CHAPTER I

INTRODUCTION

The problem of an electron moving in ionic crystal has been studied for a long time. Originally, Landau[1] was the first who proposed that it was possible for an electron to be trapped by its distortion of the polar crystal. Later, Pekar [2], who gave the name Polaron, has made the picture of an electron in the conduction band of an ionic crystal polarizing the lattice surrounding it to such an extend as to influence its physical properties such as self energy, effective mass or mobility. But the first quantitative description of the polaron is due to Froehlich [3] who make some simplified assumptions to write down the Hamiltonian of the polaron explicitly. This is called the Froehlich Hamiltonain which is a classic theory followed by many authors after then.

In general, the polaron is an electron moving in polar crystal and dragging the ion cores along by a Coulomb interaction. This means that the electron distort the lattice to deform. This deformation causes the ion cores vibrate about their equilibrium position and gives rise to phonon excitation. The phonon that arise from electron distortion together with that from thermal excitation will effect back to the electron.When an electron moves it will carry the distortion along and we regard it as a quasiparticle named the polaron.

There are many types of polaron depending on the condition imposed such as the large polaron, the small polaron, bipolaron etc. But the most fundamental one is the model proposed by Froehlich corresponding to the large polaron type. This model is based on the assumption that the electron has De Broglie wave length very much larger than the lattice spacing so that the discrete lattice can be replaced by the continuous one. We will present the review of this matter for more details in chapter I. Furthermore, the large polaron has two types, one is the electron interacting with the acoustic branch of the phonons so that the frequency of the normal modes of vibration vary with wave vector. The other is the optical polaron of which the frequency of phonon is in the range of visible light and has been assumed to be constant. The Froelich model belongs to this type.

Another class of the polaron is the small polaron which take the lattice spacing into account. In the other words, the distortion of the electron to the lattice was restricted to the vicinity of the electron so that the continuous approximation is not valid. However, this is beyond the scope of this dissertation.

It is quite natural to investigate on how one can approach the polaron problem technically. Since this is the first model in condense matter physics that provides a simple form of a particle interacting with a quantum field. The Froehlich Hamiltonian can be divided into three parts which are the electron, phonon and the interaction between electron and phonon. In the early time, the Froehlich model can be solved perturbatively only in the weak coupling regime. Field theoretical approaches have been used in this problem. For instance, Lee, Low and Pines[4], Lee and Pines[5] used the technique invented by Tomonaga in quantum field theory applying to this problem. Besides this, a variational method is applied for the intermediate coupling (Lee and Pines[5], Gurari [6], Tiablikov[7]) and the strong coupling (Pekar[2], Allcock[8]). However, these methods are illegible to solve the problem only in some certain range of the coupling constant.

Apart from the approaches in the aforementioned, Feynman's path integration formulation of quantum mechanics [9] considered to be one of the very powerful technique in physics. Regarding to the polaron problem, Feynman calculated the upper bound of the ground state energy and the effective mass of the polaron [14]. The results from this approach are sensible for the entire range of coupling constants. So to speak, Feynman's path integration approach can be applied from the ranges of weak coupling limit to the strong coupling limit. However, the drawback of this approach is that it give the less accurate results when compared to other techniques results.

Other aspects of the polaron theory, for example, the polaron in magnetic field, the bound polaron, the small polaron, the bipolaron etc. can be followed in the reviews of Mitra et al.[10], Appel[11], or in many conference proceeding such as DeVreese and Papadopoulos [12], Lakhno[13].

So far we have mentioned briefly about the basic notions of the polaron. The main theme of this thesis is to investigate the definition of the effective mass of the polaron . The concept of the effective mass of the virtual particle (or quasi-particle) is that we replace the system of a particle interacting with its surrounding by regarding this system as a free particle with finite ground state energy and mass. The quasi-particle (or the effective mass) can be defined from the kinetic energy of the extended state. The polaron is therefore, the region of distortion together with the electron can be thought as a free particle with finite effective mass (where we assume that this electron is an electron in the conduction band of an ideal polar crystal or Bloch electron).

The definition of the effective mass can be determined by various ways. The most common approach is to first looking at the following equation,

$$E = E_{\circ} + \frac{P^2}{2m_{eff}},$$

here $E_{\circ}$ is the ground state energy. The way we define the effective mass of polaron is also used in a standard perturbation or variational methods [3,4,5,6,7,8]. Alternatively, due to Feynman [14] the mass of the polaron can be determine by the off-diagonal part of the density matrix. Next is to express the density matrix in the form of a free particle as

$$\exp\left[-E_{\circ}\beta - m_{eff}\frac{\left|\vec{R}_2 - \vec{R}_1\right|}{2\beta}\right].$$

Note that Feynman did not define exactly like this (we will show it with more details in Chapter III) since he used an ad hoc assumption in order to avoid solving the integro-differential equation directly. Later many authors proposed a closed form of the polaron density matrix by various method. These can be found in Osaka [15], Sa-yakanit [16], Khandekar et al.[17], Castrigiani et al.[18], Ventriglia et al.[19], Gerlach et al.[20]. By considering this matrix at absolute zero temperature one can recover the effective mass of the polaron by above definition and the result is exactly the same as that of Feynman. However, there is another definition of the effective mass in path integration formulation given by Saitoh[21] in which an external force had been included. The effective mass was defined from the coefficient of the exponent that is proportional to the external force like

$$\rho \approx \exp\left(-\frac{f^3\beta^3}{24m_{eff}}\right).$$

This effective mass then has the meaning of an inertial mass against the force. The different point from that of Feynman is that Feynman theory has translational invariance but Saitoh theory has a broken translational symmetry due to inclusion of external force. So we can justify that these two definitions are irrelevant. There is also another definition due to Krivoglaz and Pekar [22] in which the partition function of the polaron had been calculated by the technique, so called order operator calculus [23]. However, the effective mass from this approach [22] gave numerical values greater than that of Feynman in the strong coupling limit but in agreement with each other in the weak coupling limit. Up to now, Feynman definition is the most commonly acceptable, because of its advantage in validity to all coupling and smooth interpolation between different regime of the coupling constant.

In the original work of Feynman, all the properties of the polaron had been calculated by assuming zero temperature at the first step. So there is a question that, if we start from a finite temperature theory, can we obtain the same expression for energy and effective mass of Feynman? One of the work that can answer this question is the work of Sa-yakanit[16].

By constructing the density matrix of the polaron at a finite temperature and consider it at zero temperature limit, the Feynman effective mass and the ground state energy had been recovered from the off-diagonal element of the density matrix. At the ame time, if we consider the diagonal part which proportional to the partition function of the polaron, we will find that we can make an alternative definition of the effective mass. In the other words, this definition can be taken from the prefactor of the density matrix and the expression is exactly the same as the effective mass calculated by Krivoglaz and Pekar[22]. This made us to the question that can we define a new definition wih the condition that these two mass should be the same? (although their numerical values are different). One reason for asking like this is that, in finding the effective mass, the variational parameters, which are obtained from minimizing the ground state energy, are substituted into the expression for the effective mass with no variation condition to base on. We may quote Feynman own words [14]:

"Since there is an operator analogous to the momentum which commutes with the Hamiltonian, it would be expected that there is a variational principle which minimizes the energy for each momentum. That is, we ought to be able to extend our method to yield an upper limit to the energy for each value of momentum, but we have not found the expected extension ".

From these words, we can see that the Feynman's effective mass was not correctly defined. With this reason, we may seek for a new definition of the polaron effective mass by demanding that the Feynman's mass and the Krivoglaz and Pekar mass are the same. And then use this condition to re-minimize the ground state energy. This has been presented in Chapter VI.

It is worth mentioning that there are many attempts to improve the Feynman method by various ways such as Abe and Okamoto[24] use the trial action with more variational parameters corresponding to the electron bounded by more fictitious particles . Another way is to calculate the more correction terms, i.e. adding the second cumulant expansion (Lu and Rosenfelder [25]). But they have found that the improvement is not significantly better. So Feynman's method is quite adequate.

In the next chapter, the Froehlich model will be reviewed then the Feynman 's method will be presented in chapter III. Chapter IV and V concerning about finding the finite temperature density matrix and considering the wave function of the polaron at at zero temperature limit. And the result will be presented and discussed in the last chapter.