CHAPTER V

GROUND STATE OF THE POLARON

In previous chapter we have obtained the polaron density matrix at finite temperature. Now, we may ask whether this density matrix gives the same ground state energy and effective mass as those of Feynman or not? If it does, it will convince us that this density matrix is correct. To see this, let us consider the behaviour of the density matrix at zero temperature which corresponds to the imaginary time goes to infinity. (It is noted that Feynman did not evaluate these properties from the full density matrix). The polaron density matrix reads

$$\rho(\vec{x}_2 - \vec{x}_1; \beta) = \rho_* \exp(\mathrm{A} + \int_0^\infty \int_0^\infty d\sigma d\tau (\mathrm{B} + \mathrm{E}|\vec{x}_2 - \vec{x}_1|^2)) \tag{5.1}$$

where

$$\mathrm{A} = -\frac{3}{2}\left(1 - \frac{w^2}{v^2}\right)\left(\frac{v\beta}{2}\coth(\frac{v\beta}{2}) - 1\right)$$

$$\mathrm{B} = \frac{\alpha}{2^{3/2} m^{1/2}} \int_0^\infty \frac{d^3k}{2\pi^2 \vec{k}^2} \exp\Big[i\vec{k}\cdot(\vec{x}_2 - \vec{x}_1)\mu\Big(\frac{\sinh\frac{v}{2}(\tau - \sigma)\cosh\frac{v}{2}(\beta - (\tau + \sigma))}{\sinh\frac{\beta}{2}}$$

$$\frac{(\tau - \sigma)}{M\beta}\Big) - \frac{\vec{k}^2}{2mv^2} F(|\tau - \sigma|, \beta)\Big] \frac{\cosh w(\frac{v\beta}{2} - |\tau - \sigma|)}{\sinh\frac{v\beta}{2}}$$

$$E=-\frac{C}{2}\mu^2\left(\frac{\sinh\frac{\nu}{2}(\tau-\sigma)\cosh\frac{\nu}{2}(\beta-(\tau-\sigma))}{\sinh\frac{\nu\beta}{2}}+\frac{(\tau-\sigma)}{M\beta}\right)^2\frac{\cosh w(\frac{\beta}{2}-(\tau-\sigma))}{\sinh\frac{w\beta}{2}}$$

$$F(|\tau-\sigma|,\beta)=\mu\left(\frac{2\nu\sinh\frac{\nu}{2}(\tau-\sigma)\sinh\frac{\nu}{2}(\beta-(\tau-\sigma))}{m\sinh\frac{\nu\beta}{2}}+\frac{\nu^2(\beta-(\tau-\sigma))(\tau-\sigma)}{M\beta}\right)$$

$$\rho_{\circ}(\vec{x}_2-\vec{x}_1;\beta)=\left(\frac{m}{2\pi\beta}\right)^{\frac{3}{2}}\left(\frac{\nu}{w}\frac{\sinh\frac{w\beta}{2}}{\sinh\frac{w\beta}{2}}\right)^3\exp\left[-\left(\frac{\mu\nu}{2}\coth\frac{\nu\beta}{2}+\frac{1}{2}\frac{\mu}{M\beta}\right)|\vec{x}_2-\vec{x}_1|^2\right] \quad (5.2)$$

The expression for the density matrix has been arranged so that we can see easily that the terms depending on the square of the coordinates are the off-diagonal parts. We write $\rho_{\circ}$ separately to distinguish it from the correction terms since this density matrix of trial action will give the zeroth order effective mass. (Note that the function $F(|\tau-\sigma|,\beta)$ would reduce to the function $F(x)$ of Feynman.)

From the two-particle model in previous chapter, instead of considering the coordinate of the electron, it is more convenient to transform this coordinate into the center of mass system in which

$$\vec{R}=\frac{m\vec{x}+M\vec{y}}{m+M} \quad (5.3)$$

where $\vec{x}$ is the electron coordinate

$\vec{y}$ is the fictitious particle coordinate.

Hence the center of mass coordinate are transformed as

$$\vec{R}_2 - \vec{R}_1 = \frac{m}{m_*}\left(\vec{x}_2 - \vec{x}_1\right) \tag{5.4}$$

Now we will consider the density matrix at zero temperature (β goes to infinity) and expect that the ground state energy and the effective mass of the polaron can be obtained from this density matrix. Let us firstly consider the off-diagonal part (i.e. the part depending on coordinates square) together with

$$\exp\left\{\int_0^\beta\int_0^\beta d\tau d\sigma \left[\frac{\alpha}{2^{3/2} m^{\frac{1}{2}}}\int_0^\infty \frac{dk}{3\pi} k^2 \exp\left(\frac{-k^2}{2mv^2}\right)\frac{\cosh\left(\frac{\beta}{2}-|\tau-\sigma|\right)}{\sinh\frac{\beta}{2}} - \frac{C}{2}\frac{\cosh w\left(\frac{\beta}{2}-|\tau-\sigma|\right)}{\sinh\frac{w\beta}{2}}\right]\right.$$
$$\left.\times\left(\frac{\sinh\frac{v}{2}(\tau-\sigma)\cosh\frac{v}{2}(\beta-(\tau+\sigma))}{m\ \sinh\frac{v\beta}{2}} + \frac{(\tau-\sigma)}{M\beta}\right)^2 M^2\left(\vec{R}_2-\vec{R}_1\right)^2\right\} \tag{5.5}$$

Notice that at low temperatures $\beta \to \infty$ we can show that

$$\frac{\cosh\left(\frac{\beta}{2}-|\tau-\sigma|\right)}{\sinh\frac{\beta}{2}} = \frac{\exp[\frac{\beta}{2}-|\tau-\sigma|]+\exp[-\frac{\beta}{2}+|\tau+\sigma|]}{\exp[\frac{\beta}{2}](1-\exp[-\beta])}$$

$$\xrightarrow[\beta\to\infty]{} \exp[-|\tau-\sigma|]$$

Similarly

$$\frac{\cosh w\left(\frac{\beta}{2}-|\tau-\sigma|\right)}{\sinh\frac{w\beta}{2}}\xrightarrow[\beta\to\infty]{}\exp[-w|\tau-\sigma|]$$

and the term

$$\frac{\sinh\frac{v}{2}(\tau-\sigma)\cosh\frac{v}{2}(\beta-(\tau+\sigma))}{\sinh\frac{v\beta}{2}}\approx\frac{\exp[-v\sigma]-\exp[v\tau]}{2}\xrightarrow[\beta\to\infty]{}0$$

The last expression goes to zero under the integration of the imaginary time from zero to infinity. By using the formula of Gaussian integration in the k integral, the off-diagonal part becomes

$$\exp\left\{\int_0^\beta\int_0^\beta d\tau d\sigma\left[\frac{\alpha m}{12\sqrt{\pi}}F(|\tau-\sigma|,\beta)^{-\frac{3}{2}}e^{-|\tau-\sigma|}-\frac{C}{2}e^{-w|\tau-\sigma|}\right]\frac{(\tau-\sigma)^2}{\beta^2}\left|\vec{R}_2-\vec{R}_1\right|^2\right\} \qquad (5.6)$$

To evaluate the integral in the exponent we can make approximation as

$$\int_0^\beta\int_0^\beta d\tau d\sigma\, g(|\tau-\sigma|)\approx 2\beta\int_0^\beta dx\, g(x) \qquad \text{as } \beta\to\infty$$

where $g(|\tau-\sigma|)$ is any function of its arguments, and the above equation can be shown by defining

$$f(\tau)=\int_0^\beta d\tau\, g(|\tau-\sigma|)$$

then

$$\int_0^\beta\int_0^\beta d\sigma d\tau\; g(|\tau-\sigma|) = 2\int_0^\beta\int_0^\tau d\sigma d\tau\, g(|\tau-\sigma|)$$

$$= 2\int_0^\beta d\tau f(\tau) = 2\left[\tau f(\tau)\Big|_0^\beta - \int_0^\beta d\tau\, \tau g(\tau)\right]$$

$$= 2\int_0^\beta x(\beta - x)g(x) \xrightarrow[\beta\to\infty]{} 2\beta\int_0^\infty dx g(x)$$

and then

$$\exp\left\{\int_0^\infty dx\left[\frac{\alpha m v^3}{12\sqrt{\pi}}F(x)^{-\frac{3}{2}}e^{-x} - \frac{C}{2}x^2 e^{-wx}\right]\frac{|\vec{R}_2 - \vec{R}_1|^2}{\beta^2}\right\} \tag{5.7}$$

Note that $F(x)$ is the low temperature limit of $F(|\tau-\sigma|,\beta)$ and the as those of Feynman in previous chapter. If we compare the above expression to a free particle density matrix which the effective mass can be defined as

$$\exp\left(-\frac{m_{eff}|\vec{R}_2 - \vec{R}_1|^2}{2\beta}\right)$$

Then we can find the polaron effective mass. But the expression in (5.7) is only the correction term of the zeroth order effective mass mentioned earlier so we must add it up to the zeroth order term. Then

$$m_F = m_e + \int_0^\infty dx\left(\frac{\alpha m}{3\sqrt{\pi}}v^3 x^2 e^{-x}F(x)^{-\frac{3}{2}} - 2C x^2 e^{-wx}\right). \tag{5.8}$$

The last term can be integrated to give

$$2C\int_0^{\infty} dx\, x^2 e^{-wx} = \frac{4C}{w} = M$$

This M together with m_* will give m, the mass of an electron. So we arrive at the same form of the polaron effective mass as Feynman.

$$\frac{m_F}{m} = 1 + \frac{\alpha}{3\sqrt{\pi}}\int_0^{\infty} dx v^3 x^2 e^{-x} F(x)^{-\frac{3}{2}} \qquad (5.9)$$

As pointed out by Sa-yakanit[16] that the transformation from electron coordinate to the center of mass system corresponds to replacing $\vec{x}(\tau)-\vec{x}(\sigma)$ by $U(\tau-\sigma)$. Since we know from the action that the polaron system has the translational invariance so we can approximate the classical path by straight line whereas the imaginary time interval must be small. In our case we put all the effects of the phonon field into the effect produce by a fictitious particle of mass M and the internal structures of the polaron were neglected. With this reason, the center of mass system is suitable for describing the polaron.

Now we turn to the other part of the polaron density matrix, the diagonal part which is the part independent of the polaron coordinate and this part contribute to the partition function of the system. Its expression reads

$$\left(\frac{m}{2\pi\beta}\right)^{\frac{3}{2}}\left(\frac{v}{w}\frac{\sinh\frac{w\beta}{2}}{\sinh\frac{v\beta}{2}}\right)^3 \exp\left\{\frac{\alpha}{2^{\frac{3}{2}}m^{\frac{1}{2}}}\int_0^{\beta}\int_0^{\beta} d\tau d\sigma\int_0^{\infty}\frac{d^3k}{2\pi^2k^2}\exp\left(-\frac{\vec{k}^2}{2mv^2}F(|\tau-\sigma|,\beta)\right)\right.$$

$$\times\frac{\cosh\left(\frac{\beta}{2}-|\tau-\sigma|\right)}{\sinh\frac{\beta}{2}}-\frac{3}{2}\left(1-\frac{w^2}{v^2}\right)\left[\frac{v\beta}{2}\coth\frac{v\beta}{2}-1\right] \tag{5.10}$$

Similar to the off-diagonal part, the above expression is

$$\left(\frac{m}{2\pi\beta}\right)^{\frac{3}{2}}\left(\frac{v}{w}\right)^{3}e^{\frac{3\beta}{2}(w-v)}\exp\left\{\frac{v\alpha\beta}{\sqrt{\pi}}\int_{0}^{\infty}dx\,e^{-x}F(x,\beta)^{-\frac{1}{2}}-\frac{3}{2}\left(1-\frac{w^2}{v^2}\right)\left[\frac{v\beta}{2}\coth\frac{v\beta}{2}-1\right]\right\} \tag{5.11}$$

By expanding the function $F(x,\beta)^{-\frac{1}{2}}$ with respect to $\frac{1}{\beta}$ up to first order

$$\begin{aligned}F(x,\beta)^{-\frac{1}{2}} &= F(x)^{-\frac{1}{2}}+\frac{\partial F(x,\beta)^{-\frac{1}{2}}}{\partial\frac{1}{\beta}}\frac{1}{\beta}+\ldots\\ &= F(x)^{-\frac{1}{2}}+\frac{1}{2}\frac{\mu x^2\mu^2}{M}F(x)^{-\frac{3}{2}}\frac{1}{\beta}+\ldots\end{aligned}$$

and substituting back into the density matrix we obtain

$$\begin{aligned}&\left(\frac{m}{2\pi\beta}\right)^{\frac{3}{2}}\left(\frac{v}{w}\right)^{3}e^{\frac{3\beta}{2}(w-v)}\exp\left\{\frac{\alpha v}{\sqrt{\pi}}\int_{0}^{\infty}dx\,e^{-x}F(x)^{-\frac{1}{2}}\beta+\frac{\alpha v}{\sqrt{\pi}}\int_{0}^{\infty}dx\,x^2e^{-x}F(x)^{-\frac{3}{2}}\frac{v^2\mu}{2M}\right.\\ &\left.+\frac{3}{2}\left(1-\frac{w^2}{v^2}\right)\left[\frac{v\beta}{2}\coth\frac{v\beta}{2}-1\right]\right\}.\end{aligned} \tag{5.12}$$

The terms that are independent of β can be separated out as the prefactor of the density matrix. If we demand that at ground state of the polaron, the density matrix should be the form

$$\rho \approx \left(\frac{m^*}{2\pi\beta}\right)^{\frac{3}{2}} \exp\left(-E_0\beta\right) \tag{5.13}$$

By comparing the equation (5.12) to (5.13) we found that the effective mass and the ground state energy of the polaron respectively as

$$m_{KP} = m\left(\frac{v}{w}\right)^2 \exp\left(\frac{w^2}{v^2} - 1 + \frac{w^2}{v^2}\frac{\alpha v^3}{\sqrt{\pi}}\int_0^{\infty} dx\, x^2 e^{-x} F(x)^{-\frac{3}{2}}\right) \tag{5.14}$$

$$E_0 = \frac{3}{4}\frac{(v-w)^2}{v} - \frac{\alpha v}{\sqrt{\pi}}\int_0^{\infty} dx\, e^{-x} F(x)^{-\frac{1}{2}} . \tag{5.15}$$

The expression of m_{KP} is the same as the effective mass evaluated by Krivoglaz and Pekar [22] and the energy is exactly the same as those of Feynman[14]. Now, we have found two different definitions of the polaron effective mass from the same density matrix. We may ask whether these definition would be the same or not, or if there is any relation between them. We expect that the answer should come from investigation of some properties of the density matrix. As mentioned earlier the density matrix of equation (5.1) is not exactly the real matrix that can used to describe the system. And it would give the upper bound for the ground state energy under the Feynman-Jansen inequality. So the assumption that the polaron at ground state behaves like a free particle is only an approximation. For the effective mass, unlike the energy we have no criterion to justify which one is true or which one is better (for the ground state energy, the lower is the better). Nevertheless, we will consider further on the wave function of the polaron.

By collecting all the diagonal and off-diagonal part of the polaron density matrix we can write

$$\rho\left(\vec{R}_2-\vec{R}_1;\beta\to\infty\right)\approx\left(\frac{m^*}{2\pi\beta}\right)^{\frac{3}{2}}\exp\left(-E_0\beta-\frac{m_F\left|\vec{x}_2-\vec{x}_1\right|^2}{2\beta}\right). \qquad (5.16)$$

We can extract the wave function of the polaron from this density matrix by considering

$$\int_{-\infty}^{\infty} d^3k\ \exp\left[-\frac{2\pi^2\beta}{m^*}\vec{k}^2+2\pi\, i\vec{k}\cdot\left|\vec{R}_2-\vec{R}_1\right|\sqrt{\frac{m_F}{m^*}}\right]=\left(\frac{m^*}{2\pi\beta}\right)^{\frac{3}{2}}\exp\left(-\frac{m_F\left|\vec{R}_2-\vec{R}_1\right|^2}{2\beta}\right)$$

Substitute this and the density matrix reads

$$\rho=\int_{-\infty}^{\infty} d^3k\ \exp\left[i\vec{k}\cdot\left|\vec{R}_2-\vec{R}_1\right|2\pi\sqrt{\frac{m_F}{m^*}}\right]\exp\left[-E_0-\frac{2\pi^2\vec{k}^2}{m^*}\right], \qquad (5.17)$$

We change variable $\vec{k}$ by identifying the term in front of the coordinate as the momentum of the particle

$$\vec{p}=2\pi\sqrt{\frac{m_F}{m^*}}\,\vec{k}$$

and the measure

$$d^3k=\frac{d^3p}{\left(2\pi\sqrt{\frac{m_F}{m^*}}\right)^3}$$

Then the density matrix reads

$$\rho = \int \frac{Vd^3p}{(2\pi)^3}\left(\frac{m^*}{m_F}\right)^{\frac{3}{2}} \frac{1}{V}\exp\left[i\vec{p}\cdot\left|\vec{R}_2-\vec{R}_1\right|-\left(E_\circ+\frac{\vec{p}^2}{2m_F}\right)\beta\right] \tag{5.18}$$

From the relation

$$\rho(\vec{x}_2,\vec{x}_1;\beta)=\sum_n \Psi^*(\vec{x}_2)\Psi(\vec{x}_1)\exp(-E_n\beta)$$

We can separate out the wave function and the energy as

$$\Psi_p(\vec{R})=\frac{1}{\sqrt{V}}\sqrt{\frac{m^*}{m_F}}\exp[i\vec{p}\cdot\vec{R}], \tag{5.19}$$

$$E_p=E_\circ+\frac{\vec{p}^2}{2m_F}. \tag{5.20}$$

Note that the energy is the excitation state that depend on the momentum. If we consider about the normalization condition of the polaron wave function we find that

$$\int d^3R\,\Psi^*(\vec{R})\Psi(\vec{R})=\left(\frac{m^*}{m_F}\right)^{\frac{3}{2}}=1, \tag{5.21}$$

so we can conclude that the mass defined by Krivoglaz and Pekar should be the same value as the Feynman mass. What we can do is evaluation of these quantities numerically at various coupling constant by the same set of variational parameters which will be presented in the next chapter.