

## CHAPTER IV

### THE POLARON DENSITY MATRIX

In previous chapter, the polaron action has been derived by integrating out the phonon coordinates. Instead of directly calculating the phonon part, this part is regarded as a transformation function and is evaluated by using the ground state wave function and the density matrix of a free harmonic oscillator. In order to find the action at a finite temperature, we must calculate the path integrals involving the phonon coordinates which will be shown in section 4.1. Previously, we did not derive the trial action, so we will present detailed calculations in section 4.2. The generating functional will be constructed from this trial action since the quantities that have contributions to the density matrix are easily derived from this functional. This material will be presented in sections 4.3 and 4.4 .

#### 4.1 The Finite Temperature Polaron Action

In the original paper of Feynman [5], the polaron action was evaluated in real time and the phonon coordinates were removed by viewing the phonon parts of the density matrix as a transformation function (Feynman and Hibbs[9]). This function can be evaluated by using the ground state wave function of a forced harmonic oscillator. The result is an action which is a functional of an electron coordinates. Then the real time was replaced by an imaginary time,  $\tau = -i\beta$ , where the Planck

constant is set to be unity. In this section we will do a more general case, which we calculate the phonon part directly in the imaginary time at the first step. If one is interest in the ground state behavior of the polaron, the imaginary time must be taken to go to infinity. We can write the polaron density matrix

$$\rho = \int D\vec{r}(\tau) \exp\left(-\frac{1}{2} \int_0^{\beta} d\tau \dot{\vec{r}}^2(\tau)\right) \prod_k \int d\vec{Q}_k \exp\left[\frac{\mu}{2} \dot{\vec{Q}}_k^2 - \vec{Q}_k^2 + \gamma_k \vec{Q}_k\right], \quad (4.1)$$

where the terms involving  $\vec{Q}_k$  are the phonon part, the phonon frequency was set to be unity and  $\gamma_k$  is the force defined by

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

The phonon part can be evaluated easily by setting the two end points to be equal, this corresponds to the partition function of the phonon system. Then the classical action for each momentum  $\vec{k}$  reads

$$S_d^k = -\frac{m}{2i \sinh \beta} \left[ 2(\cosh \beta - 1) Q_k^2 - \frac{2Q_k}{m} \int_0^{\beta} d\tau \gamma_k(\tau) (\sinh \tau + \sinh(\beta - \sigma)) \right. \\ \left. - \frac{2}{m^2} \int_0^{\beta} \int_0^{\beta} d\sigma d\tau \gamma_k(\tau) \gamma_k(\sigma) \sinh \tau \sinh(\beta - \sigma) \right]. \quad (4.2)$$

Then the density matrix corresponds to above action will be integrated overall coordinate  $Q_k$  which can be done easily since it is a Gaussian integral.

$$\int dQ_k \rho_{ph}(Q_k, \beta; Q_k, 0) = \left( \frac{m}{2\pi \sinh \beta} \right)^{\frac{3}{2}} \int dQ_k \exp(S_{cl}^k)$$

$$= \left( \frac{1}{2 \sinh \beta/2} \right) \exp \left[ \frac{\alpha}{2^{\frac{3}{2}}} \int_0^\beta \int_0^\beta d\tau d\sigma \frac{1}{|\bar{r}(\tau) - \bar{r}(\sigma)|} \frac{\cosh(\beta - |\tau - \sigma|)}{\sinh \frac{\beta}{2}} \right] \quad (4.3)$$

Adding the exponent to the equation (4.1) gives the finite temperature polaron action

$$S = -\frac{1}{2} \int_0^\beta d\tau \dot{\bar{r}}^2(\tau) + \frac{\alpha}{2^{\frac{3}{2}}} \int_0^\beta \int_0^\beta d\sigma d\tau \frac{1}{|\bar{r}(\tau) - \bar{r}(\sigma)|} \frac{\cosh(\beta - |\tau - \sigma|)}{\sinh \frac{\beta}{2}} \quad (4.4)$$

We can check the correctness of the above expression by taking the imaginary time to go to infinity, then the hyperbolic term is

$$\frac{\cosh(\beta - |\tau - \sigma|)}{\sinh \frac{\beta}{2}} \xrightarrow{\beta \rightarrow \infty} e^{-|\tau - \sigma|}. \quad (4.5)$$

So the action in equation (4.4) reduce to Feynman action at zero-temperature limit.

## 4.2 The Finite Temperature Trial Action

In the Feynman original paper [14], he introduced a trial action which has the physical meaning of the two particles attached together and the potential depends only on the difference between their coordinates. We will show in this section that the system of an electron bound by a fictitious particle of mass  $M$  and spring constant  $k$  will lead to the Feynman trial action.

As mentioned previously in Chapter III, the potential should be of the form of equation (3.12). The Lagrangian reads

$$L = \frac{1}{2} \left[ m\dot{\bar{r}}^2(t) + M\dot{\bar{y}}^2(t) - k(\bar{r}(t) - \bar{y}(t))^2 \right] \quad (4.6)$$

Where  $\bar{y}(t)$  is the coordinate of a fictitious particle which would be eliminated like the phonon. We can write above Lagrangian to consisted of free and force harmonic oscillators.

$$L = \frac{1}{2} \left[ m\dot{\bar{r}}^2(t) - k\bar{r}^2(t) \right] + \frac{1}{2} \left[ M\dot{\bar{y}}^2 - k\bar{y}^2 \right] + k\bar{r}(t)\bar{y}(t). \quad (4.7)$$

The path integrals for this Lagrangian involves two paths for  $\bar{r}(t)$  and  $\bar{y}(t)$ .

Consider the fictitious particle first, its path integrals read

$$\int D\bar{y}(\tau) \exp \left( -\frac{1}{2} \int_0^{\beta} d\tau (M\dot{\bar{y}}^2(\tau) - k\bar{y}^2 + k\bar{r}(\tau)\bar{y}(\tau)) \right) = \left( \frac{mw}{2\pi \sinh \beta w} \right)^{\frac{3}{2}} \exp(S_{cl}) \quad (4.8)$$

where  $w = \sqrt{\frac{k}{M}}$  and the classical path is available in many books [9,26]

$$S_{cl}[\bar{y}(\tau)] = \frac{-Mw}{2i \sinh w\beta} \left[ 2(\cosh w\beta - 1)\bar{y}_1\bar{y}_2 - \frac{2\bar{y}_2 k}{Mw} \int_0^{\beta} d\tau \bar{r}(\tau) \sinh w\tau \right. \\ \left. - \frac{2\bar{y}_1 k}{Mw} \int_0^{\beta} d\tau \bar{r}(\tau) \sinh w(\beta - \tau) - \frac{2k^2}{M^2 w^2} \int_0^{\beta} \int_0^{\tau} d\sigma d\tau \bar{r}(\tau)\bar{r}(\sigma) \sinh w(\beta - \tau) \sinh w\sigma \right] \quad (4.9)$$

This phonon part of the density matrix can be simplified by regarding it as a heat bath and averaging it out. This can be done by setting the phonon end points to be equal and integrating it overall phonon coordinates.

$$\begin{aligned}
\rho_{\text{polaron}}(\bar{r}_2, \bar{r}_1; \beta) &= \int \int d\bar{y}_1 d\bar{y}_2 \delta(\bar{y}_2 - \bar{y}_1) \rho(\bar{r}_2, \bar{r}; \bar{y}_2, \bar{y}_1; \beta) \\
&= \left( \frac{mw}{2\pi \sinh w\tau} \right)^{\frac{3}{2}} \int D\bar{r}(\tau) \exp \left( -\frac{m}{2} \int_0^\beta d\tau \dot{\bar{r}}^2 - \frac{k}{2} \int_0^\beta d\tau \bar{r}^2 \right) \\
&\times \int d\bar{y} \exp \left\{ \frac{-Mw\bar{y}^2}{\sinh w\beta} (\cosh w\beta - 1) - k\bar{y} \int_0^\beta d\tau \bar{r}(\tau) \left( \frac{\sinh w\tau + \sinh w(\beta - \tau)}{\sinh w\beta} \right) \right. \\
&\quad \left. - \frac{k^2}{Mw} \int_0^\beta \int_0^\tau d\sigma d\tau \bar{r}(\tau) \bar{r}(\sigma) \frac{\sinh w(\beta - \tau) \sinh w\sigma}{\sinh w\beta} \right\} \quad (4.10)
\end{aligned}$$

The integral involving  $\bar{y}$  is a Gaussian type and can be evaluated easily. Then the trial action is of the form

$$S. = -\frac{m}{2} \int_0^\beta d\tau \dot{\bar{r}}^2(\tau) - \frac{k\omega}{8} \int_0^\beta \int_0^\beta d\sigma d\tau (\bar{r}(\tau) - \bar{r}(\sigma)) \frac{2 \cosh w \left( \frac{\beta}{2} - |\tau - \sigma| \right)}{\sinh \frac{w\beta}{2}} \quad (4.11)$$

### 4.3 Construction of the Generating Functional

In this section the construction of the generating functional will be reviewed

By the definitions  $C = \frac{Mw^3}{4}$  and  $w^2 = \frac{k}{m}$ , the action in equation (4.11) can be written as

$$S. = -\frac{m}{2} \int_0^\beta d\tau \dot{\bar{r}}^2(\tau) - \frac{C}{2} \int_0^\beta \int_0^\beta d\sigma d\tau (\bar{r}(\tau) - \bar{r}(\sigma)) \frac{2 \cosh w \left( \frac{\beta}{2} - |\tau - \sigma| \right)}{\sinh \frac{w\beta}{2}} \quad (4.12)$$

Since we cannot evaluate the density matrix for this trial action directly so the variational principle may be applied. By using the Feynman-Jensen inequality we have

$$\rho(\bar{r}_2, \bar{r}_1; \beta) \geq \rho(\bar{r}_2, \bar{r}_1; \beta) \exp\left(\langle S - S_0 \rangle_S\right) \quad (4.13)$$

We will see that the exponent in equation(4.13) contained with the averaging over quantities like  $\langle \bar{r}(\tau) \rangle$  or  $\langle \bar{r}(\tau) \bar{r}(\sigma) \rangle$ . And these quantities can be extracted from the generating functional defined as

$$\left\langle \exp\left(\int_0^{\beta} d\tau \bar{f}(\tau) \bar{r}(\tau)\right)\right\rangle = \frac{\int D\bar{r}(\tau) \exp\left(S_0 + \int_0^{\beta} d\tau \bar{f}(\tau) \bar{r}(\tau)\right)}{\int D\bar{r}(\tau) \exp(S_0)} \quad (4.14)$$

with end points condition

$$\bar{r}(\tau) = \bar{r}_2 \quad , \quad \bar{r}(\tau) = \bar{r}_1$$

and  $f(\tau)$  is an arbitrary function of imaginary time. By following the standard way of evaluation of the path integration, we substitute  $\bar{r}(\tau)$  by

$$\bar{r}(\tau) = \bar{r}_c(\tau) + \bar{y}(\tau),$$

with  $\bar{y}(\beta) = 0 = \bar{y}(0)$ .

We know from Feynman and Hibbs [9] that the term linear in  $\bar{y}(\tau)$  that appear together with  $\bar{f}(\tau)$  will vanish due to above condition. So the remaining terms of  $\bar{y}(\tau)$  of the denominator and numerator should be the same and cancelled out. The term left us is the exponential of the two classical action, that is

$$\left\langle \exp\left(\int_0^\beta d\tau \bar{f}(\tau) \bar{r}(\tau)\right) \right\rangle_s = \exp(\bar{S}_f, -\bar{S}_s). \quad (4.15)$$

Hence, we can see that the quantities of interest can be extracted from above formula by performing the functional differentiation with respect to  $\bar{f}(\tau)$  and setting it to be zero. In evaluating of equation (4.15), we encounter the problem of finding the classical action  $\bar{S}_f$ , that is we must evaluate out the classical path. Since  $S_s$ , the quadratic action which we can obtain the path integral exactly, comes from the two particle model, we can find the classical path from the Lagrangian (4.6) with external force

$$L = \frac{1}{2} [m\dot{\bar{r}}^2(t) + M\dot{\bar{y}}^2(t) - k(\bar{r}(t) - \bar{y}(t))^2] + \bar{f}(t)\bar{r}(t). \quad (4.16)$$

By using the center of mass coordinates

$$\bar{x} = \bar{r} - \bar{y}, \quad \bar{R} = \frac{m\bar{r} + M\bar{y}}{m+M}, \quad m_s = m+M$$

$$\mu = \frac{mM}{m+M}, \quad v^2 = \frac{k}{\mu}, \quad w^2 = \frac{k}{M}, \quad (4.17)$$

so the Lagrangian can be written as containing two couple systems of forced harmonic oscillators

$$L = \frac{1}{2} (\mu \dot{\bar{x}}^2 - k\bar{x}^2) + \frac{\mu}{m} \bar{f} \cdot \bar{x} + \frac{1}{2} m_s \dot{\bar{R}}^2 + \bar{f} \cdot \bar{R}. \quad (4.18)$$

This Lagrangian will give two differential equations:

$$\ddot{\bar{x}}(t) - v^2 \bar{x}(t) = -\bar{f}(t), \quad (4.19)$$

$$\ddot{\bar{R}}(t) = -\frac{\bar{f}(t)}{m}, \quad (4.20)$$

which can be solved easily by the Green function method. The Green function of equations (4.19) and (4.20) respectively are

$$\begin{aligned} G_x(t, s) &= -\frac{\sinh vt}{v} (\coth vt - \coth v\beta \sinh vs) H(t-s) \\ &= -\frac{\sinh vt}{v} (\coth v\beta - \coth v\beta \sinh vs) H(s-t), \end{aligned} \quad (4.21)$$

$$G_R(t, s) = \frac{(t-\beta)}{\beta} s H(t-s) + \frac{t}{\beta} (s-\beta) H(s-t). \quad (4.22)$$

With the conditions of the end points

$$\bar{x}(0) = \bar{x}_1, \quad \bar{x}(\beta) = \bar{x}_2 \quad ; \quad \bar{R}(0) = \bar{R}_1, \quad \bar{R}(\beta) = \bar{R}_2 \quad (4.23)$$

where the solution of the differential equation is in the form

$$\bar{r}(t) = \bar{r}(\beta)G(\beta, t) - \bar{r}(0)G(0, t) - \int_0^\beta \bar{f}(s)G(t, s)dt \quad (4.24)$$

So the classical path can be determined and substituted into the action to give

$$\bar{S}_x = \frac{\mu v}{2 \sinh v\beta} [ -(\bar{x}_2^2 + \bar{x}_1^2) \cosh v\beta + 2\bar{x}_2 \bar{x}_1 ] + \frac{2\bar{x}_2}{v} \int_0^\beta dt \bar{f}(t) \sinh vt$$

$$+ \frac{2\bar{x}_1}{v} \int_0^\beta dt \bar{f}(t) \sinh v(\beta-t) + \frac{2}{v^2} \int_0^\beta \int_0^\beta d\sigma d\tau \bar{f}(\tau) \bar{f}(\sigma) \sinh v(\beta-t) \sinh v\sigma$$

(4.25)

$$\bar{S}_R = -\frac{m}{2} \frac{(\bar{R}_2 - \bar{R}_1)^2}{\beta} + \bar{R}_2 \int_0^\beta dt \bar{f}(t) \frac{t}{\beta} + \bar{R}_1 \int_0^\beta dt \bar{f}(t) \frac{(\beta-t)}{\beta}$$

$$+ \frac{1}{m} \int_0^\beta \int_0^t dt ds \bar{f}(t) \bar{f}(s) (\beta-t) \frac{s}{\beta} \quad (4.26)$$

The next step is to transform the coordinates  $\bar{R}$  and  $\bar{x}$  back to the original one so that we can distinguish the coordinate of the fictitious particle and integrate it out. Again, this can be done by setting the end points of the fictitious particle to be equal. We obtain

$$\rho = \int \int d\bar{y}_2 d\bar{y}_1 \rho(\bar{r}_2, \bar{r}_1; \bar{y}_2, \bar{y}_1) \delta(\bar{y}_2 - \bar{y}_1).$$

The generating functional with its exponent can be written as

$$\begin{aligned} \bar{S}_f = & - \left[ \frac{v\mu}{4} \coth \frac{v\beta}{2} + \frac{\mu}{2M\beta} \right] |\bar{r}_2 - \bar{r}_1|^2 \\ & + \bar{r}_1 \int_0^\beta d\tau \bar{f}(\tau) \left[ \frac{\mu}{m} \left( \frac{\sinh v(\beta-\tau)}{\sinh v\beta} + \frac{\sinh \frac{v}{2}(\beta-\tau) \sinh \frac{v}{2}\tau}{\cosh \frac{v}{2}\beta} \right) + \frac{\mu(\beta-\tau)}{M\beta} \right] \\ & + \bar{r}_2 \int_0^\beta d\tau \bar{f}(\tau) \left[ \frac{\mu \sinh v\tau}{m \sinh v\beta} + \frac{\sinh \frac{v}{2}(\beta-\tau) \sinh \frac{v}{2}\tau}{\cosh \frac{v}{2}\beta} + \frac{\mu\tau}{M\beta} \right] \end{aligned}$$

$$\begin{aligned}
& + \int_0^\beta \int_0^\beta d\sigma d\tau \bar{f}(\tau) \bar{f}(\sigma) \left( \frac{\mu}{v \sinh v\beta} \left\{ \sinh v(\beta - \tau) \sinh v\sigma - 4 \sinh \frac{v}{2}(\beta - \tau) \sinh \frac{v}{2}\tau \right. \right. \\
& \left. \left. \times \sinh \frac{v}{2}(\beta - \sigma) \sinh \frac{v}{2}\sigma \right\} + \frac{\mu}{M} \frac{(\beta - \tau)\sigma}{\beta} \right). \quad (4.27)
\end{aligned}$$

And  $\bar{S}_.$  can be found by setting  $\bar{f}(\tau)$  to be zero in the equation (4.27) and is

$$\bar{S}_. = - \left[ \frac{v\mu}{4} \coth \frac{v\beta}{2} + \frac{\mu}{2M\beta} \right] |\bar{r}_2 - \bar{r}_1|^2. \quad (4.28)$$

#### 4.4 The Polaron Density Matrix

From the Feynman-Jansen inequality, we can write the density matrix that gives the upper bound of the ground state energy of the polaron as equation (4.13)

$$\rho(\bar{r}_2, \bar{r}_1; \beta) \geq \rho_0(\bar{r}_2, \bar{r}_1; \beta) \exp(\langle S - S_0 \rangle_{S_0})$$

where  $\rho_0$  is in the form

$$\rho_0(\bar{r}_2, \bar{r}_1; \beta) = \left( \frac{m}{2\pi\beta} \right)^{\frac{3}{2}} \left( \frac{v \sinh w\beta/2}{w \sinh v\beta/2} \right)^3 \exp(\bar{S}_0). \quad (4.29)$$

The average in the exponent of equation (4.13) can be determined from the generating functional in previous section. Then

$$\langle S - S_0 \rangle = \langle S' \rangle - \langle S'_0 \rangle \quad (4.30)$$

where  $S'$  and  $S'_.$  are the last terms of the action of the polaron and the trial action respectively. The bracket means averaging with respect to the trial action  $S_.$

The next step is to evaluate  $\langle S' \rangle$ , writing its form explicitly

$$\langle S' \rangle = \frac{\alpha}{2^{\frac{3}{2}}} \int_0^{\beta} \int_0^{\beta} d\sigma d\tau \frac{\cosh w(\beta/2 - |\tau - \sigma|)}{\sinh w\beta/2} \int \frac{d^3 \bar{k}}{2\pi^2 k^2} \exp(i\bar{k} \cdot \bar{A} - k^2 B) \quad (4.31)$$

where

$$\langle \exp(i\bar{k} \cdot (\bar{r}_\tau - \bar{r}_\sigma)) \rangle = \exp\left\{ i\bar{k} \cdot \langle \bar{r}_\tau - \bar{r}_\sigma \rangle - \frac{k^2}{2} \left( \frac{1}{3} \langle (\bar{r}_\tau - \bar{r}_\sigma)^2 \rangle - \langle \bar{r}_\tau - \bar{r}_1 \rangle^2 \right) \right\}$$

For the sake of typing convenience, the imaginary times which are the arguments of the coordinates are given as subscripts. We then obtain

$$\begin{aligned} \bar{A} = \langle \bar{r}_\tau - \bar{r}_\sigma \rangle &= \left. \frac{\delta S'_\tau}{\delta f_\tau} \right|_{f=0} - \left. \frac{\delta S'_\sigma}{\delta f_\sigma} \right|_{f=0} \\ &= \bar{r}_2 \left[ \frac{\mu \cosh v\beta/2}{\sinh v\beta} (\sinh v(\tau - \beta/2) - \sinh v(\sigma - \beta/2)) + \frac{\mu}{M\beta} (\tau - \sigma) \right] \\ &\quad - \bar{r}_1 \left[ \frac{\mu \sinh v(\sigma - \tau)/2}{\sinh v\beta} (\sinh v(\tau - \sigma)/2 + \cosh v(\beta - (\tau + \sigma)/2)) - \frac{\mu}{M\beta} (\tau - \sigma) \right] \end{aligned} \quad (4.32)$$

This expression can be simplified by letting  $\tau > \sigma$  and becomes

$$\bar{A} = \langle \bar{r}_\tau - \bar{r}_\sigma \rangle = \mu \left( \frac{\sinh v(\tau - \sigma)/2 \cosh v(\beta - \tau - \sigma)/2}{m \sinh v\beta/2} + \frac{(\tau - \sigma)}{M\beta} \right) |\bar{r}_\tau - \bar{r}_\sigma|, \quad (4.33)$$

and

$$B = \frac{1}{6} \left[ \langle (\bar{r}_\tau - \bar{r}_\sigma)^2 \rangle - A^2 \right]. \quad (4.34)$$

The first term in the square bracket can be expanded and calculated from the generating functional

$$\begin{aligned} \langle (\bar{r}_\tau - \bar{r}_\sigma)^2 \rangle &= \langle \bar{r}_\tau^2 \rangle + \langle \bar{r}_\sigma^2 \rangle - 2 \langle r_\tau r_\sigma \rangle \\ &= \frac{3\mu}{m} \left( \frac{2 \sinh \frac{v}{2}(\tau - \sigma) \sinh \frac{v}{2}(\beta - (\tau - \sigma))}{mv \sinh \frac{v}{2}\beta} + \frac{[\beta - (\tau - \sigma)](\tau - \sigma)}{M\beta} \right) \\ &\quad + \mu^2 \left( \frac{\sinh \frac{v}{2}(\tau - \sigma) \cosh \frac{v}{2}(\beta - (\tau + \sigma))}{m \sinh \frac{v}{2}\beta} + \frac{(\tau - \sigma)}{M\beta} \right)^2 |\bar{r}_\tau - \bar{r}_\sigma|^2. \end{aligned} \quad (4.35)$$

Substitute this into (4.34) together with (4.33) then we can find **B**. From the relation

$$\langle S' \rangle = C \frac{\delta}{\delta C} \ln \rho. \quad (4.36)$$

we recall that  $C = \frac{w}{4}(v^2 - w^2)$ . Equation (4.36) then becomes

$$\begin{aligned}
\langle S_i \rangle = & -\frac{3}{2} \left(1 - \frac{w^2}{v^2}\right) \left(\frac{v\beta}{2} \coth \frac{v\beta}{2} - 1\right) - \frac{(\bar{r}_\tau - \bar{r}_\sigma)^2}{2\beta} \left\{ -\left(1 - \frac{w^2}{v^2}\right)^2 \left(\frac{v\beta}{2} \operatorname{cosech}^2 \frac{v\beta}{2}\right. \right. \\
& \left. \left. + \left(1 - \frac{w^2}{v^2}\right) \frac{v\beta}{2} \coth \frac{v\beta}{2} - \frac{1}{2} \left(1 - \frac{w^2}{v^2}\right)^2 \frac{v\beta}{2} \coth \frac{v\beta}{2} - \frac{w^2}{v^2} \left(1 - \frac{w^2}{v^2}\right) \right\}. \quad (4.37)
\end{aligned}$$

Collecting all terms and substituting into the equation (4.13) gives us the full form of the density matrix which will be presented in the next chapter.

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