CHAPTER VI

AN IMPROVEMENT OF THE POLARON THEORY AT FINITE TEMPERATURES

In this chapter, we shall discuss an improvement of the polaron theory at finite temperatures based upon the use of a new trial action which resembles that of Osaka but which has two additional parameters.

VI.1 Statement of the Problem

In the previous chapters, the polaron theory at absolute zero temperature was first presented and then it was shown how this theory had been improved by Abe and Okamoto[13]. It is therefore of interest to attempt to improve in a corresponding manner the polaron theory at finite temperatures as already discussed in Chapter V. It is reasonable to expect that the polaron energy thus obtained will be accurate and will have a slightly lower value than that obtained by using Osaka's original treatment.

To evaluate the polaron energy, the canonical partition function Z is required. Since

$$Z = \int_{-\infty}^{\infty} d\underset{\sim}{r}_{el}\, \rho(\underset{\sim}{r}_{el}, \underset{\sim}{r}_{el}; \beta) \quad , \tag{6.1}$$

then the density matrix of the system must be determined first. To do this, we have to evaluate the path integral

$$\rho(\underset{\sim}{r}_{el}, \underset{\sim}{r}_{el}; \beta) = \int \mathcal{D}\underset{\sim}{r}_{el}(t)\, \exp S \quad , \tag{6.2}$$

where S is the polaron action, given by

$$S = -\frac{1}{2}\int_0^\beta \left(\frac{d\underset{\sim}{r}_{el}(t)}{dt}\right)^2 dt + \frac{\alpha}{2^{3/2}}\left\{\frac{e^\beta}{e^\beta-1}\iint_0^\beta dt\,ds\,\frac{e^{-|t-s|}}{|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|} + \frac{1}{e^\beta-1}\iint_0^\beta dt\,ds\,\frac{e^{|t-s|}}{|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|}\right\}. \quad (6.3)$$

The difficulty with the path integral (6.2) is that the polaron action S is not quadratic in $\underset{\sim}{r}_{el}$ and $\dot{\underset{\sim}{r}}_{el}$. Since only quadratic actions lead to integrable path integrals, we must then introduce a trial action S_1 which is integrable and resembles the exact action.

VI.2 The New Trial Action

Osaka has made a choice of trial action S_1 at finite temperatures as

$$S_1 = -\frac{1}{2}\int_0^\beta \left(\frac{d\underset{\sim}{r}_{el}(t)}{dt}\right)^2 dt - \frac{c}{2}\left\{\frac{e^{\beta\omega}}{e^{\beta\omega}-1}\iint_0^\beta dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega|t-s|} + \frac{1}{e^{\beta\omega}-1}\iint_0^\beta dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{\omega|t-s|}\right\}. \quad (6.4)$$

We shall consider instead the trial action

$$S_1 = -\frac{1}{2}\int_0^\beta \left(\frac{d\underset{\sim}{r}_{el}(t)}{dt}\right)^2 dt - \frac{c_1}{2}\left\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}\iint_0^\beta dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_1|t-s|} + \frac{1}{e^{\beta\omega_1}-1}\iint_0^\beta dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{\omega_1|t-s|}\right\}$$
$$-\frac{c}{2}\left\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}\iint_0^\beta dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{-\omega_2|t-s|} + \frac{1}{e^{\beta\omega_2}-1}\iint_0^\beta dt\,ds\,|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2 e^{\omega_2|t-s|}\right\}, \quad (6.5)$$

which roughly approximates the exact action S, and where the inverted distance terms are replaced by the parabolic terms $|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(S)|^2$. The physical meaning of the trial action S_1 is that of an electron interacting with two fictitious particles. The strength of the interaction is described by a harmonic potential, and the frequencies can be varied by means of the parameters C_1, C_2 and ω_1, ω_2. The four variable parameters will be later adjusted to minimize the polaron energy. We note that the trial action (6.5) resembles that of Osaka closely, but that the former has two more adjustable parameters.

VI.3 Evaluation of the Polaron Energy

In order to evaluate the polaron free energy, consider first the partition function Z which is given as

$$Z = e^{-\beta F} \quad , \tag{6.6}$$

and

$$Z = \int_{-\infty}^{\infty} d\underset{\sim}{r}_{el}\, \rho(\underset{\sim}{r}_{el}, \underset{\sim}{r}_{el}; \beta) \quad , \tag{6.7}$$

where

$$\rho(\underset{\sim}{r}_{el}, \underset{\sim}{r}_{el}; \beta) = \int_{r_{el}}^{r_{el}} d\underset{\sim}{r}_{el}(t)\, e^{S} \quad . \tag{6.8}$$

The partition function can be expressed in terms of path integrals. By substituting (6.8) for (6.7), we obtain

$$Z = \int_{-\infty}^{\infty}\int_{r_{el}}^{r_{el}} \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S}\, d\underset{\sim}{r}_{el} = e^{-\beta F} \quad . \tag{6.9}$$

Similarly the partition function associated with the trial action S_1 can be written as

$$Z_1 = \int_{-\infty}^{\infty}\int_{r_{el}}^{r_{el}} \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}\, d\underset{\sim}{r}_{el} = e^{-\beta F_1} \quad . \tag{6.10}$$

So that

$$\frac{\int_{-\infty}^{\infty}\int_{r_{el}}^{r_{el}} \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S}\, d\underset{\sim}{r}_{el}}{\int_{-\infty}^{\infty}\int_{r_{el}}^{r_{el}} \mathcal{D}\underset{\sim}{r}_{el}(t)\, e^{S_1}\, d\underset{\sim}{r}_{el}} = e^{-\beta(F - F_1)} \quad . \tag{6.11}$$

By using $e^{S} = e^{S - S_1} . e^{S_1}$ the above equation can be reduced to

$$\frac{\int_{-\infty}^{\infty}\int_{r_{el}}^{r_{el}} \mathcal{D} r_{el}(t)\, e^{S-S_1} \cdot e^{S_1} d r_{el}}{\int_{-\infty}^{\infty}\int_{r_{el}}^{r_{el}} \mathcal{D} r_{el}(t)\, e^{S_1} d r_{el}} = e^{-\beta(F-F_1)} , \qquad (6.12)$$

i.e.
$$\langle e^{S-S_1} \rangle = e^{-\beta(F-F_1)} , \qquad (6.13)$$

where the average value of e^{S-S_1} is taken over all paths with the same initial and final points and the weight of each path is $e^{S_1}\mathcal{D} \underset{\sim}{r}_{el}(t)$, including all possible values of $\underset{\sim}{r}_{el}$ in the averaging process.

By using the general inequality

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

for any variable x, (6.13) becomes

$$e^{-\beta(F-F_1)} \geq e^{\langle S-S_1 \rangle} . \qquad (6.14)$$

Therefore we obtain the variational principle

$$\beta(F-F_1) \leq -\langle S-S_1 \rangle$$

or

$$F \leq F_1 - \frac{1}{\beta}\langle S \rangle + \frac{1}{\beta}\langle S_1 \rangle . \qquad (6.15)$$

We note that the Feynman variational principle of the ground state polaron energy is now replaced by the variational principle of the free energy. The problem is to find the trial free energy

$$F_{tr} = F_1 - \frac{1}{\beta}\langle S \rangle + \frac{1}{\beta}\langle S_1 \rangle = -\frac{1}{\beta}(\ln z_1 + \langle S \rangle + \langle S_1 \rangle) , \qquad (6.16)$$

and then to minimize with respect to the four variable parameters. Thus we require the values of $\langle S \rangle$ and $\langle S_1 \rangle$ which are given by

$$\langle S \rangle = \frac{\alpha}{2^{3/2}} \iint_0^{\beta} dt\,ds \left\{ \frac{e^{\beta}}{e^{\beta}-1} e^{-|t-s|} + \frac{1}{e^{\beta}-1} e^{|t-s|} \right\} \langle |\underset{\sim}{r}_{el}(t) - \underset{\sim}{r}_{el}(s)|^{-1} \rangle , \qquad (6.17)$$

and

$$\langle S_1\rangle = -\frac{C_1}{2}\int_0^\beta\int dt\,ds\left\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}\cdot e^{-\omega_1|t-s|}+\frac{1}{e^{\beta\omega_1}-1}e^{\omega_1|t-s|}\right\}\langle|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2\rangle$$
$$-\frac{C_2}{2}\int_0^\beta\int dt\,ds\left\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}\cdot e^{-\omega_2|t-s|}+\frac{1}{e^{\beta\omega_2}-1}e^{\omega_2|t-s|}\right\}\langle|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2\rangle. \quad (6.18)$$

In order to calculate $\langle S\rangle$, it is necessary to evaluate $\langle|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^{-1}\rangle$ which is expressed by a Fourier transform as

$$\langle|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^{-1}\rangle = \int\frac{d^3\underset{\sim}{K}}{2\pi K^2}\langle\exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s))]\rangle \quad . \quad (6.19)$$

Therefore our problem is to find $\langle\exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s))]\rangle$, and to subsequently apply the second order differentiation with respect to $\underset{\sim}{K}$ on this form. The averages $\langle S\rangle$ and $\langle S_1\rangle$ can then be obtained if $\langle\exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s))]\rangle$ given by

$$\langle\exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\rangle = \frac{\int\mathcal{D}\underset{\sim}{r}_{el}(t)\exp[\int\underset{\sim}{f}(t)\cdot\underset{\sim}{r}_{el}(t)\,dt]\,e^{S_1}}{\int\mathcal{D}\underset{\sim}{r}_{el}(t)\,e^{S_1}}, \quad (6.20)$$

where $\underset{\sim}{f}(t) = i\underset{\sim}{K}(\delta(t-\tau)-\delta(t-\sigma))$, can be determined.

Since the three rectangular components of the electron motions (6.18) can be separated, we need to consider explicitly only one component, say the x-component. Hence, aside from a normalization factor, (6.20) can be reduced to

$$\langle\exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\rangle = \int\mathcal{D}x(t)\exp\Big[-\frac{1}{2}\int_0^\beta\left(\frac{dx(t)}{dt}\right)^2dt-\frac{C_1}{2}\Big\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}\int_0^\beta\int dt\,ds[x(t)-x(s)]^2e^{-\omega_1|t-s|}$$
$$+\frac{1}{e^{\beta\omega_1}-1}\int_0^\beta\int dt\,ds\,[x(t)-x(s)]^2e^{\omega_1|t-s|}\Big\}-\frac{C_2}{2}\Big\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}\int_0^\beta\int dt\,ds\cdot$$
$$[x(t)-x(s)]^2e^{-\omega_2|t-s|}+\frac{1}{e^{\beta\omega_2}-1}\int_0^\beta\int dt\,ds[x(t)-x(s)]^2e^{\omega_2|t-s|}\Big\}$$
$$+\int_0^\beta f_x(t)\,x(t)\,dt\Big].$$

The integration is carried out after substitution of $x(t)$ by $\bar{x}(t) + y(t)$, where $\bar{x}(t)$ is the classical path and $y(t)$ is now the variable of integration. The integration terms of $y(t)$ give an unimportant constant independent of f_x. Then we obtain

$$\langle \exp[iK_x(x(\tau)-x(\sigma))]\rangle = \exp\Big[-\frac{1}{2}\int_0^\beta \dot{\bar{x}}^2(t)dt - \frac{c_1}{2}\Big\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}\iint_0^\beta dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2 e^{-\omega_1|t-s|}$$
$$+ \frac{1}{e^{\beta\omega_1}-1}\iint_0^\beta dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2 e^{\omega_1|t-s|}\Big\} - \frac{c_2}{2}\Big\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}\cdot$$
$$\iint_0^\beta dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2 e^{-\omega_2|t-s|} + \frac{1}{e^{\beta\omega_2}-1}\iint_0^\beta dt\,ds\,[\bar{x}(t)-\bar{x}(s)]\times$$
$$e^{\omega_2|t-s|}\Big\} + \int f_x(t)\,\bar{x}(t)\,dt\Big], \qquad (6.21)$$

where the classical path $\bar{x}(t)$ satisfies the principle of least action. The action corresponding to the above expression is

$$S' = -\frac{1}{2}\int_0^\beta \dot{\bar{x}}^2(t)dt - \frac{c_1}{2}\iint_0^\beta dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2\Big\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}e^{-\omega_1|t-s|} + \frac{1}{e^{\beta\omega_1}-1}e^{\omega_1|t-s|}\Big\}$$
$$-\frac{c_2}{2}\iint_0^\beta dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2\Big\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}e^{-\omega_2|t-s|} + \frac{1}{e^{\beta\omega_2}-1}e^{\omega_2|t-s|}\Big\}$$
$$+\int_0^\beta f_x(t)\,\bar{x}(t)\,dt\ . \qquad (6.22)$$

Hence

$$\delta S' = 0 = -\frac{1}{2}\int_0^\beta 2\dot{\bar{x}}(t)\,\delta\dot{\bar{x}}(t)dt - \frac{c_1}{2}\iint_0^\beta dt\,ds\,2[\bar{x}(t)-\bar{x}(s)]\,\delta(\bar{x}(t)-\bar{x}(s))\,\{A_1\}$$
$$-\frac{c_2}{2}\iint_0^\beta dt\,ds\,2[\bar{x}(t)-\bar{x}(s)]\,\delta(\bar{x}(t)-\bar{x}(s))\,\{A_2\}$$
$$+\int_0^\beta f_x(t)\,\delta\bar{x}(t)\,dt\ , \qquad (6.23)$$

where

$$A_1 = \left\{ \frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1} \cdot e^{-\omega_1|t-s|} + \frac{1}{e^{\beta\omega_1}-1} e^{\omega_1|t-s|} \right\} , \qquad (6.24a)$$

and

$$A_2 = \left\{ \frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1} \cdot e^{-\omega_2|t-s|} + \frac{1}{e^{\beta\omega_2}-1} e^{\omega_2|t-s|} \right\} . \qquad (6.24b)$$

By interchanging the imaginary time variables t and s of some terms in (6.23), we obtain

$$0 = -\dot{\bar{x}}(x)\delta\bar{x}(t)\Big|_0^\beta + \int_0^\beta \ddot{\bar{x}}(t)\,\delta\bar{x}(t)dt - c_1 \iint_0^\beta dt\,ds[\bar{x}(t)-\bar{x}(s)]\,\delta\bar{x}(t)\,\{A_1\}$$

$$+ c_1 \iint_0^\beta ds\,dt[\bar{x}(s)-\bar{x}(t)]\,\delta\bar{x}(t)\,\{A_1\} - c_2 \iint_0^\beta dt\,ds[\bar{x}(t)-\bar{x}(s)]\,\delta\bar{x}(t)\,\{A_2\}$$

$$+ c_2 \iint_0^\beta ds\,dt[\bar{x}(s)-\bar{x}(t)]\,\delta\bar{x}(t)\{A_2\} + \int_0^\beta f_x(t)\,\delta\bar{x}(t)dt$$

$$= \int_0^\beta dt\left[\ddot{\bar{x}}(t) - 2c_1\int_0^\beta ds[\bar{x}(t)-\bar{x}(s)]\,\{A_1\} - 2c_2\int_0^\beta ds[\bar{x}(t)-\bar{x}(s)]\{A_2\} + f_x(t)\right]\delta\bar{x}(t).$$

Thus

$$\ddot{\bar{x}}(t) = 2c_1\bar{x}(t)\int_0^\beta ds\{A_1\} - 2c_1\int_0^\beta ds\,\bar{x}(s)\{A_1\} + 2c_2\bar{x}(t)\int_0^\beta ds\{A_2\} - 2c_2\int_0^\beta ds\,\bar{x}(s)\{A_2\} - f_x(t). \qquad (6.25)$$

Consider the values of $\int_0^\beta ds\,\{A_1\}$ and $\int_0^\beta ds\,\{A_2\}$.

We have

$$\int_0^\beta ds\{A_1\} = \int_0^\beta ds\left\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1} e^{\omega_1|t-s|} + \frac{1}{e^{\beta\omega_1}-1} e^{\omega_1|t-s|}\right\}$$

$$= \frac{e^{\beta\omega_1}}{(e^{\beta\omega_1}-1)\omega_1}\left[1 - e^{-\omega_1 t} - e^{\omega_1(t-\beta)} + 1\right] + \frac{1}{(e^{\beta\omega_1}-1)\omega_1}\left[-1 + e^{\omega_1 t} + e^{-\omega_1(t-\beta)} - 1\right]$$

$$= \frac{2}{\omega_1} . \qquad (6.26a)$$

Similarly $$\int_0^\beta ds\,\{A_2\} = \frac{2}{\omega_2} . \qquad (6.26b)$$

We remark that the result of the integration does not depend on β. Therefore if we take $\beta=\infty$, (6.26a) becomes

$$\int_0^\beta ds\, e^{-\omega_1|t-s|} = \frac{2}{\omega_1}, \qquad (6.26c)$$

which proves the validity of certain expressions that we have used in the previous chapters.

By using (6.26a) and (6.26b) for (6.25), we obtain the equation of motion of the classical path $\bar{x}(t)$ as

$$\frac{d^2\bar{x}(t)}{dt^2} = \frac{4C_1}{\omega_1}\bar{x}(t) - 2C_1\int_0^\beta ds\,\bar{x}(s)\left\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}\cdot e^{-\omega_1|t-s|} + \frac{1}{e^{\beta\omega_1}-1}\cdot e^{\omega_1|t-s|}\right\}$$

$$+\frac{4C_2}{\omega_2}\bar{x}(t) - 2C_2\int_0^\beta ds\,\bar{x}(s)\left\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}\cdot e^{-\omega_2|t-s|} + \frac{1}{e^{\beta\omega_2}-1}\cdot e^{\omega_2|t-s|}\right\} - f_x(t), \qquad (6.27)$$

with the boundary conditions $\bar{x}(0) = \bar{x}(\beta) = 0$.

Eq.(6.21) can be written as

$$\langle \exp[iK_x(x(\tau)-x(\sigma))]\rangle = \exp\Big[-\frac{1}{2}\dot{\bar{x}}(t)\bar{x}(t)\Big|_0^\beta + \frac{1}{2}\int_0^\beta \ddot{\bar{x}}(t)\bar{x}(t)\,dt - \frac{C_1}{2}\int_0^\beta\!\!\int dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2\{A_1\}$$

$$-\frac{C_2}{2}\int_0^\beta\!\!\int dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2\{A_2\} + \int_0^\beta f_x(t)\,\bar{x}(t)\,dt\Big].$$

After substituting (6.25) in the above equation, it becomes

$$\langle \exp[iK_x(x(\tau)-x(\sigma))]\rangle = \exp\Big[C_1\int_0^\beta\!\!\int dt\,ds\,(\bar{x}(t)-\bar{x}(s))\,\bar{x}(t)\,\{A_1\} - C_2\int_0^\beta\!\!\int dt\,ds\,(\bar{x}(t)-\bar{x}(s))\,\bar{x}(t)\{A_2\}$$

$$-\frac{1}{2}\int_0^\beta f_x(t)\bar{x}(t)\,dt - \frac{C_1}{2}\int_0^\beta\!\!\int dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2\{A_1\}$$

$$-\frac{C_2}{2}\int_0^\beta\!\!\int dt\,ds\,[\bar{x}(t)-\bar{x}(s)]^2\{A_2\} + \int_0^\beta f_x(t)\,\bar{x}(t)\,dt\Big]$$

$$= \exp\left[\frac{iKx}{2}\left(\bar{x}(\tau)-\bar{x}(\sigma)\right)\right]. \qquad (6.28)$$

We note that the above relation is the same as those obtained from the polaron state at absolute zero temperature, viz.(3.51) and (4.9), but the classical path $\bar{x}$ is now the solution of the more complicated integro-differential equation (6.27), which can be converted to an ordinary differential equation by introducing

$$Y(t) = \frac{\omega_1}{2}\int_0^\beta ds\,\bar{x}(s)\left\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}\cdot e^{-\omega_1|t-s|} + \frac{1}{e^{\beta\omega_1}-1}\,e^{\omega_1|t-s|}\right\}, \tag{6.29}$$

and

$$Z(t) = \frac{\omega_2}{2}\int_0^\beta ds\,\bar{x}(s)\left\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}\cdot e^{-\omega_2|t-s|} + \frac{1}{e^{\beta\omega_2}-1}\cdot e^{\omega_2|t-s|}\right\}, \tag{6.30}$$

thus

$$\frac{d^2\bar{x}(t)}{dt^2} = \frac{4c_1}{\omega_1}\bar{x}(t) - \frac{4c_1}{\omega_1}Y(t) + \frac{4c_2}{\omega_2}\bar{x}(t) - \frac{4c_2}{\omega_2}Z(t) - f_x(t). \tag{6.31}$$

By performing the second order differentiation with respect to time t on (6.29) and (6.30) we obtain

$$\frac{d^2Y(t)}{dt^2} = \omega_1^2\left[Y(t) - \bar{x}(t)\right], \tag{6.32}$$

and

$$\frac{d^2Z(t)}{dt^2} = \omega_2^2\left[Z(t) - \bar{x}(t)\right]. \tag{6.33}$$

The equations of motion of $\bar{x}(t)$, $Y(t)$, and $Z(t)$ can be easily separated. The differential equation of motion of the classical path $\bar{x}(t)$ is

$$\left\{D^6 - (\nu_1^2+\nu_2^2)D^4 + (\nu_2^2\omega_1^2+\nu_1^2\omega_2^2-\omega_1^2\omega_2^2)D^2\right\}\bar{x}(t) = -(D^2-\omega_2^2)(D^2-\omega_1^2)f_x(t), \tag{6.34}$$

which can be solved by using Laplace transform. After the transformation we obtain.

$$p^6 f(p) - p^5 \bar{x}(0) - p^4 \dot{\bar{x}}(0) - p^3 \ddot{\bar{x}}(0) - p^2 \dddot{\bar{x}}(0) - p \ddddot{\bar{x}}(0) - \overset{.....}{\bar{x}}(0) = -\int_0^\infty e^{-p\tau}(D^2-\omega_2^2)(D^2-\omega_1^2) f_x(t)\,dt \,.$$

$$-(v_1^2+v_2^2)\left[p^4 f(p) - p^3 \bar{x}(0) - p^2 \dot{\bar{x}}(0) - p \ddot{\bar{x}}(0) - \dddot{\bar{x}}(0)\right] \qquad (6.35)$$

$$+ (v_2^2\omega_1^2 + v_1^2\omega_2^2 - \omega_1^2\omega_2^2)\left[p^2 f(p) - p\bar{x}(0) - \dot{\bar{x}}(0)\right]$$

We have neglected the transient terms in the case of polaron at absolute zero temperature. But for the polaron at finite temperatures, which we are now dealing with, the time interval $(0, \beta)$ is finite. Therefore the terms $\dot{\bar{x}}(0)$, $\ddot{\bar{x}}(0)$, $\dddot{\bar{x}}(0)$,..... ...., $\overset{.....}{\bar{x}}(0)$ must also be considered; Eq.(6.35) then becomes

$$f(p) = \frac{-iK_x\left[p^4-(\omega_1^2+\omega_2^2)p^2+\omega_1^2\omega_2^2\right](e^{-p\tau}-e^{-p\sigma})}{p^6-(v_1^2+v_2^2)p^4+Ap^2} + \frac{(c_1p^4+b_2p^2+b_3)+(c_2p^3+b_4p)}{p^6-(v_1^2+v_2^2)p^4+Ap^2}, \qquad (6.35a)$$

where $\dot{\bar{x}}(0) = c_1$, $\ddot{\bar{x}}(0) = c_2$,.........., $\overset{.....}{\bar{x}}(0) = c_5$,

$$A = v_2^2\omega_1^2 + v_1^2\omega_2^2 - \omega_1^2\omega_2^2 ,$$

and

$$b_2 = c_3 - (v_1^2+v_2^2)c_1 ,$$

$$b_3 = c_3 - (v_1^2+v_2^2)c_3 + Ac_1 ,$$

$$b_4 = c_4 - (v_1^2+v_2^2)c_2 .$$

The classical path $\bar{x}(t)$ can be directly determined by applying inverse Laplace transform to (6.35a) The result is

$$\bar{x}(t) = \bar{x}(t)\Big|_{T=0,\,4\text{ Parameters}} + B_1\sinh Q_1t + B_2\sinh Q_2t + B_3\sinh Q_3t + D_1\cosh Q_1t$$
$$+ D_2\cosh Q_2t + D_3\cosh Q_3t , \qquad (6.36)$$

where

$$B_1 = \frac{(c_1Q_1^4+b_2Q_1^2+b_3)}{Q_1(Q_1^2-Q_2^2)(Q_1^2-Q_3^2)}, \quad B_2 = \frac{(c_1Q_2^4+b_2Q_2^2+b_3)}{Q_2(Q_2^2-Q_1^2)(Q_2^2-Q_3^2)}, \quad B_3 = \frac{(c_1Q_3^4+b_2Q_3^2+b_3)}{Q_3(Q_3^2-Q_1^2)(Q_3^2-Q_2^2)}$$

and

$$D_1 = \frac{(C_2 Q_1^3 + b_4 Q_1)}{Q_1(Q_1^2-Q_2^2)(Q_1^2-Q_3^2)}, \quad D_2 = \frac{(C_2 Q_2^3 + b_4 Q_2)}{Q_2(Q_2^2-Q_1^2)(Q_2^2-Q_3^2)}, \quad D_3 = \frac{(C_2 Q_3^3 + b_4 Q_3)}{Q_3(Q_3^2-Q_1^2)(Q_3^2-Q_2^2)} .$$

The values of B_1, B_2, B_3, and D_1, D_2, D_3 are obtained by using the boundary conditions

$$\bar{x}(0) = \bar{x}(0) \Big| + D_1 + D_2 + D_3 = 0 ,$$

$$D_1 + D_2 + D_3 = 0 ,$$

and

$$\bar{X}(\beta) = \bar{x}(\beta)\Big|_{T=0,4P} + B_1 \sinh Q_1\beta + B_2 \sinh Q_2\beta + B_3 \sinh Q_3\beta = 0$$

$$- iK_x\Big[U_1(\sinh Q_1(\beta-\tau) - \sinh Q_1(\beta-\sigma)) + U_2(\sinh Q_2(\beta-\tau) - \sinh Q_2(\beta-\sigma))$$

$$+ U_3(\sinh Q_3(\beta-\tau) - \sinh Q_3(\beta-\sigma)\Big] = -(B_1 \sinh Q_1\beta + B_2 \sinh Q_2\beta + B_3 \sinh Q_3\beta),$$

where the problem is considered under the special condition $D_1 = D_2 = D_3 = 0$.

Hence

$$B_1 = \frac{iK_x U_1(\sinh Q_1(\beta-\tau) - \sinh Q_1(\beta-\sigma))}{\sinh Q_1\beta}, \quad U_1 = \frac{(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)}{Q_1(Q_1^2-Q_2^2)(Q_1^2-Q_3^2)}, \tag{6.37a}$$

$$B_2 = \frac{iK_x U_2(\sinh Q_2(\beta-\tau) - \sinh Q_2(\beta-\sigma))}{\sinh Q_2\beta}, \quad U_2 = \frac{(Q_2^2-\omega_1^2)(Q_2^2-\omega_2^2)}{Q_1(Q_2^2-Q_3^2)(Q_2^2-Q_1^2)}, \tag{6.37b}$$

$$B_3 = \frac{iK_x U_3(\sinh Q_3(\beta-\tau) - \sinh Q_3(\beta-\sigma))}{\sinh Q_3\beta}, \quad U_3 = \frac{(Q_3^2-\omega_1^2)(Q_3^2-\omega_2^2)}{Q_3(Q_3^2-Q_2^2)(Q_3^2-Q_1^2)} . \tag{6.37c}$$

Since Q_1^2, Q_2^2, and Q_3^2, satisfy the cubic equation

$$P^6 - (v_1^2 - v_2^2)P^4 + (v_2^2\omega_1^2 + v_1^2\omega_2^2 - \omega_1^2\omega_2^2)P^2 = 0 ,$$

one root of which is equal to zero, then (6.36) becomes

$$\bar{X}(t) = -iK_x\Big\{U_1'\big[H(t-\tau)\sinh Q_1(t-\tau) - H(t-\sigma)\sinh Q_1(t-\sigma)\big]$$

$$+U_2'\big[H(t-\tau)\sinh Q_2(t-\tau) - H(t-\sigma)\sinh Q_2(t-\sigma)\big]$$

$$+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}\Big[H(t-\tau)\frac{\sinh Q_3(t-\tau)}{Q_3}\Big|_{Q_3=0} - H(t-\sigma)\frac{\sinh Q_3(t-\sigma)}{Q_3}\Big]\Big\}$$

$$-iK_x\Big\{U_1'\frac{(\sinh Q_1(\beta-\tau) - \sinh Q_1(\beta-\sigma))}{\sinh Q_1\beta}\sinh Q_1 t$$

$$+U_2'\frac{(\sinh Q_2(\beta-\tau) - \sinh Q_2(\beta-\sigma))}{\sinh Q_2\beta}\sinh Q_2 t$$

$$+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}\frac{(\sinh Q_3(\beta-\tau) - \sinh Q_3(\beta-\sigma))/Q_3}{(\sinh Q_3\beta)/Q_3}\cdot\frac{\sinh Q_3 t}{Q_3}\Big|_{Q_3=0}\Big\}, \qquad (6.38)$$

where $U_1' = \dfrac{(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)}{Q_1^3(Q_1^2-Q_2^2)}$ and $U_2' = \dfrac{(Q_2^2-\omega_1^2)(Q_2^2-\omega_2^2)}{Q_2^3(Q_2^2-Q_1^2)}$.

From (6.38), we have

$$\bar{X}(t) = -iK_x\Big\{U_1'\Big[H(t-\tau)\sinh Q_1(t-\tau) - H(t-\sigma)\sinh Q_1(t-\sigma) - \frac{(\sinh Q_1(\beta-\tau) - \sinh Q_1(\beta-\sigma))\sinh Q_1 t}{\sinh Q_1\beta}\Big]$$

$$+U_2'\Big[H(t-\tau)\sinh Q_2(t-\tau) - H(t-\sigma)\sinh Q_2(t-\sigma) - \frac{(\sinh Q_2(\beta-\tau) - \sinh Q_2(\beta-\sigma))\sinh Q_2 t}{\sinh Q_2\beta}\Big]$$

$$+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}\Big[H(t-\tau)(t-\tau) - H(t-\sigma)(t-\sigma) + \frac{(\tau-\sigma)}{\beta}t\Big]\Big\}. \qquad (6.39)$$

Substituting (6.39) for (6.28), we obtain

$$\langle\exp[iK_x(x(\tau)-x(\sigma))]\rangle = \exp\Big[\frac{K_x^2}{2}\Big\{U_1'\Big[-\cosh Q_1|\tau-\sigma| + e^{-Q_1|\tau-\sigma|} + 4\cosh Q_1\big(\beta-\tfrac{\tau+\sigma}{2}\big)\sinh Q_1\tfrac{|\tau-\sigma|}{2}\cdot$$

$$\frac{4\cosh Q_1\frac{(\tau+\sigma)}{2}\sinh Q_2\frac{|\tau-\sigma|}{2}}{\sinh Q_1\beta}\Big]$$

$$+U_2'\Big[-\cosh Q_2|\tau-\sigma| + e^{-Q_2|\tau-\sigma|} + \frac{4\cosh Q_2\big(\beta-\frac{\tau+\sigma}{2}\big)\sinh Q_2\frac{|\tau-\sigma|}{2}}{\sinh Q_2\beta}$$

$$\cosh Q_2\frac{(\tau+\sigma)}{2}\sinh Q_2\frac{|\tau-\sigma|}{2}\Big]$$

$$+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}\Big[-|\tau-\sigma|\Big(1-\frac{|\tau-\sigma|}{\beta}\Big)\Big]\Big\}\Big]. \qquad (6.40)$$

Referring to the average of exp $\left[i\underset{\sim}{K}\cdot(\underset{\sim}{r}(\tau)-\underset{\sim}{r}_{el}(\sigma)\right]$ given in Chapter V, if the coordinate R_1 is integrated under the conditions $R_2 = R_1$ and $r_1 = r_2 = 0$, we shall obtain the condition $\tau + \sigma = \beta$. The boundary conditions of the problem under consideration are given by $\underset{\sim}{r}_{el}(0) = \underset{\sim}{r}_{el}(\beta) = 0$. The condition $\tau + \sigma = \beta$ is applied to (6.40) to give

$$\left\langle \exp\left[iK_x\left(x(\tau)-x(\sigma)\right)\right]\right\rangle = \exp\Big[-\frac{K_x^2}{2}\Big\{U_1'\Big[(\cosh Q_1|\tau-\sigma|-1)+(1-e^{-Q_1|\tau-\sigma|})-\coth\frac{Q_1\beta}{2}\cdot(\cosh Q_1|\tau-\sigma|-1)\Big]+U_2'\Big[(\cosh Q_2|\tau-\sigma|-1)+(1-e^{-Q_2|\tau-\sigma|})-\coth\frac{Q_2\beta}{2}(\cosh Q_2|\tau-\sigma|-1)\Big]+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}|\tau-\sigma|\left(1-\frac{|\tau-\sigma|}{\beta}\right)\Big\}\Big]. \tag{6.41}$$

Hence

$$\langle\exp[i\underset{\sim}{K}_x(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\rangle = \exp\left[-\frac{K^2}{2}\,G\left[|t-s|\right]\right], \tag{6.42}$$

where

$$G[|t-s|] = \frac{1}{V_+^2-V_-^2}\Big[\frac{(V_+^2-\omega_1^2)(V_+^2-\omega_2^2)}{V_+^3}\Big\{(1-e^{-V_+|t-s|})+(1-\coth\frac{V_+\beta}{2})(\cosh V_+|\tau-\sigma|-1)\Big\}+\frac{(V_+^2-\omega_2^2)(\omega_1^2-V_-^2)}{V_-^3}\Big\{(1-e^{-V_-|t-s|})+(1-\coth\frac{V_-\beta}{2})(\cosh V_-|\tau-\sigma|-1)\Big\}\Big]+\frac{\omega_2^2\omega_1^2}{V_+^2V_-^2}|\tau-\sigma|\left(1-\frac{|\tau-\sigma|}{\beta}\right), \tag{6.43}$$

and

$$Q_{1,2}^2 = V_{+,-}^2 = \frac{1}{2}\left[V_1^2+V_2^2 \pm\left\{(V_1^2-V_2^2)^2+64\,\frac{C_1C_2}{\omega_1\omega_2}\right\}^{\frac{1}{2}}\right], \tag{6.44}$$

$$V_1^2 = \omega_1^2+\frac{4C_1}{\omega_1}, \quad V_2^2 = \omega_2^2+\frac{4C_2}{\omega_2}. \tag{6.45}$$

The variables C_1 and C_2 are represented by $V_\pm$, ω_1, ω_2 as

$$\frac{4C_1}{\omega_1} = -\frac{1}{\omega_1^2-\omega_2^2}(V_+^2-\omega_1^2)(V_-^2-\omega_1^2), \tag{6.46}$$

$$\frac{4C_2}{\omega_2} = \frac{1}{\omega_1^2-\omega_2^2}(V_+^2-\omega_2^2)(V_-^2-\omega_2^2). \tag{6.47}$$

Although the method we have just used for the determination of $\left\langle \exp\left[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s))\right]\right\rangle$ can under suitable circumstances lead to the desired results in a relatively simple manner, it is not very generally applicable. A more general method will now be introduced.

Owing to the difficulties in solving the complicated integro-differential equation (6.27) in the general case, the polaron model that corresponds to the trial action S_1 will be introduced. Since the physical meaning of S_1 in (6.5) is that of an electron interacting with two fictitious particles through the harmonic potential, we can represent the action S_1 of this simple physical system by means of the model Lagrangian L' for the three coupled particle model, viz.,

$$L' = \frac{1}{2}\dot{\underset{\sim}{r}}^2 + \frac{1}{2}M_1\dot{\underset{\sim}{R}}_1^2 - \frac{1}{2}k_1\cdot(\underset{\sim}{r}-\underset{\sim}{R}_1)^2 + \frac{1}{2}M_2\dot{\underset{\sim}{R}}_2^2 - \frac{1}{2}k_2(\underset{\sim}{r}-\underset{\sim}{R}_2)^2, \tag{6.48}$$

where m_1, m_2 refer to the masses of the two fictitious particles. By a method similar to that used in Section V.2, we obtain the motion of the electron that is described by the trial action S_1 as the solution of (6.48), and we can represent $\underset{\sim}{r}_{el}(t)$ by $\underset{\sim}{r}(t)$ under the conditions $k_1 = \frac{4C_1}{\omega_1}$, $\omega_1' = \omega_1$, $M_1\omega_1'^3 = 4C_1$ and $k_2 = \frac{4C_2}{\omega_2}$, $\omega_2' = \omega_2$, $M_2\omega_2'^3 = 4C_2$.

Then the path integral of the trial actions S_1 is replaced by the path integral of the Lagrangian L'. The path integral of (6.20) can therefore be replaced by the following Lagrangian

$$L = \frac{1}{2}\dot{\underset{\sim}{r}}^2 + \frac{1}{2}M_1\dot{\underset{\sim}{R}}_1^2 - \frac{1}{2}k_1(\underset{\sim}{r}-\underset{\sim}{R}_1)^2 + \frac{1}{2}M_2\dot{\underset{\sim}{R}}_2^2 - \frac{1}{2}k_2(\underset{\sim}{r}-\underset{\sim}{R}_2)^2 + \underset{\sim}{f}(t)\cdot\underset{\sim}{r} \,. \tag{6.49}$$

Let us introduce new variables in the center of mass coordinate system as follows

$$\underset{\sim}{q}_1 = \underset{\sim}{r} - \underset{\sim}{R}_1 \quad , \quad \underset{\sim}{q}_2 = \underset{\sim}{r} - \underset{\sim}{R}_2 \quad , \quad \underset{\sim}{Q}_o = \frac{\underset{\sim}{r} + M_1\underset{\sim}{R}_1 + M_2\underset{\sim}{R}_2}{1 + M_1 + M_2} . \qquad (6.50)$$

Then the Lagrangian (6.50) is written as

$$L = \frac{1}{2} A\dot{\underset{\sim}{q}}_1^2 - \frac{1}{2} k_1\underset{\sim}{q}_1^2 + \frac{M_1}{M_T} \underset{\sim}{f}(t).\underset{\sim}{q}_1 + \frac{1}{2} B\dot{\underset{\sim}{q}}_2^2 - \frac{1}{2} k_2\underset{\sim}{q}_2^2$$
$$+ \frac{M_2}{M_T} \underset{\sim}{f}(t).\underset{\sim}{q}_2 - C\dot{\underset{\sim}{q}}_1\dot{\underset{\sim}{q}}_2 + \frac{M_T}{2} \dot{\underset{\sim}{Q}}_o^2 + \underset{\sim}{Q}_o.\underset{\sim}{f}(t), \qquad (6.51)$$

where the total mass of the system is given by $M_T = 1+M_1+M_2$, and

$$A = \frac{M_1(M_2 +1)}{M_T} \quad , B = \frac{M_2(M_1 +1)}{M_T} \quad , \quad C = \frac{M_1M_2}{M_T} \quad . \qquad (6.52)$$

The equations of motion of $\underset{\sim}{q}_1$, $\underset{\sim}{q}_2$ and $\underset{\sim}{Q}_o$ can be derived from the principle of least action. Since we have used the imaginary time in the trial action then the Lagrangian (6.51) must also be written in the from involving the imaginary time and we thus obtain

$$\delta S = 0 = -A\dot{\underset{\sim}{q}}_1.\delta\underset{\sim}{q}_1\Big|_0^\beta - B\dot{\underset{\sim}{q}}_2.\delta\underset{\sim}{q}_2\Big|_0^\beta + C\dot{\underset{\sim}{q}}_1 . \delta\underset{\sim}{q}_2\Big|_0^\beta - M_T\dot{\underset{\sim}{Q}}_o.\delta\underset{\sim}{Q}_o\Big|_0^\beta$$
$$+ \int_0^\beta \Big\{\Big[A\ddot{\underset{\sim}{q}}_1 - k_1\underset{\sim}{q}_1 + \frac{M_1}{M_T}\underset{\sim}{f}(t) - C\ddot{\underset{\sim}{q}}_2\Big]\delta\underset{\sim}{q}_1 + \Big[B\ddot{\underset{\sim}{q}}_2 - k_2\underset{\sim}{q}_2 - C\ddot{\underset{\sim}{q}}_1 + \frac{M_2}{M_1}\underset{\sim}{f}(t)\Big]\delta\underset{\sim}{q}_2$$
$$+ \Big[M_T\ddot{\underset{\sim}{Q}}_o + \underset{\sim}{f}(t)\Big].\delta\underset{\sim}{Q}_o\Big\} dt \quad .$$

It follows that

$$A\ddot{\underset{\sim}{q}}_1 - C\ddot{\underset{\sim}{q}}_2 - k_1\underset{\sim}{q}_1 + \frac{M_1}{M_T} \underset{\sim}{f}(t) = 0 \quad , \qquad (6.53)$$

$$B\ddot{\underset{\sim}{q}}_2 - C\ddot{\underset{\sim}{q}}_1 - k_2\underset{\sim}{q}_2 + \frac{M_2}{M_T} \underset{\sim}{f}(t) = 0 \quad , \qquad (6.54)$$

$$\ddot{\underset{\sim}{Q}}_0 = -\frac{f(t)}{M_T} . \tag{6.55}$$

The variables $\underset{\sim}{q}_1$ and $\underset{\sim}{q}_2$ in equations of motion (6.53) and (6.54) can be separated. The results are

$$[(AB-C^2)D^4-(k_2A+k_1B)D^2+k_1k_2]\underset{\sim}{q}_1 + \frac{[M_1(BD^2-k_2)+CD^2M_2)]}{M_T}\underset{\sim}{f}(t) = 0 , \tag{6.56}$$

$$[(AB-C^2)D^4-(K_2A+k_1B)D^2-C^2D^2]\underset{\sim}{q}_2 + \frac{[M_2(AD^2-k_1)+CD^2M_1]}{M_T}\underset{\sim}{f}(t) = 0 , \tag{6.57}$$

where $D = \frac{d}{dt}$.

We rewrite (6.56) in the simple form

$$(D^2-Q_1^2)(D^2-Q_2^2)\underset{\sim}{q}_1 = \frac{-[(M_1B+CM_2)D^2-k_2M_1]}{M_1M_2}\underset{\sim}{f}(t) , \tag{6.58}$$

where

$$Q_{1,2}^2 = \frac{(k_2A+k_1B)\pm[(k_2A+k_1B)^2-4(AB-C^2)k_1k_2]^{\frac{1}{2}}}{2(AB-C^2)}$$

$$= \frac{1}{2}\left[(V_2^2+V_1^2)\pm\left\{(V_1^2-V_2^2)^2+64\frac{C_1C_2}{\omega_1\omega_2}\right\}^{\frac{1}{2}}\right] , \tag{6.59}$$

under the conditions

$$\frac{M_1}{M_1+1} = \frac{k_1}{V_1^2} = \frac{4C_1}{V_1^2\omega_1} , \quad \frac{M_2}{M_2+1} = \frac{k_2}{V_2^2} = \frac{4C_2}{V_2^2\omega_2} .$$

To solve (6.58) for $\underset{\sim}{q}_1$ we apply Laplace transform, thus

$$[p^4-(Q_1^2+Q_2^2)p^2+Q_1^2Q_2^2]f(p)-[p^3-(Q_1^2+Q_2^2)p]q_{11} = -i\underset{\sim}{k}\left[\frac{(BM_1+CM_2)p^2-K_2M_1}{M_TM_2}\right](e^{-p\tau}-e^{-p\sigma}),$$

$$-[p^2-(Q_1^2-Q_2^2)]\dot{\underset{\sim}{q}}_1(0)$$

under the conditions $q_1(0) = q_{11}$, $q_1(0) = q_{12}$ and $\ddot{q}(0) = 0$, $\dddot{q}_1(0) = 0$.

The variable $q_1(t)$ can be obtained directly by applying inverse Laplace transform to

$$f(p) = \frac{-i\underset{\sim}{K}}{M_1M_2}\,\frac{[(BM_1+CM_2)p^2-k_2M_1]}{(p^2-Q_1^2)(p^2-Q_2^2)}\,(e^{-p\tau}-e^{-p\sigma}) + \frac{[p^3-(Q_1^2+Q_2^2)p]}{(p_1^2-Q_1^2)(p^2-Q_2^2)}\,q_{11}$$

$$+\frac{[p^2-(Q_1^2+Q_2^2)]}{(p^2-Q_1^2)(p^2-Q_2^2)}\,\dot{\underset{\sim}{q}}(0) \quad .$$

Hence

$$\underset{\sim}{q}_1(t) = \frac{-i\underset{\sim}{K}}{M_1M_2}\Big\{U_1\big[H(t-\tau)\sinh Q_1(t-\tau)-H(t-\sigma)\sinh Q_1(t-\sigma)\big]$$

$$+U_2\big[H(t-\tau)\sinh Q_2(t-\tau)-H(t-\sigma)\sinh Q_2(t-\sigma)\big]\Big\}$$

$$-q_{11}\left\{\frac{Q_2^2}{(Q_1^2+Q_2^2)}\cosh Q_1t+\frac{Q_1^2}{(Q_2^2-Q_1^2)}\cosh Q_2t\right\}$$

$$-\dot{\underset{\sim}{q}}_1(0)\left\{\frac{Q_2^2}{Q_1(Q_1^2-Q_2^2)}\sinh Q_1t+\frac{Q_1^2}{Q_2(Q_2^2-Q_1^2)}\sinh Q_2t\right\}, \qquad (6.60)$$

where

$$U_1 = \frac{[(BM_1+CM_2)Q_1^2-k_2M_1]}{Q_1(Q_1^2-Q_2^2)}, \quad U_2 = \frac{[(BM_1+CM_2)Q_2^2-k_2M_1]}{Q_2(Q_2^2-Q_1^2)} . \qquad (6.60a)$$

Now

$$\underset{\sim}{q}_1(\beta) = q_{12} = \frac{-i\underset{\sim}{K}}{M_1M_2}\Big\{U_1\big[\sinh Q(\beta-\tau)-\sinh Q_1(\beta-\sigma)\big]+U_2\big[\sinh Q_2(\beta-\tau)-\sinh Q_2(\beta-\sigma)\big]\Big\}$$

$$\frac{-q_{11}}{(Q_1^2-Q_2^2)}\left\{Q_2^2\cosh Q_1\beta-Q_1^2\cosh Q_2t\right\}$$

$$-\dot{\underset{\sim}{q}}_1(0)\left\{\frac{Q_2^2}{Q_1^2(Q_1^2-Q_2^2)}\sinh Q_1t+\frac{Q_1^2}{Q_2(Q_2^2-Q_1^2)}\sinh Q_2t\right\} .$$

After substituting $\dot{\underset{\sim}{q}}_1(0)$ obtained from the above equation for (6.60) we obtain

$$q_1(t) = \frac{-iK}{M_1M_2}\Big\{U_1\Big[H(t-\tau)\sinh Q_1(t-\tau) - H(t-\sigma)\sinh Q_1(t-\sigma)\Big] + U_2\Big[H(t-\tau)\sinh Q_2(t-\tau)$$

$$-H(t-\sigma)\sinh Q_2(t-\sigma)\Big] + \Big[U_1(\sinh Q_1(\beta-\tau) - \sinh(\beta-\sigma)) + U_2($$

$$\sinh Q_2(\beta-\tau) - \sinh Q_2(\beta-\sigma))\Big] / (Q_2^3 \sinh Q_1\beta - Q_1^3 \sinn Q_2\beta) \cdot$$

$$[Q^3 \sinh Q_1 t - Q_1^2 \cosh Q_2 t]\Big\}$$

$$- \frac{g_{11}}{(Q_1^2 - Q_2^2)}\Big\{(Q_2^2 \cosh Q_1 t - Q_1^2 \cosh Q_2 t) - \frac{(Q_2^2 \cosh Q_1\beta - Q_1^2 \cosh Q_2\beta)}{(Q_2^3 \sinh Q_1\beta - Q_1^3 \sinh Q_2\beta)} \cdot$$

$$(Q_2^3 \sinh Q_1 t - Q_1^3 \sinh Q_2 t)\Big\} - g_{12}\,\frac{(Q_2^3 \sinh Q_1 t - Q_1^3 \sinh Q_2 t)}{(Q_2^3 \sinh Q_1 \beta - Q_1^3 \sinh Q_2\beta)}. \qquad (6.61)$$

Similarly, Eq.(6.57) can be solved for $q_2(t)$. The result is

$$q_2(t) = \frac{-iK}{M_1M_2}\Big\{U_1'\Big[H(t-\tau)\sinh Q_1(t-\tau) - H(t-\sigma)\sinh Q_1(t-\sigma)\Big]$$

$$+U_2'\Big[\sinh Q_1(\beta-\tau) - \sinh Q_1(\beta-\sigma)\Big]$$

$$+\left[\frac{U_1'(\sinh Q_1(\beta-\tau) - \sinh Q_1(\beta-\sigma) + U_2'(\sinh Q_2(\beta-\tau) - \sinh Q_2(\beta-\sigma))}{(Q_2^3 \sinn Q_1\beta - Q_1^3 \sinh Q_2\beta)}\right] \cdot$$

$$[Q_2^3 \sinh Q_1 t - Q_1^3 \sinh Q_2 t]\Big\}$$

$$- \frac{g_{21}}{(Q_1^2 - Q_2^2)}\Big\{(Q_2^2 \cosh Q_1 t - Q_1^2 \cosh Q_2 t) - \frac{(Q_2^2 \cosh Q_1\beta - Q_1^2 \cosh Q_2\beta)}{(Q_2^3 \sinh Q_1\beta - Q_1^3 \sinh Q_2\beta)} \cdot$$

$$(Q_2^3 \sinh Q_1 t - Q_1^3 \sin Q_2 t)\Big\} - g_{22}\,\frac{(Q_2^3 \sinh Q_1 T - Q_1^3 \sinh Q_2 t)}{(Q_2^3 \sinh Q_1\beta - Q_1^3 \sinh Q_2\beta)}, \qquad (6.62)$$

under the conditions $\underset{\sim}{q}_2(0) = q_{21}$, $\underset{\sim}{q}_2(\beta) = q_{22}$, and $\ddot{\underset{\sim}{q}}_2(0) = \dddot{\underset{\sim}{q}}_2(0) = 0$, with the substitutions

$$U_1' = \frac{[(AM_2+CM_1)Q_1^2 - k_1 M_2]}{Q_1(Q_1^2-Q_2^2)} \quad , \quad U_2' = \frac{[(AM_2+CM_2)Q_2^2 - k_1 M_2]}{Q_2(Q_2^2-Q_1^2)} \;. \quad (6.62\,a)$$

We have already solved the differential equation in the same form as (6.55) in Chapter V. The solution of (6.55) can thus be obtained easily under the conditions $\underset{\sim}{Q}_o(0) = Q_1$ and $\underset{\sim}{Q}_o(\beta) = Q_2$. The result is

$$\underset{\sim}{Q}_o(t) = Q_1 + \left\{(Q_2-Q_1) - \frac{i\underset{\sim}{k}}{M_T}(\tau-\sigma)\right\}\frac{t}{\beta} - \frac{i\underset{\sim}{k}}{M_T}\left\{(t-\tau)H(t-\tau) - (t-\sigma)H(t-\sigma)\right\} . \quad (6.63)$$

Consider the value of M_T in the form of ω_1^2, ω_2^2, Q_1^2 and Q_2^2 obtained from (6.59), we have

$$\frac{1}{M_T} = \frac{\omega_1^2\omega_2^2}{Q_1^2 Q_2^2} \quad . \quad (6.64)$$

By substitution of (6.64) for (6.63), we obtain

$$\underset{\sim}{Q}_o(t) = Q_1 + \left\{(Q_2-Q_1) - i\underset{\sim}{k}\frac{\omega_1^2\omega_2^2}{Q_1^2 Q_2^2}(\tau-\sigma)\right\}\frac{t}{\beta} - i\underset{\sim}{k}\frac{\omega_1^2\omega_2^2}{Q_1^2 Q_2^2}\left\{(t-\tau)H(t-\tau) - (t-\sigma)H(t-\sigma)\right\} . (6.65)$$

By using (6.53), (6.54), and (6.56), the path integration (6.20) can be carried out with the use of the Gaussian integral method, thus

$$\left\langle \exp[i\underset{\sim}{k}\cdot(\underset{\sim}{r}_{el}(\tau) - \underset{\sim}{r}_{el}(\sigma))]\right\rangle_{\substack{q_{11},\, q_{12} \\ q_{21},\, q_{22} \\ Q_2,\, Q_1,\, \beta}} = \exp\left\{\int_0^\beta \left[-\tfrac{1}{2}A\dot{\underset{\sim}{q}}_1^2 - \frac{k_1}{2}\underset{\sim}{q}_1^2 + \frac{M_1}{M_T}\underset{\sim}{f}(t)\cdot\underset{\sim}{q}_1 - \tfrac{1}{2}B\dot{\underset{\sim}{q}}_2^2 \right.\right.$$
$$\left.\left. + \frac{M_2}{M_T}\underset{\sim}{f}(t)\cdot\underset{\sim}{q}_2 + C\dot{\underset{\sim}{q}}_1\cdot\dot{\underset{\sim}{q}}_2 + \frac{M_T}{2}\dot{\underset{\sim}{Q}}_o^2 + \underset{\sim}{Q}_o\cdot\underset{\sim}{f}(t)\right]dt\right\}$$

$$\langle \exp[i\underset{\sim}{\kappa}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\rangle = \exp\Big\{-\frac{A}{2}\dot{\underset{\sim}{q}}_1\underset{\sim}{q}_1\Big|_0^\beta - \frac{B}{2}\dot{\underset{\sim}{q}}_2\underset{\sim}{q}_2\Big|_0^\beta + \frac{C}{2}\Big[\dot{\underset{\sim}{q}}_1\underset{\sim}{q}_2+\underset{\sim}{q}_1\dot{\underset{\sim}{q}}_2\Big]\Big|_0^\beta$$

$$-\frac{M_T}{2}\dot{\underset{\sim}{Q}}_0\underset{\sim}{Q}_0\Big|_0^\beta + \frac{1}{2}\int_0^\beta\Big[\frac{M_1}{M_T}\underset{\sim}{f}(t)\cdot\underset{\sim}{q}_1 + \frac{M_2}{M_T}\underset{\sim}{f}(t)\underset{\sim}{q}_2 + \underset{\sim}{Q}_0\cdot\underset{\sim}{f}(t)\Big]dt\Big\}$$

$$= \Big\{\exp[i\underset{\sim}{\kappa}(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\Big\}_{\substack{q_{11},q_{12}\\ q_{21},q_{22},\beta}} \cdot \Big\{\exp[i\underset{\sim}{\kappa}(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\Big\}_{Q_1,Q_2,\beta}, \qquad (6.66)$$

where the first part is given by

$$\exp\Big\{-\frac{M_1(M_2+1)}{2(1+M_1+M_2)}\big(\dot{\underset{\sim}{q}}_1(\beta)\underset{\sim}{q}_1(\beta)-\dot{\underset{\sim}{q}}_1(0)\underset{\sim}{q}_1(0)\big) + \frac{i\underset{\sim}{\kappa}}{2}\frac{M_1}{(1+M_1+M_2)}\big(\underset{\sim}{q}_1(\tau)-\underset{\sim}{q}_1(\sigma)\big)$$

$$-\frac{M_2(M_1+1)}{2(1+M_1+M_2)}\big(\dot{\underset{\sim}{q}}_2(\beta)\underset{\sim}{q}_2(\beta)-\dot{\underset{\sim}{q}}_2(0)\underset{\sim}{q}_2(0)\big) + \frac{i\underset{\sim}{\kappa}}{2}\frac{M_2}{(1+M_1+M_2)}\big(\underset{\sim}{q}_2(\tau)-\underset{\sim}{q}_1(\sigma)\big)$$

$$+\frac{M_1M_2}{2(1+M_1+M_2)}\Big[\big(\dot{\underset{\sim}{q}}_1(\beta)\cdot\underset{\sim}{q}_2(\beta)-\dot{\underset{\sim}{q}}_1(0)\cdot\underset{\sim}{q}_2(0)\big)+\big(\underset{\sim}{q}_1(\beta)\dot{\underset{\sim}{q}}_2(\beta)-\underset{\sim}{q}_1(0)\dot{\underset{\sim}{q}}_2(0)\big)\Big]\Big\},$$

and the second part is given by

$$\exp\Big\{-\frac{(1+M_1+M_2)}{2}\big(\dot{\underset{\sim}{Q}}_0(\beta)\cdot\underset{\sim}{Q}_0(\beta)-\dot{\underset{\sim}{Q}}_0(0)\underset{\sim}{Q}_0(0)\big)+\frac{i\underset{\sim}{\kappa}}{2}\big(Q_0(\tau)-Q_0(\sigma)\big)\Big\}.$$

By substituting $\dot{Q}_0(\beta)$, $\dot{Q}_0(0)$, and $Q_0(\tau)$, $Q_0(\sigma)$ obtained from (6.65) for the second part of (6.66), we obtain

$$\Big\{\exp[i\underset{\sim}{\kappa}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\Big\}_{Q_2,Q_1,\beta} = \exp\Big\{-\frac{(1+M_1+M_2)}{2\beta}(Q_2-Q_1)\Big[(Q_2-Q_1)-i\underset{\sim}{\kappa}\,\omega_1^2\omega_2^2\,|\tau-\sigma|\Big]$$

$$+\frac{i\underset{\sim}{\kappa}}{2}\Big[(Q_2-Q_1)-i\underset{\sim}{\kappa}\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}|\tau-\sigma|\Big]\frac{|\tau-\sigma|}{\beta}$$

$$+\frac{(i\underset{\sim}{\kappa})^2}{2}\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}|\tau-\sigma|\Big\}. \qquad (6.67)$$

By substituting (6.61) and (6.62) for the first part of (6.66), we obtain

$$\left\{\exp[i\underset{\sim}{K}\cdot(\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma))]\right\}_{\substack{q_{11},q_{12}\\ q_{21},q_{22},\beta}} = \exp\left\{\frac{(i\underset{\sim}{K})^2}{2}\frac{1}{M_T M_2}\left\{U_1\sinh Q_1|\tau-\sigma|+U_2\sinh Q_2|\tau-\sigma|\right.\right.$$

$$+[U_1(\sinh Q_1(\beta-\tau)-\sinh Q_1(\beta-\sigma))+U_2(\sinh Q_2(\beta-\tau)$$

$$-\sinh Q_2(\beta-\sigma))]\,\cdot$$

$$\frac{Q_2^3(\sinh Q_1\tau-\sinh Q_1\sigma)-Q_1^3(\sinh Q_2\tau-\sinh Q_2\sigma)}{Q_2^3\sinh Q_1\beta-Q_1^3\sinh Q_2\beta}$$

$$+\frac{(i\underset{\sim}{K})^2}{2}\frac{1}{M_T M_1}\left\{U_1'\sinh Q_1|\tau-\sigma|+U_2'\sinh Q_2|\tau-\sigma|\right.$$

$$+[U_1'(\sinh Q_1(\beta-\tau)-\sinh Q_1(\beta-\sigma))+U_2'\cdot$$

$$(\sinh Q_2(\beta-\tau)-\sinh Q_2(\beta-\sigma))]\times\cdot$$

$$\frac{Q_2^3(\sinh Q_1\tau-\sinh Q_1\sigma)-Q_1^3(\sinh Q_2\tau-\sinh Q_2\sigma)}{(Q_2^3\sinh Q_1\beta-Q_1^3\sinh Q_2\beta)}$$

$$-\frac{(i\underset{\sim}{K})^2}{2}\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}|\tau-\sigma|\left(\frac{|\tau-\sigma|}{\beta}-1\right)$$

$$\left.+\text{terms depend on } q_{11},q_{12},q_{21},q_{22},Q_1,Q_2\right\} \tag{6.68}$$

After substituting (6.67) and (6.68) for (6.66) and connecting the variables q_{11}, q_{21}, Q_1 and q_{12}, q_{22}, Q_2 in the Lagrangian L with the variables r_1, R_{11}, R_{21} and r_1, R_{12}, R_{22}, we obtain

$$\langle \exp i\underset{\sim}{K}\cdot[\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)]\rangle = \exp\Big[\frac{K^2}{2}\Big\{\frac{(M_1U_1+M_2U_1')}{M_TM_1M_2}\Big[(e^{-Q_1|\tau-\sigma|}-1)+(1-\cosh Q_1|\tau-\sigma|)$$

$$+\frac{\sinh Q_1(\beta-\tau)-\sinh Q_1(\beta-\sigma)}{Q_2^3\sinh Q_1\beta-Q_1^3\sinh Q_1\beta}\times$$

$$[Q_2^3(\sinh Q_1\tau-\sinh Q_1\sigma)-Q_1^3(\sinh Q_2\tau-\sinh Q_2\sigma)]$$

$$+\frac{(M_1U_2+M_2U_2')}{M_TM_1M_2}\Big[(e^{-Q_2|\tau-\sigma|}-1)+(1-\cosh Q_2|\tau-\sigma|)$$

$$+\frac{\sinh Q_2(\beta-\tau)-\sinh Q_2(\beta-\sigma)}{Q_2^3\sinh Q_2\beta-Q_1^3\sinh Q_2\beta}\times$$

$$[Q_2^3(\sinh Q_1\tau-\sinh Q_1\sigma)-Q_1^3(\sinh Q_2\tau-\sinh Q_2\sigma)]$$

$$-\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}|\tau-\sigma|\Big(1-\frac{|\tau-\sigma|}{\beta}\Big)\Big\}\Big], \qquad (6.69)$$

aside from some terms that depend on q_{11}, q_{21}, Q_1 and q_{12}, q_{22}, Q_2, which must be integrated out under the condition $R_2=R_1$. By using the relations (6.60a), (6.62a), and (6.52), the coefficient terms $\frac{(M_1U_1+M_2U_1')}{M_TM_1M_2}$ and $\frac{(M_1U_2+M_2U_2')}{M_TM_1M_2}$ can be given in terms of Q_1^2, Q_2^2, ω_1^2 and ω_2^2 as

$$\frac{M_1U_1+M_2U_1'}{M_TM_1M_2}=\frac{(Q_1^2-\omega_1^2)(Q_2^2-\omega_2^2)}{Q_1^3(Q_1^2-Q_2^2)}, \qquad \frac{M_1U_2+M_2U_2'}{M_TM_1M_2}=\frac{(Q_2^2-\omega_2^2)(\omega_1^2-Q_2^2)}{Q_2^3(Q_1^2-Q_2^2)}.$$

(6.70)

Using the above relations for (6.69), we obtain

$$\langle \exp i\underset{\sim}{K}\cdot[\underset{\sim}{r}_{el}(\tau)-\underset{\sim}{r}_{el}(\sigma)]\rangle = \exp\Big[-\frac{K^2}{2}\Big\{\frac{(Q_1^2-\omega_1^2)(Q_1^2-\omega_2^2)}{Q_1^3(Q_1^2-Q_2^2)}\Big[(1-e^{-v_+|\tau-\sigma|})+(1-\cosh v_+|\tau-\sigma|)$$

$$+\frac{\sinh Q_1(\beta-\tau)-\sinh Q_1(\beta-\sigma)}{Q_2^3\sinh Q_1\beta-Q_1^3\sinh Q_1\beta}\cdot\Big[Q_2^3(\sinh Q_1\tau-\sinh Q_1\sigma)$$

$$-Q_1^3(\sinh Q_2\tau-\sinh Q_2\sigma)\Big]+\frac{\omega_1^2\omega_2^2}{Q_1^2Q_2^2}|\tau-\sigma|\Big(1-\frac{|\tau-\sigma|}{\beta}\Big)\Big\}\Big]$$

$$= \exp\Big[-\frac{K^2}{2}G[|\tau-\sigma|]\Big] . \qquad (6.71)$$

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The average of the exact action S can be determined by using (6.17), (6.19), (6.42) and (6.71)

$$\langle S\rangle = \frac{\alpha}{2^{3/2}}\int_0^\beta\!\!\int dtds\Big\{\frac{e^\beta}{e^\beta-1}e^{-|t-s|}+\frac{1}{e^\beta-1}e^{|t-s|}\Big\}\int_{-\infty}^{\infty}\frac{K^2 4\pi dk}{2\pi K^2}\exp\Big[\frac{-K^2}{2}G[|t-s|]\Big]$$

$$= \frac{\alpha}{\pi^{1/2}}\beta\int_0^\beta d\tau\Big\{\frac{e^\beta}{e^\beta-1}e^{-\tau}+\frac{1}{e^\beta-1}e^{\tau}\Big\}\sqrt{G|\tau|} . \qquad (6.72)$$

The average of the trial action S_1 is determined by applying the second order differentiation with respect to $\underset{\sim}{K}$ to $\langle \exp i\underset{\sim}{K}\cdot[r_{el}(\tau)-r_{el}(\sigma)]\rangle$, and then $\langle |r_{el}(t)-r_{el}(s)|^2\rangle$ is obtained by taking the limit of $\underset{\sim}{K}$ to zero as

$$\langle|\underset{\sim}{r}_{el}(t)-\underset{\sim}{r}_{el}(s)|^2\rangle = 3\,G[|t-s|] . \qquad (6.73)$$

Substitution of the above relation in (6.18) leads to

$$\langle S_1\rangle = -\frac{C_1}{2}\cdot 3\int_0^\beta\!\!\int dtds\Big\{\frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}e^{-\omega_1|t-s|}+\frac{1}{e^{\beta\omega_1}-1}e^{\omega_1|t-s|}\Big\}G[|t-s|]$$

$$-\frac{C_2}{2}\cdot 3\int_0^\beta\!\!\int dtds\Big\{\frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}e^{-\omega_2|t-s|}+\frac{1}{e^{\beta\omega_2}-1}e^{\omega_2|t-s|}\Big\}G[|t-s|].$$

$$\langle S_1 \rangle = -\frac{3C_1\beta}{2}\int_0^{\beta} d\tau \left\{ \frac{e^{\beta\omega_1}}{e^{\beta\omega_1}-1}\cdot e^{-\omega_1\tau} + \frac{1}{e^{\beta\omega_1}-1} e^{\omega_1\tau} \right\} G[|\tau|]$$

$$-\frac{3C_2\beta}{2}\int_0^{\beta} d\tau \left\{ \frac{e^{\beta\omega_2}}{e^{\beta\omega_2}-1}\cdot e^{-\omega_2\tau} + \frac{1}{e^{\beta\omega_2}-1}\cdot e^{\omega_2\tau} \right\} G[|\tau|] \quad . \quad (6.74)$$

After substituting for $G[|\tau|]$ in (6.74) and (6.72) and integrating the expression out explicitly by using a digital computer, the trial free energy (6.16) can in principle be evaluated completely. The trial free energy can then be minimized with respect to the four variable parameters v_+, v_-, and ω_1 , ω_2 . When the free energy is known , the self energy and the average energy can be determined by using the relation

$$E_S = \frac{\delta(\beta F)}{\delta\beta} - \frac{3}{2}KT \quad , \qquad (6.75)$$

and

$$\bar{E} = \frac{\delta(\beta F)}{\delta\beta} \quad . \qquad (6.76)$$