CHAPTER VI

RESULTS, DISCUSSIONS AND CONCLUSION

As mentioned earlier, the polaron mass defined by Feynman is somewhat questionable. Firstly, he substituted the distance between two polaron end points by an imaginary velocity $\vec{U}$ multiplied by imaginary time as $\vec{x}_2 - \vec{x}_1 = \vec{U}\tau$ and used it to determine the generating functional and find the effective mass from this functional. This means that he neglected all the quantum fluctuation since the distance between two points are replaced by a straight line. The reason that can support this idea, as pointed out by Sa-yakanit [16], is that the distance and the momentum of the polaron must be small. Secondly, the numerical values of the effective masses which obtained by using variational parameters were determined from minimization of the ground state energy. At this point, the correct way should be extension of minimizing the energy for each momentum of the polaron but, as pointed out by Feynman himself, we have not found the expected extension [14].

The first discrepancy can be fixed by the result that Sa-yakanit has shown. The polaron effective mass can be determined rigorously from the off-diagonal part of the density matrix at zero temperature limit and the result corresponds to that of Feynman. For the second one, there is still no variational principle for this definition. The aim of this work is to find a more physical definition of the effective mass. The variational parameters that determine mass assumed to be obtained from a different argument of Feynman.

From the results in previous chapter, the ground state wave function of the polaron was found from the plaron density matrix and we obtained a condition that if we demand the wave function to be normalized the two definition of the effective mass, i.e. the definition by Feynman and by Krivoglaz and Pekar should be equal. By setting

$$m_{KP}(v,w) = m_F(v,w), \qquad (6.1)$$

we obtain

$$1+\frac{\alpha v^3}{3\sqrt{\pi}}\int_0^{\infty} dx \frac{x^2 e^{-x}}{F(x)^{\frac{3}{2}}} = \left(\frac{v}{w}\right)^2 \exp\left[\frac{w^2}{v^2} - 1 + \frac{w^2}{v^2}\frac{\alpha v^3}{3\sqrt{\pi}}\int_0^{\infty} dx \frac{x^2 e^{-x}}{F(x)^{\frac{3}{2}}}\right] \qquad (6.2)$$

where $F(x) = w^2 x + v\left(1-\frac{w^2}{v^2}\right)\left(1-e^{-vx}\right).$

We use equation (6.2) to determine one of the parameters and use the other to minimize the ground state energy. The numerical results is presented in table 6.1 (see Appendix). It is noted that the new parameters satisfy our assumption, i.e. these parameters satisfy the equation (6.2) and at the same time minimize the energy. For comparison we present also the values calculated from the expressions by Feynman and Krivoglaz and Pekar in table 6.2. Comparison between our results and Feynman's results are presented in tables 6.3 and 6.4. The effective masses will be plotted in figure 6.1.

Table 6.1 The variational parameters obtained from the minimization of the ground state energies and then the effective mass was re-calculated.

α	v	w	m_{new}	E_{new}
1	2.716	2.48	1.19819	-1.01293
2	2.841	2.33	1.48568	-2.05494
3	3.028	2.18	1.93148	-3.13234
4	3.264	1.99	2.68936	-4.25447
5	3.663	1.80	4.13918	-5.43697
6	4.396	1.61	7.45220	-6.70704
7	5.575	1.43	15.2030	-8.10945
8	7.414	1.30	35.5344	-9.69335
9	9.877	1.22	65.5548	-11.4846
10	12.72	1.17	118.221	-13.4888
11	15.34	1.13	184.296	-15.7094
12	19.00	1.11	293.163	-18.1419
13	22.40	1.09	422.105	-20.7901
14	25.51	1.07	568.366	-23.6497
15	29.62	1.06	781.014	-26.7234
16	33.72	1.05	1031.17	-30.0085

Table 6.2 The ground state energies and the effective masses of the polaron by the definition of Krivoglaz-Pekar and Feynman. The variational parameter comes from minimizing the ground state energy[1].

α	v	w	m_{kp}	m_F	E_F
1	3.06	2.83	1.19494	1.19466	-1.01302
2	3.237	2.716	1.47361	1.47264	-2.05536
3	3.42	2.56	1.89153	1.88846	-3.13333
4	3.663	2.368	2.38875	2.57774	-4.25648
5	4.04	2.14	3.90995	3.89417	-5.44014
6	4.667	1.874	6.87053	6.83690	-6.71087
7	5.81	1.604	14.4544	14.3908	-8.11269
8	7.588	1.403	31.6807	31.5851	-9.69537
9	9.851	1.283	62.8567	62.7329	-11.4858
10	12.48	1.210	111.992	111.849	-13.4904
11	15.41	1.162	183.215	183.066	-15.7098
12	18.67	1.136	281.742	281.499	-18.1434
13	22.17	1.110	412.442	412.218	-20.7907
14	25.99	1.090	582.859	582.681	-23.6513
15	30.08	1.077	797.441	797.250	-26.7249
16	34.46	1.067	1064.22	1064.28	-30.0114

[1] This data are taken from the results calculated by Lu and Rosenfelder [25].

Table 6.3 Comparison of Feynman's energies, E_F with our results, E_{new} at various coupling constants.

α	E_F	E_{new}	%different
1	-1.01302	-1.01293	0.008885
2	-2.05536	-2.05494	0.020436
3	-3.13333	-3.13234	0.031601
4	-4.25648	-4.25447	0.047233
5	-5.44014	-5.43697	0.058288
6	-6.71087	-6.70704	0.057088
7	-8.11269	-8.10945	0.039945
8	-9.69537	-9.69335	0.020837
9	-11.4858	-11.4846	0.010448
10	-13.4904	-13.4888	0.011861
11	-15.7098	-15.7094	0.002546
12	-18.1434	-18.1419	0.008268
13	-20.7907	-20.7901	0.002886
14	-23.6513	-23.6497	0.006765
15	-26.7249	-26.7234	0.005613
16	-30.0114	-30.0085	0.009663

Table 6.4 Comparison of Feynman's masses, m_F with our results, m_{new} at various coupling constants.

α	m_F	m_{new}	%different
1	1.19466	1.19819	0.29
2	1.47361	1.48568	0.82
3	1.89153	1.93148	2.25
4	2.38875	2.68936	4.24
5	3.90995	4.13918	6.09
6	6.83690	7.45220	8.61
7	14.3908	15.2030	5.49
8	31.5851	35.5344	11.77
9	62.7329	65.5548	4.39
10	111.849	118.221	5.54
11	183.066	184.296	0.50
12	281.499	293.163	4.06
13	412.218	422.105	2.37
14	582.681	568.366	2.49
15	797.250	781.014	2.06
16	1064.28	1031.17	3.16

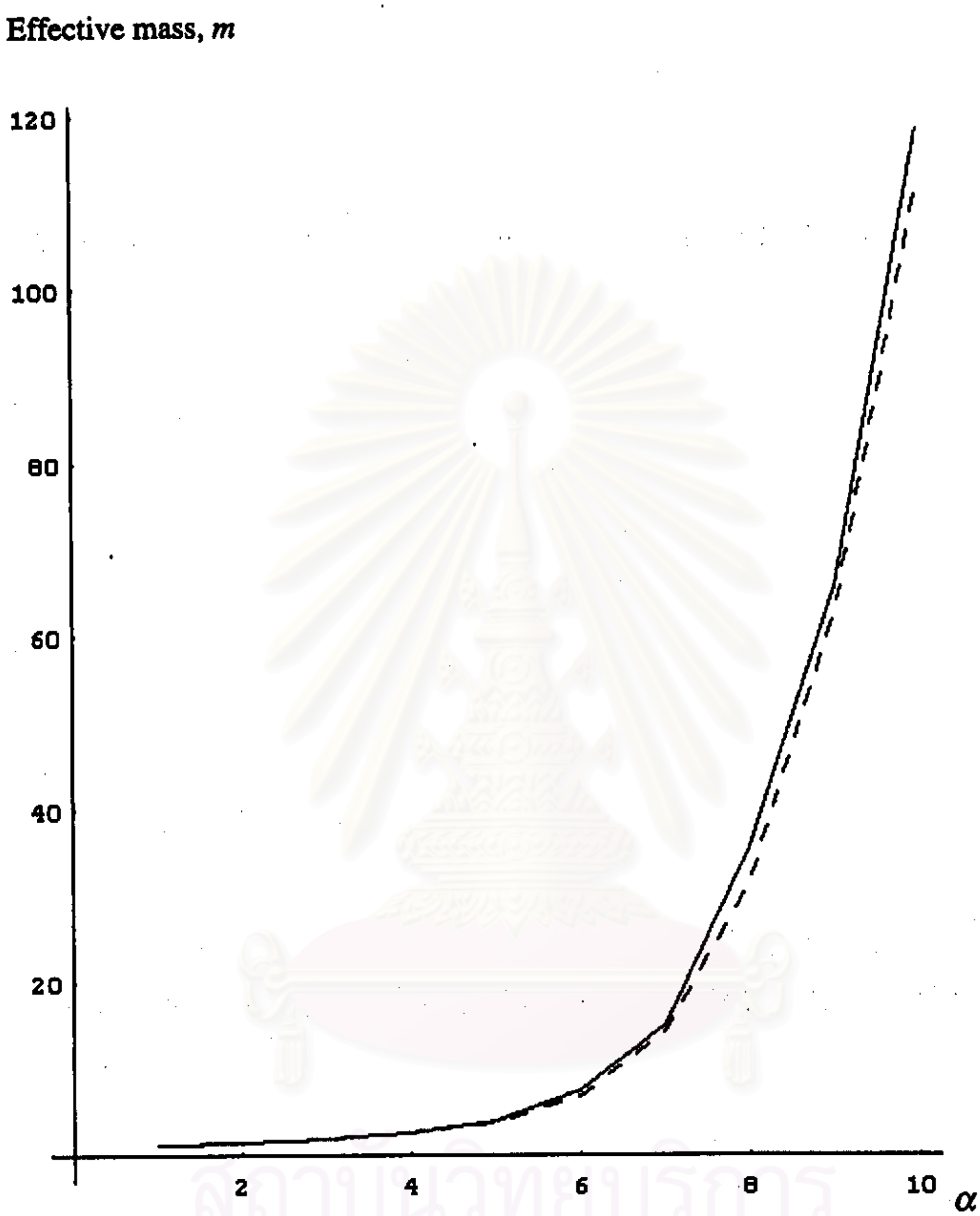

Figure 6.1 The polaron effective massed plotting versus the coupling constants. The dashed line denotes the result by Feynman. The solid line is our result.

We can see from the graphs that the numerical values of our effective masses are a little greater than the results calculated from Feynman's definition. The differences grow more in the intermediate coupling. The most difference is not more than 12 %. At the ground state energies, the differences between our results and Feynman's are very small. This is not an improvement since the energies must be as low as possible. Our results are slightly higher than Feynman's energies. For all coupling, the differences do not exceed approximately 0.06 % which can be improved by the more accurate calculation (minimization).

In fact, we cannot judge which definitions are right. Feynman's definition is better in the sense that the energies are lower, which following the Feynman-Jansen inequality. Our definition is superior for it satisfying the normalized-wave function condition that we impose. The very small deviations in energies make us claim that our definition is consistent with the theory and is an alternative way to define the effective mass.

Another aspect of the effective mass of the polaron we have considered is the momentum dependence of the mass. In the process that we obtained the Feynman's effective mass from the finite-temperature density matrix, we have collected only the terms up to the 2nd order of the coordinates of the electron which is enough for the case of low momentum limit which is Feynman's work. It is interesting to investigate the higher order terms and we may proceed by expanding the exponential involving the coordinates, $\left(\vec{R}_2 - \vec{R}_1\right)$ in the equation (5.5). The 3rd order term will vanish since it is an odd function under integration over $\vec{k}$, and the 4th order term will be kept. The mass depends on the momentum as

$$\frac{\left(\vec{R}_2 - \vec{R}_1\right)^4}{\beta^4}. \tag{6.3}$$

As mentioned previously, the effective mass can be defined from the coefficients of the coordinates squared. So this 4th order term can be added up to the effective mass by separating out the 4th power to be 2nd power terms. Remark that this can be done by assuming that we can neglect the correlation of the momentum. The result is the effective mass that depends on the momentum as

$$\frac{m_F}{m}=1+\frac{\alpha}{3\sqrt{\pi}}\int_0^{\infty}dx\frac{v^3x^2e^{x}}{F^{\frac{3}{2}}(x)}+\frac{\alpha}{18\sqrt{\pi}}\int_0^{\infty}dx\frac{v^5x^4e^{-x}}{F^{\frac{5}{2}}(x)}\vec{P}^2. \tag{6.4}$$

For low momenta, we can neglect this correction term and the expression of the effective mass reduces to the case of Feynman. We have performed the numerical calculation of the effective mass and the relation between this mass and the polaron momentum can be shown in figure 6.2

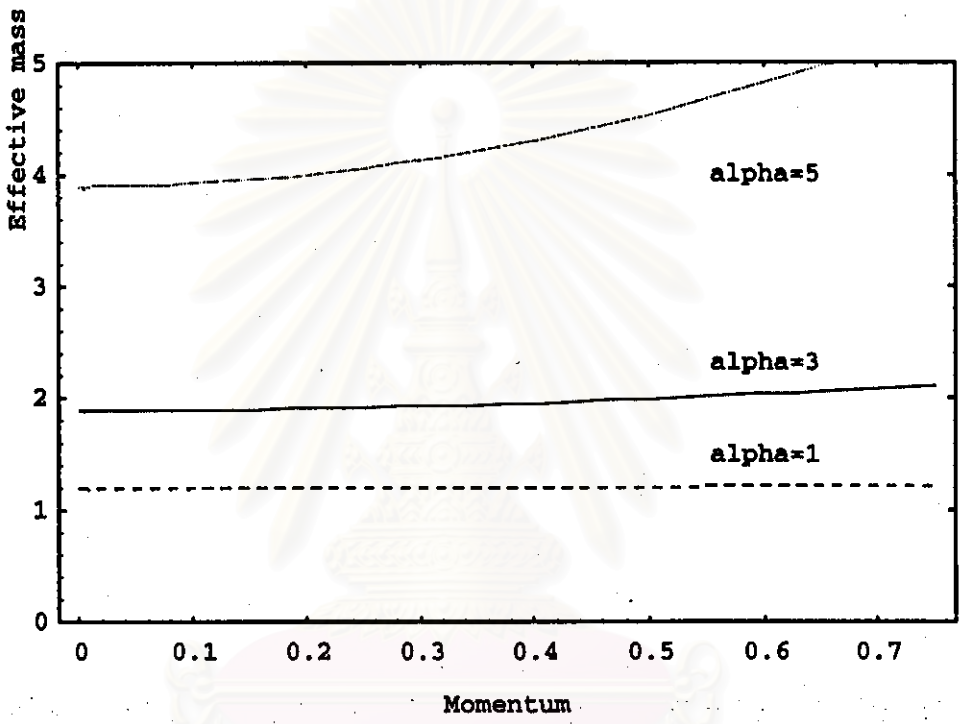

Figure 6.2 Relations between the polaron effective mass and its momentum plotting for various coupling constant (alpha means the coupling constant).

We can see that for weak coupling, the mass is nearly independent on the momentum (the dashed curve is nearly straight line). This is also true for the higher momentum. For the strong coupling, the masses depend quadratically to the momentum. We have tried to seek for the physical description of these results but we have not found it yet and later we will quote the work by other authors to compare their results to ours. Before going to that materials, we will present the relation between the energy and the momentum of the polaron as followed.

We know from the concepts of the quasi-particle that its self energy can be defined in the form of excitation energy like

$$E(\vec{P}) = E_0 + \frac{\vec{P}^2}{2m_{eff}}. \tag{6.5}$$

where E_0 is the ground state energy and m_{eff} is an effective mass

So if the quasi-particle behaves like a free particle then its total energy must depend on its momentum quadratically. In our case, instead of regarding the effective mass as a constant, we may substitute our effective mass in equation (6.4) into equation (6.5). The result can be summarized by figure 6.3.

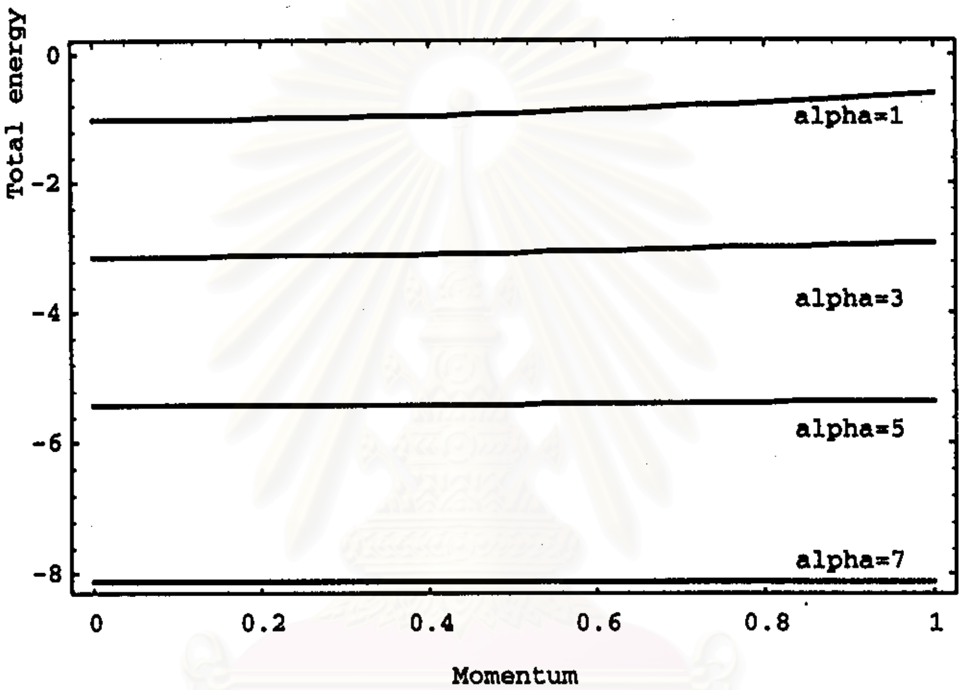

Figure 6.3 Relations between the energy and momentum of the polaron at various coupling constants.

This results correspond to previous figure involving mass since for weak coupling the energy dispersion looks like that of a free particle but for the larger coupling the momentum dependence decreases.

Recently, there is a work by Wang et. al. [29] concerning the properties of the moving polaron. By using the method of Lee, Low and Pines [5] they came to the results that are similar to ours which are presented in figures 6.4 and 6.5. Note that these figures are taken from reference [29].

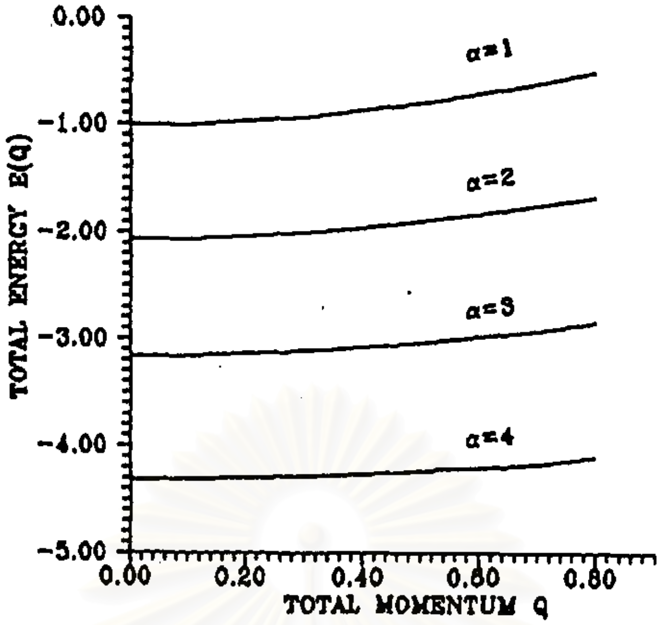

Figure 6.4 Total energy $E(Q)$ versus the total momentum Q of the electron and phonon with different coupling constants for $Q < 1.0$.

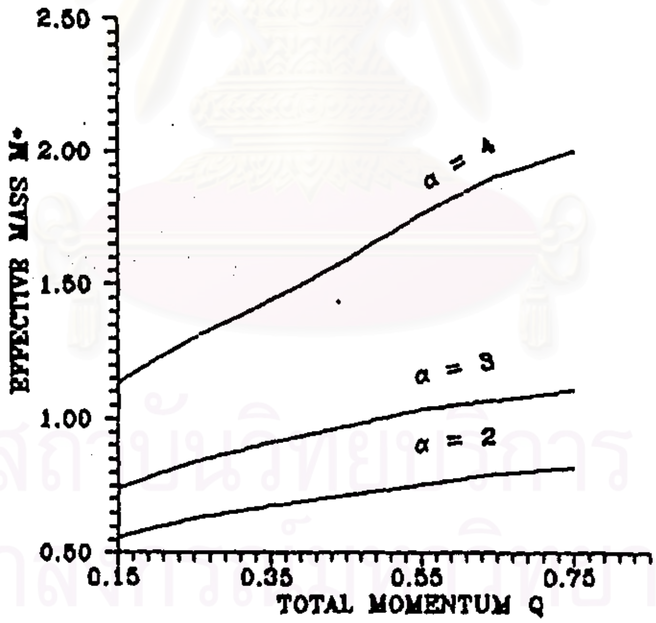

Figure 6.5 The effective mass as a function of total momentum with various coupling constants.

When we compare these figures to our results in figures 6.2 and 6.3 at the same range of momenta, we will see some similarity. Although we cannot say that these are the equivalent results but this reminds us for its implication. The work by Wang et. al. was concerned only the weak coupling regime (remember that Lee, Low and Pines method is a perturbation theory) so it could be applied to some values of momenta and coupling constants. In that work, they introduced the phonon momenta together with electron momentum which constitute to the total momentum of the system as we mentioned above. This is different from ours which the polaron coordinates was eliminated at the first step, then the momentum left is the momentum of the polaron itself. So we may interpret our momentum as the total momentum of the polaron system. They remarked further that, if we take the total momentum $Q=0$, we are able to return to the case of the static polaron. This is consistent with our result, as mentioned previously, if we let the momentum to be small, the correction term can be neglected and the mass reduces to that of Feynman. We have questioned earlier about the physical implication of the momentum dependent mass. From the view of path integral formulation we cannot see anything but if we compare it to the work by Wang et. al., and presume that it is equivalent to the path integration method we may find the interpretation from this work. Wang et. al. pointed out that when the momentum increases the total phonon number will increase, as does the binding energy of the system, thus, it will prevent increasing of the kinetic energy and make the total energy to be a constant with momentum. However, we cannot insist that our theory are equivalent to that of Wang et. al. since there is no rigorous proof for this similarity.

So far, we can summarize all the material we have presented as follow. By starting from the simplified model of the polaron, we can write down the Lagrangian. In order to evaluate the ground state energy and the effective mass of the polaron from this Lagrangian, we choose to follow the method of path integration which is superior than other methods as it can be applied for all ranges of the coupling constants. This method is based on the variation principle so the ground state energies we calculated are only the estimated upper bound of the real energies. In finding the effective mass, there is no variation principle to define this quantity so an ad hoc assumption was made. Although the numerical values of the effective mass defined by Feynman are in accord with the values obtained by other methods, we still want to find a better definition.

Our aim in this work is to look for a new definition of the effective mass that is consistent with the basic principle of quantum mechanics, i.e. the normalization condition of the wave functions of the polaron. These wave functions were extracted from the polaron density matrix at zero temperature limit. Together with this, we obtained the expression for energy excited state as well. We have found that if we demand the wave functions are normalizable, the mass defined from two different places of the density matrix must be equal and we can use this equality to be the condition that leads to the desired definition.

The numerical results of the masses and energies that have been re-minimized are very close to the values calculated from Feynman's expressions, especially the energies differ by no more than 0.06 % which can be improved further by a more accurate minimization. The masses deviate more but there is no criterion to judge which ones is correct. We may say that our definition is superior since it satisfied the condition proposed above. Demanding of an accurate numerical vales of the mass made us investigate further. If we consider the higher order terms of expansion of an exponential in density matrix, we will find that the first survived term depends on the momentum. If we substitute this mass into the energy excited states, we will obtain a dispersion relation that is similar to the one obtain by Wang et. al. [29]. If we suspect that this result is equivalent to the result by Wang et. al. or not, a rigorous proof is needed.