}{\nu^2}\right)^2\right) + \frac{1}{3}\cdot\frac{2^{-\frac{3}{2}}}{4\pi^{1/2}}\alpha\cdot 2\beta\int_0^\beta\int_0^\beta dt\, ds\Big((\bar{n}+1)e^{-|t-s|} +$$
$$+ \bar{n}e^{|t-s|}\Big)B'^{2}A^{-\frac{3}{2}}\Big]\Big\}, \qquad (5.49)$$

where we have exclude $(\vec{r}'' - \vec{r}')$ from the expression of $\vec{B}$ and defined the remaining as $\vec{B}'$.

At very low temperature $T \to \infty$ or as $\beta \to \infty$, we look for terms inside the square bracket of the above expression which are independent of β, clearly, the third one is required and the fourth one needs further consideration.

Partial integration of the fourth term yields

$$\beta\int_0^\beta\int_0^\beta dt\,ds\left((\bar{n}+1)e^{-|t-s|} + \bar{n}e^{|t-s|}\right)B'^{2}(\beta,t,s;\nu,\omega)\,A^{-3/2}(\beta,t-s;\nu,\omega)$$

$$= 2\beta^2\int_0^\beta ds\left((\bar{n}+1)e^{-|\beta-s|} + \bar{n}e^{|\beta-s|}\right)\left[\frac{\left(1-\frac{\omega^2}{\nu^2}\right)\sinh\nu\left(\frac{\beta-s}{2}\right)\cosh\frac{\nu s}{2}}{\sinh\frac{\nu\beta}{2}} + \frac{\omega^2}{\nu^2}\left(1-\frac{s}{\beta}\right)\right]^2 \times$$

$$\times\left[\frac{1}{\nu}\left(1-\frac{\omega}{\nu}\right)\frac{\sinh\nu(\frac{\beta}{2}-s)\sinh\frac{\nu s}{2}}{\sinh\frac{\nu\beta}{2}}+\frac{\omega^2}{2\nu^2}s\left(1-\frac{s}{\beta}\right)\right]^{-\frac{3}{2}} \tag{5.50}$$

For large β ,

$$\left[(\bar{n}+1)e^{-|\beta-s|}+\bar{n}e^{|\beta-s|}\right]\simeq\left[\frac{e^{\beta}e^{-|\beta-s|}}{e^{\beta}-1}+\frac{e^{|\beta-s|}}{e^{\beta}-1}\right]\simeq e^{-s},$$

$$\frac{\sinh\nu(\frac{\beta-s}{2})\cosh\frac{\nu s}{2}}{\sinh\frac{\nu\beta}{2}}\simeq\frac{1}{2}\left(1+e^{-\nu s}\right)$$

and

$$\frac{\sinh\nu(\frac{\beta-s}{2})\sinh\frac{\nu s}{2}}{\sinh\frac{\nu\beta}{2}}\simeq\frac{1}{2}\left(1-e^{-\nu s}\right). \tag{5.51}$$

Eq. (5.50) in the limit $\beta>>1$ becomes

$$2\beta^2\int_0^{\beta}ds\,e^{-s}\left[\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1+e^{-\nu s}\right)+\frac{\omega^2}{\nu^2}\left(1-\frac{s}{\beta}\right)\right]^2\times$$

$$\times\left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{\omega^2}{2\nu^2}s\left(1-\frac{s}{\beta}\right)\right]^{-\frac{3}{2}} \tag{5.52}$$

Next, we expand each radical term in powers of $\frac{1}{\beta}$, the multiplication of the two series gives 3 terms proportional to $\frac{1}{\beta^2}$ and this in turn make the whole (5.52) independent of β . Let us write down explicitly the β-independent contributions to $\rho_1(\vec{r}''\vec{r}';\beta)$ in the limits $|\vec{r}''-\vec{r}'|\to\infty$ and $\beta\to\infty$

$$\rho_1(\vec{r}''\vec{r}';\beta)\sim\exp\left\{-\frac{|\vec{r}''-\vec{r}'|^2}{2\beta}\left[\left(1-\left(1-\frac{\omega^2}{\nu^2}\right)^2\right)+\frac{1}{3}\cdot\frac{2^{-\frac{3}{2}}}{4\pi^{\frac{1}{2}}}\alpha\cdot 4\times\right.\right.$$

$$\times\int_0^{\infty}ds\,e^{-s}\left\{\frac{\omega^4}{\nu^4}\cdot s^2\left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{1}{2}\frac{\omega^2}{\nu^2}s\right]^{-3/2}-\right.$$

$$-\frac{3}{2}\frac{\omega^4}{\nu^4}s^3\left[\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{\omega^2}{\nu^2}\right]\left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{1}{2}\frac{\omega^2}{\nu^2}s\right]^{-\frac{5}{2}}$$

$$+\frac{3\times5}{16}\frac{\omega^4}{\nu^4}s^4\left[\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1+e^{-\nu s}\right)+\frac{\omega^2}{\nu^2}\right]^2\left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{\omega^2}{2\nu^2}s\right]^{-\frac{7}{2}}\Bigg\}$$

(5.53)

Express this asymptotic form of $\rho_1(\vec{r}''\vec{r}';\beta)$ as

$$\rho_1(\vec{r}''\vec{r}';\beta) \sim \exp\left\{-\frac{\overset{*}{m}}{2\beta}|\vec{r}''-\vec{r}'|^2\right\},$$

we suddenly obtain the approximation to the polaron effective mass $\overset{*}{m}$ at extremely low temperatures, as

$$\overset{*}{m} = 1-\left(1-\frac{\omega^2}{\nu^2}\right)+\frac{1}{3}\cdot 2^{-\frac{3}{2}}\pi^{-\frac{1}{2}}\alpha\frac{\omega^4}{\nu^4}\int_0^\infty ds\, e^{-s}\Bigg\{s^2\left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{1}{2}\frac{\omega^2}{\nu^2}\cdot s\right]^{-\frac{3}{2}}$$

$$-\frac{3}{2}s^3\left[\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1+e^{-\nu s}\right)+\frac{\omega^2}{\nu^2}\right]\left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{1}{2}\frac{\omega^2}{\nu^2}\cdot s\right]^{-\frac{5}{2}}$$

$$+\frac{3\times5}{16}s^4\left[\frac{1}{2}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{\omega^2}{\nu^2}\right]^2\left[\frac{1}{2\nu}\left(1-\frac{\omega^2}{\nu^2}\right)\left(1-e^{-\nu s}\right)+\frac{1}{2}\frac{\omega^2}{\nu^2}s\right]^{-\frac{7}{2}}\Bigg\},$$

(5.54)

in which we recall that the two parameters ν and ω to be employed so as to attain the optional value of $\overset{*}{m}$ are those obtained by Feynman in Chapter III.

Obviously, for $\alpha=0$; $\nu=\omega$ the polaron effective mass reduces to

$$\overset{*}{m} = 1 \qquad \text{or} \qquad \frac{\overset{*}{m}}{m_{eff}} = 1 , \tag{5.55}$$

the effective mass of bare electron in absence of electron-lattice interaction.

In case of weak coupling, $\alpha \simeq 0$, in which $\nu \simeq \omega$, setting $\nu = (1+\epsilon)\omega$; $\epsilon \ll 1$ in (5.54) and keeping the order of expansions in powers of ϵ up to ϵ^2 or $\alpha\epsilon$, we find

$$\overset{*}{m} = 1-4\epsilon^2+\frac{1}{3}\cdot 2^{-\frac{3}{2}}\pi^{-\frac{1}{2}}\alpha\,(1-4\epsilon)\int_0^\infty ds\, e^{-s}\Big\{\frac{s^{-\frac{1}{2}}}{2^{-3/2}}\Big[1-\frac{3\epsilon}{\omega}\cdot\frac{1}{s}(1-e^{-\omega s}-\omega s)\Big]$$

$$-\frac{3}{2}\cdot\frac{s^{\frac{1}{2}}}{2^{-\frac{5}{2}}}\Big[\epsilon(e^{-\omega s}-1)+1-\frac{5\epsilon}{\omega}\cdot\frac{1}{s}\left(1-e^{-\omega s}-\omega s\right)\Big]$$

$$+\frac{3\times 5}{16}\frac{s^{\frac{1}{2}}}{2^{-7/2}}\Big[2\epsilon\,(e^{-\omega s}-1)+1-\frac{7\epsilon}{\omega}\cdot\frac{1}{s}(1-e^{-\omega s}-\omega s)\Big] \qquad (5.56)$$

Performing the integrations and ignoring terms of order higher than α^2, we have, in terms of ϵ and ω ,

$$\overset{*}{m} = 1-4\epsilon^2+\frac{7}{24}\alpha+\frac{\epsilon-\alpha}{3}\Big[-\frac{19}{8}-\frac{3\times 19}{4\omega}+\frac{3\times 19}{4\omega(1+\omega)^{1/2}}+\frac{3\times 3}{4\,(1+\omega)^{3/2}}\Big]. \quad (5.57)$$

In this limit the appropriate values of ω and ϵ and (5.57) found to be

$$\omega = 3 \quad \text{and} \quad \epsilon = \frac{2\alpha}{27} \quad ,$$

therefore our $\overset{*}{m}$ in terms of coupling constant α is

$$\overset{*}{m} = 1+\frac{7}{24}\alpha+\alpha^2\,(-0.017-0.022)$$

$$= 1+0.291\alpha-0\,(\alpha^2) \qquad (5.58)$$

For strong coupling, $\alpha \gg 1;\ \nu \gg 1$; $\frac{\omega}{\nu} \ll 1$, expanding the radical terms in (5.54) in powers of $\frac{1}{\nu}$, and neglecting $e^{-\nu s}$, we finally arrive at

$$\overset{*}{m} = \frac{1}{3}2^{-3/2}\pi^{-\frac{1}{2}}\alpha\,\frac{\omega^4}{\nu^4}\int_0^\infty ds\, e^{-s}\Big\{s^2\left(\frac{1}{2\nu}\right)^{-\frac{3}{2}}\Big[1-\frac{3}{2}\frac{\omega^2}{\nu}s\Big]-\frac{3}{2}s^3\cdot\frac{1}{2}\left(\frac{1}{2\nu}\right)^{-\frac{5}{2}}\Big[1-\frac{5}{2}\frac{\omega^2}{\nu}s\Big]$$

$$+\frac{3\times 5}{16}s^4\cdot\frac{1}{4}\left(\frac{1}{2\nu}\right)^{-\frac{7}{2}}\Big[1-\frac{7}{2}\frac{\omega^2}{\nu}s\ \Big] \qquad (5.59)$$

Keeping only zeroth-order terms in the expansion, we have

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

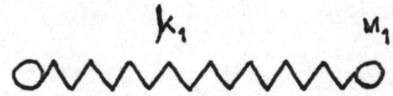
$$= \pi^{-\frac{1}{2}}\alpha\omega^4\Big[\frac{2}{3\nu^{5/2}}-\frac{3}{\nu^{3/2}}+\frac{5\times 3}{2.\nu^{1/2}}\Big]. \qquad (5.60)$$

The suitable ω and ν to be used in this case are

$$\omega = 1 \quad \text{and} \quad \nu \simeq \left(\frac{4}{9}\,\frac{\alpha^2}{\pi}\right)$$

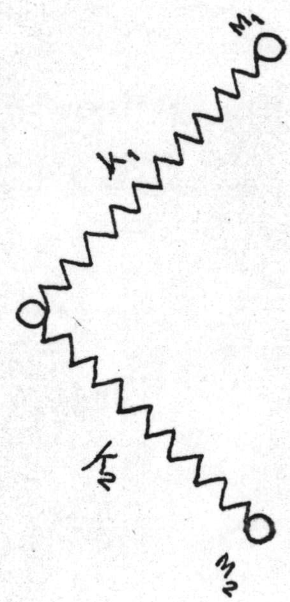
As a result, the value of $\overset{*}{m}$ takes the anomalous form:

$$\overset{*}{m} = O(\alpha^{-4}) - O(\alpha^{-2}) + \frac{45}{4} \tag{5.61}$$



$K_1 = M_1\omega_1^2, \quad 4C_1 = M_1\omega_1^3$

Fig.IV The Two Coupled Particle Model



$K_1 = M_1\omega_1^2, \quad 4C_1 = M_1\omega_1^3$

$K_2 = M_2\omega_2^2, \quad 4C_2 = M_2\omega_2^3$

Fig.V The Three Coupled Particle Model