

## CHAPTER I

### INTRODUCTION

#### I.1 The Polaron Problem

Several drastic assumptions are generally made in attacking many-electron problems of solid state theory. Practically, one-electron problems are considered with the effects of other electrons treated statistically. In most cases, the crystal is assumed perfect without any impurities or defects and the ions are supposed to be fixed rigidly in their lattice positions. However, in studying particular aspects of the solid, some approximations are inapplicable, for example, the rigid lattice assumption must be abandoned in considering thermal properties of a crystal. As far as mathematical techniques are available, one hopes to deal with the less idealized situations in which most of the general approximations are still valid but some of these have to be remedied.

Our problem is to study a system of a slow conduction electron in an ionic crystal, commonly known as a polaron. Qualitatively, when an electron moves through the crystal it polarizes-and thus distorts-the lattice in its neighborhood. The polarization induces a dipole electric field which in turn acts back on the electron. As the electron moves, the polarization field always moves with it or, in quantum field theory language, the electron is dressed by the cloud of virtual phonons. Because of the strong interaction between the electron and the large electric dipole moments associated with the longitudinal optical modes of lattice vibration, it is unjustified to

neglect the interaction between the electron and these lattice vibrations. Such electron-lattice interaction affects both static and dynamic properties: it lowers the energy of the electron at rest, adds more inertia, or equivalently, effective mass to the electron and gives rise to scattering of the electron by the phonons. We shall focus our attention merely on the static properties, particularly on the effective mass of the polaron with extremely weak and strong interaction strength.

The polaron problem has first come into theoretical interest in 1933 when Landau proposed the idea of self-trapping electron in a sodium chloride crystal in an attempt to explain F-centers. The polaron concept was introduced later by Pekar in 1954. Various methods have been developed and applied to investigate polaron-related properties. The enthusiasm in this problem was aroused by the following reasons: it is a simple example of non-relativistic particle-quantum field interaction problems; it leads to the understanding of the validity of the less rigorous assumptions made about the lattice vibrations in the study of metal and metallic conductivity and especially to gain more information about polar semiconductors and insulators.

The principal mathematical device used in this research is the path integration technique formulated by Feynman and Hibbs<sup>(1)</sup>. It

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<sup>1</sup> R.P. Feynman, and A.R. Hibbs, Quantum Mechanics and Path Integral, New York: McGraw-Hill (1965) 26.

has been numerically proved by Schultz<sup>(2)</sup> to be the one that gives superior self-energy and effective mass of the polaron for a wide range of coupling strength as compared with other earlier polaron theories<sup>(3-4)</sup>.

Generally, a critical step in solving quantum mechanical problems is to set up the Hamiltonian, or classically, the Lagrangian of the systems. We thus begin the first chapter with a brief account for the derivation of the Frohlich Hamiltonian. All assumptions involved throughout the process will be summarized systematically. In the remaining sections of this chapter, we present a qualitative survey on how the polaron self-energy and effective mass depend upon the interaction strength,  $\alpha$ , in two limiting cases, i.e., for small and large  $\alpha$ . The path integral formalism of quantum mechanics with its particular illustration applied mainly in this thesis will be introduced together with its close relation to the density matrix in Chapter II. Chapter III is devoted to a study of Feynman's effective

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<sup>2</sup> T.D. Schultz, "Slow Electrons in Polar Crystals: Self Energy, Mass and Mobility.", Physical Review, 116 (1959) 526.

<sup>3</sup> T.D. Lee, and D. Pines, "Interaction of a Nonrealistic Particle with a Scalar Field with Application to Slow Electrons in Polar Crystal.", Physical Review, 92 (1953) 883.

<sup>4</sup> E.P. Gross, "Small Oscillation Theory of the Interaction of a Particle and Scalar Field.", Physical Review, 100 (1955) 1571.

approach to the polaron ground state energy and effective mass since it is the original work that proves the success of the path integral method. The results will be carried out in detail, especially on the effective mass. Various results based on different definitions of the effective mass worked out by other authors<sup>(5-8)</sup> will be given in the following chapter. In Chapter V, we extend the evaluation of the polaron effective mass to a slightly more general state by considering the density matrix instead of the propagator or the partition function of the problem. In the last chapter we compare our results of the polaron effective mass with those mentioned previously. Finally, further possible improvements of the results will be discussed.

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<sup>5</sup> See Reference (2) P. 528

<sup>6</sup> J.T. Marshall, and M.S. Chawla, "Feynman Path-Integral Calculation of the Polaron Effective Mass.", Physical Review B, 2 (1970) 4283.

<sup>7</sup> M.A. Krivoglaz, and S.I. Pekar, "The Method of Traces for Conduction Electrons in Semiconductors." (Part II), Bull. Acad. Sci. USSR Phys. Ser. (English Translation) 21 (1957) 13.

<sup>8</sup> R.W. Hellwarth, and P.W. Platzman, "Magnetization of Slow Electrons in a Polar Crystal.", Physical Review, 128 (1962) 1599.

## I.2 Classical Lagrangian and Hamiltonian of the System

The Hamiltonian describing the behavior of an electron in a lattice field was first derived by Fröhlich<sup>(9)</sup>. According to various simplifying assumptions made during the course of his work, it was later well known as an idealized polaron model. Since the mathematical details of the Fröhlich derivation are available in the original and review papers concerning with this problem, we shall give here only a short mathematical account for this, and shall, instead, concentrate on physical interpretations.

As an electron is filled into the conduction band of a perfect ionic crystal, contributions to the energy of the system come from: the kinetic energy of the electron and the potential energy of interaction between the electron and the rigidly fixed lattice. The latter includes Coulomb and exchange interactions with other electrons. In one-electron approximation, this can be represented by a single periodic function of the electron position  $\vec{r}$ ,  $V(\vec{r})$ .

If the lattice is distorted, there will be three additional terms in the total energy: the lattice potential energy associated with the deformation, the additional interaction caused by the change in interaction  $V(\vec{r})$  of the electron with its deforming environment, and the lattice kinetic energy associated with the rate of lattice deformation.

One may ask, at this step, which modes of lattice vibration are likely to be interacted by the electron. Let us review briefly

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<sup>9</sup> H. Fröhlich, "Electrons in Lattice Fields.", Advances in Physics, 3 (1954) 3.

the dynamical properties of the lattice based upon the theory of Born and Huang<sup>(10)</sup>. In ionic crystals, there are two oppositely charged ions per unit cell giving rise to one longitudinal and two transverse optical modes and one longitudinal and two transverse acoustic modes for each wave vector  $\hat{k}$ . In the acoustic modes the two ions within each cell vibrate essentially in phase, the vibrations from cell to cell differing in phase depending on  $\hat{k}$ . In the optical modes, the two ions within each cell vibrate essentially out of phase, the vibrations from cell to cell still differing in phase depending on  $\hat{k}$ , however, as the main contributions to the lattice potential energy are from the interactions within a unit cell, the frequencies of these modes are not very sensitive to the phase relations between cells and the frequencies  $\omega_{\hat{k}}$  are frequently assumed to be independent of  $\hat{k}$ ,  $\omega_{\hat{k}} = \omega_L$ . This approximation may not be good for short wavelengths where the phase differences between cells are significant. The important characteristic of the longitudinal optical modes is that they give rise to a polarization field to be interacted with the electron whereas this field vanishes for transverse modes. Furthermore the long-wavelength acoustic phonons do not produce any polarization of the lattice. In other words, the long range interaction between the longitudinal optical modes and the electron is much stronger than the other short range contributions to the electron-lattice interaction term, so it is the only one considered.

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<sup>10</sup> M. Born, and K. Huang, Dynamical Theory of Crystal Lattices, Oxford: Clarendon Press (1956) 91.

According to the classification of energy mentioned above, the total Hamiltonian of the electron-lattice system can be written formally:

$$H = H_{el} + H_{field} + H_{int} \quad (1.1)$$

$H_{el}$  represents the energy contribution when we consider the motion of the electron in a rigidly fixed lattice, it is simply written  $\frac{m_{eff}\dot{r}^2}{2}$ , where  $m_{eff}$  stands for the electron effective mass. By replacing the free electron mass by its band mass, we have implicitly taken into account the effect of the periodic potential  $V(\vec{r})$ .

To obtain the expression for the free longitudinal optical phonons Hamiltonian  $H_{field}$ , it is necessary to compute the lattice potential energy associated with a polarization field which will occur during the course of the lattice vibrations. The energy per unit volume needed to produce an infinitesimal change in polarization  $d\vec{P}$  in a crystal with electric displacement  $\vec{D}$  is  $\vec{D} \cdot d\vec{P}$ . The polarization  $\vec{P}_i$  is related to  $\vec{D}_i$  and the electric field intensity  $\vec{E}_i$  in the crystal by

$$\vec{D}_i = \vec{E}_i + 4\pi\vec{P}_i \quad (1.2)$$

If the displacement  $\vec{D}_i$  is slowly created, it varies directly with the intensity  $\vec{E}_i$  through:

$$\vec{D}_i = \epsilon \vec{E}_i \quad (1.3)$$

where  $\epsilon$  is the static dielectric constant. Substitution of  $\vec{E}_i$  in (1.2) gives

$$\vec{P}_i = \frac{\epsilon - 1}{4\pi\epsilon} \vec{D}_i \quad (1.4)$$

Thus the total lattice potential energy per unit volume necessary to produce the polarization  $\vec{F}_i$  with the displacement  $\vec{D}_i$  is

$$\int_0^{F_i} \vec{D}_i \cdot d\vec{F} = \frac{4\pi\epsilon}{\epsilon-1} \frac{F_i^2}{2} = \frac{\epsilon-1}{4\pi\epsilon} \frac{D_i^2}{2}. \quad (1.5)$$

Now, if the external field is turned off quickly,  $\vec{D}_i$  will be decreased to zero. The relation (1.3) becomes

$$d\vec{D} = \epsilon_\infty d\vec{E}, \quad (1.6)$$

where  $\epsilon_\infty$  is the high frequency dielectric constant due to electronic polarization only. Thus

$$d\vec{F} = \frac{\epsilon_\infty - 1}{4\pi\epsilon_\infty} d\vec{D}, \quad (1.7)$$

and the work performed per unit volume in turning off the field is

$$\int_{D_i}^0 \frac{\epsilon_\infty - 1}{4\pi\epsilon_\infty} \vec{D} \cdot d\vec{D} = -\frac{\epsilon_\infty - 1}{4\pi\epsilon_\infty} \frac{D_i^2}{2}. \quad (1.8)$$

Combination of (1.5) and (1.8) gives total work  $U[\vec{F}]$  required to attain the desired final state  $\vec{F}(\vec{r})$  as

$$U[\vec{F}] = \frac{1}{4\pi} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon} \right) \int \frac{D_i^2}{2} d^3r, \quad (1.9)$$

and the final polarization is

$$\begin{aligned} \vec{F} &= \vec{F}_i + \int_{\vec{F}_i}^{\vec{F}} d\vec{F} = \frac{\epsilon-1}{4\pi\epsilon} \vec{D}_i + \frac{\epsilon_\infty-1}{4\pi\epsilon_\infty} \int_{\vec{D}_i}^0 d\vec{D} \\ &= \frac{1}{4\pi} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon} \right) \vec{D}_i. \end{aligned} \quad (1.10)$$

is now defined by

$$\vec{D}_i = \frac{4\pi}{\bar{\epsilon}} \vec{F}, \quad (1.11)$$

where  $\bar{\epsilon} = \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon} \right)$ , the effective dielectric constant. Thus the potential energy associated with an ionic displacement corresponding



to a polarization field  $\vec{F}(\vec{r})$  made slowly for the intrinsic electrons to respond is

$$U(\vec{F}) = \int \frac{\vec{F} \cdot \vec{D}}{2} d^3\vec{r} = \frac{2\pi}{\epsilon} \int \vec{F}^2 d^3\vec{r} \quad (1.12)$$

Saying that all longitudinal modes oscillate with the same frequency  $\omega_L$  implies that the kinetic energy of the polarization field is related to the potential energy in the same way as for a simple harmonic oscillator of frequency  $\omega_L$ . Thus the kinetic energy of the free phonons is readily

$$T(\vec{F}) = \frac{2\pi}{\epsilon\omega_L^2} \int \dot{\vec{F}}^2 d^3\vec{r} \quad (1.13)$$

We finally consider electron-lattice Hamiltonian,  $H_{int}$ , i.e., the potential energy of a point charge  $-e$  at position  $\vec{r}$  interacts with the polarization field  $\vec{F}(\vec{r})$ . The electric displacement field at  $\vec{r}'$  produced by the charge is defined by

$$\vec{D}(\vec{r}'; \vec{r}) = -\nabla_{r'} \frac{e}{|\vec{r}' - \vec{r}|} \quad (1.14)$$

Neglecting the electromagnetic self-energy of the electron, the  $H_{int}$  is obtained from

$$\begin{aligned} H_{int} &= -\int \vec{D}(\vec{r}'; \vec{r}) \cdot \vec{F}(\vec{r}') d^3\vec{r}' \\ &= e \int \nabla_{r'} \left( \frac{1}{|\vec{r}' - \vec{r}|} \right) \cdot \vec{F}(\vec{r}') d^3\vec{r}' \end{aligned} \quad (1.15)$$

The total Lagrangian for the electron-lattice system is then

$$L = \frac{m^* \dot{\vec{r}}^2}{2} + \frac{4\pi}{\epsilon\omega_L^2} \int \frac{\dot{\vec{F}}^2(\vec{r}') - \omega_L^2 \vec{F}^2(\vec{r}')}{2} d^3\vec{r}' - e \int \nabla_{r'} \left( \frac{1}{|\vec{r}' - \vec{r}|} \right) \cdot \vec{F}(\vec{r}') d^3\vec{r}' \quad (1.16)$$

Equivalently, the total Hamiltonian of the system is

$$H = \frac{p^2}{2m_{eff}} + \frac{1}{2} \int \left( \frac{\vec{G}^2(\vec{r}')}{M_f} + M_f \omega_L^2 \vec{F}^2(\vec{r}') \right) d^3\vec{r}' + e \int \nabla_{r'} \left( \frac{1}{|\vec{r}' - \vec{r}|} \right) \cdot \vec{F}(\vec{r}') d^3\vec{r}' \quad (1.17)$$

where  $\vec{P}$  and  $\vec{G}(\vec{r})$  are taken to be canonically-conjugate momenta of the canonical coordinates  $\vec{r}$  and  $\vec{P}(\vec{r})$  respectively, and where we have set

$$M_f = \frac{4\pi}{\epsilon \omega_L^2} \quad (1.18)$$

to play the role of a mass for the normal mode oscillators.

A number of assumptions have been made during the course of the Lagrangian derivation. Let us summarize the principal ones as follows:

(1) Band mass approximation for the electron to take care of the effect of the periodic potential  $V(\vec{r})$ . This claim is reasonable providing the effect of the electron-lattice interaction is not so strong that the electron is localized in a region the order of the lattice spacing, and it is restricted to the case of slow electrons.

(2) Continuum approximation: the lattice is treated to be a polarizable continuous medium. In view of the spreading of the electron wave-packet, this approximation is valid in the less ionic crystals and seems not too bad for more ionic crystals such as the alkali-halides.

(3) Electron-phonon interaction is limited to longitudinal optical phonons with long wavelength.

(4) The dispersion of those modes of vibration is neglected, assume that all modes have the same frequency  $\omega_L$ .

(5) The relativistic and magnetic effects are ignored.

(6) Intrinsic electrons of the crystal are assumed to follow the ionic displacements produced by the electron inertialessly.

(7) Harmonicity approximation: the vibration of the ions is represented by that of a harmonic oscillator.

In conclusion, the Fröhlich Hamiltonian is well justified for describing the behavior of a so called "large polaron"<sup>(11)</sup>.

### I.3 Qualitative Theories of Polarons

The purpose of this section is to give a broad physical idea on how the self-energy and the effective mass of polarons depend upon the electron-lattice interaction strength by means of Fröhlich's simple theory of polarons<sup>(12)</sup>.

#### (I.3.1) Self-energy

Basing on Fröhlich's simple theory, the size of polaron is characterized by the radius outside which the electron appears as a static charge and the lattice polarization assumes its full static value. The two limiting cases, static and dynamic situations, are considered respectively.

Firstly, if the electron velocity is much higher than that of the ions, this will give rise to a polaron model in which the electronic wave function is treated as a static charge distribution and becomes localized in a lattice. At large distances the field produced by the

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<sup>11</sup> J. Apple, "Polaron.", in Solid State Physics, 21, Eds. F. Seitz, D. Turnbull, and H. Ehrenreich, New York and London: Academic Press (1968) 195.

<sup>12</sup> H. Fröhlich, "Introduction to the Theory of the Polaron.", in Polarons and Excitons, Eds. C.G. Kuper, and G.D. Whitfield, Edinburgh and London: Oliver and Boyd (1962) 5.

electron is assumed Coulombic. Because of the electron's finite extension, the potential is taken to be constant, say, within distance  $l_1$ , as shown in Fig. I. The potential energy of the system is roughly  $-\frac{e^2}{\bar{\epsilon}l_1}$ . For the system restricted to a dimension of order  $l_1$ , from the uncertainty relation, its kinetic energy is of order  $\frac{4\pi^2\hbar^2}{2m_{\text{eff}}l_1^2}$ . Thus the approximate total energy of the electron in the lattice is

$$u_1 \approx -\frac{e^2}{\bar{\epsilon}l_1} + \frac{4\pi^2\hbar^2}{2m_{\text{eff}}l_1^2} \quad (1.19)$$

Minimizing the energy  $u_1$  with respect to  $l_1$  yields the most likely size of the polaron as

$$l_1 = \frac{4\pi^2\hbar^2\bar{\epsilon}}{m_{\text{eff}}e^2} \quad (1.20)$$

Substituting  $l_1$  into (1.19), the energy  $u_1$  is now expressed in terms of known quantities as

$$u_1 = -\frac{m_{\text{eff}}e^4}{8\pi^2\hbar^2\bar{\epsilon}^2}$$

Secondly, we have the case of slow electron or the dynamic case in which the lattice vibrational frequency  $\omega_L$  is so high that the lattice would adjust to the electron's motion, this leads to consideration of dynamical problem of an electron with velocity  $v$  interacting with a lattice of natural frequency  $\omega_L$ . The electron is seen to be effectively static only at distances from the electron at which the angular distance  $d_1$  travelled by the electron in a time  $\omega_L^{-1}$  is sufficiently small. This requires  $\frac{v}{\omega_L d_1} \ll 1$ . Hence the limiting distance is  $d_1 \sim \frac{v}{\omega_L}$ . On the other hand, the electron's size  $d_2$  can be related to its velocity by the uncertainty principle as  $d_2 \sim \frac{2\pi\hbar}{m_{\text{eff}}v}$

which must not exceed  $d_1$ . The intersection of curves  $d_1$  and  $d_2$  plotted as a function of  $v$  at  $v = \sqrt{\frac{\hbar \omega_L}{m_{\text{eff}}}}$  gives the radius  $l_2$  in this case:

$$l_2 = \sqrt{\frac{\hbar}{m_{\text{eff}} \omega_L}} \quad (1.22)$$

Neglecting the kinetic energy, only the potential energy corresponding to an electron distributed over a sphere of radius  $l_2$  contributes to the total energy  $U_2$  which is

$$U_2 = -\frac{e^2}{\epsilon l_2} = -\frac{e^2}{\epsilon} \sqrt{\frac{m_{\text{eff}} \omega_L}{2 \pi \hbar}} \quad (1.23)$$

Comparing the self energies obtained in the two models with the phonon energy  $\hbar \omega_L$  yields the important information:

$$-\frac{U_1}{\hbar \omega_L} = \frac{1}{8 \pi^2} \cdot \frac{e^4 m_{\text{eff}}}{\epsilon \hbar^3 \omega_L} = -\frac{1}{4 \pi} \left( \frac{U_2}{\hbar \omega_L} \right)^2, \quad (1.24)$$

which leads to the desirability of introducing a dimensionless coupling constant  $\alpha$  as

$$\alpha = \frac{e^2}{\epsilon} \sqrt{\frac{m_{\text{eff}}}{2 \omega \hbar^3}}. \quad (1.25)$$

This  $\alpha$  implies the strength of electron-phonon interaction in polaron theories.

Now it is convenient to express  $U_1$  and  $U_2$  in terms of  $\alpha$  :

$$U_1 \sim -\frac{\alpha^2}{4 \pi} \hbar \omega_L, \quad \text{static case.}$$

And

$$U_2 \sim -\frac{\alpha}{\pi^2} \hbar \omega_L, \quad \text{dynamic case.}$$

To determine which case is most applicable for a given crystal,  $\alpha$  is then evaluated, if  $\alpha$  is large, note that  $|U_1| > |U_2|$ , thus in this case the first approximation is better.

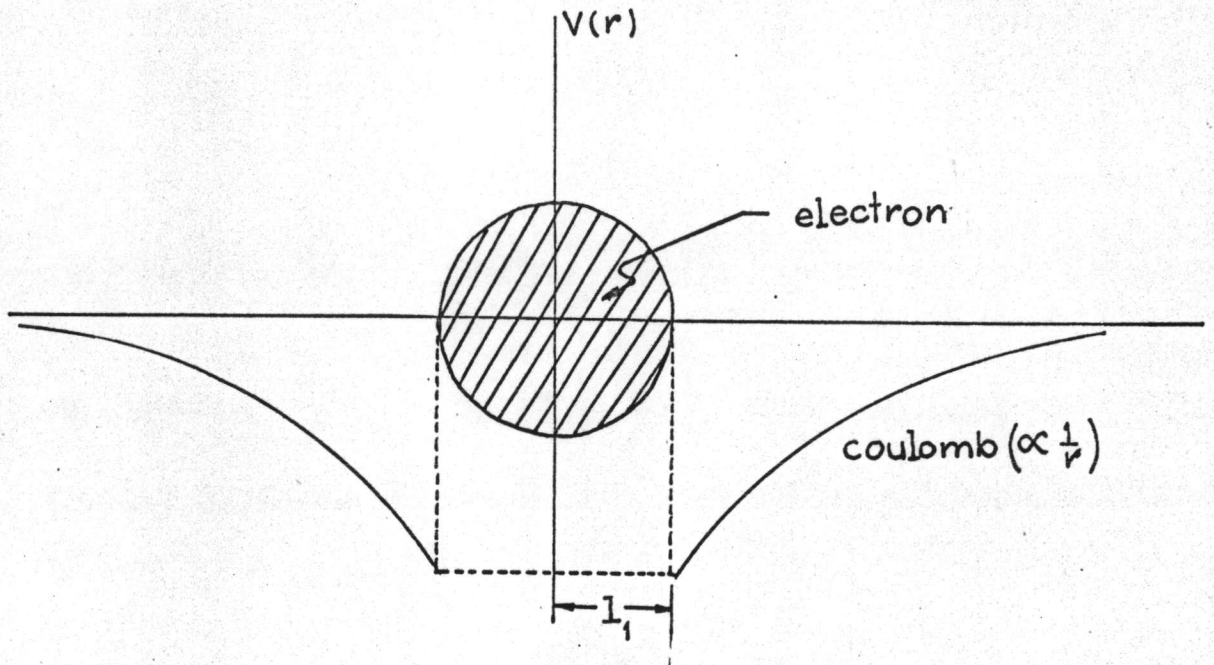


Fig. I The Field Produced by the Electron in the Static Case

(I.3.2) Effective mass

As a simple theory, Frohlich regards the polaron effective mass,  $m_{Fr}^*$  as defined by the equation:

$$\frac{1}{2} m_{Fr}^* v^2 = \frac{1}{2} m_{eff} v^2 + T_{ion} \quad (1.28)$$

where  $T_{ion}$  represents the total kinetic energy of the ions. Treating the lattice as a dielectric continuum,  $T_{ion}$  can be obtained conventionally by

$$T_{ion} = \frac{1}{2} M N_0 \int (\dot{\vec{d}}(\vec{r}'))^2 d^3 r', \quad (1.29)$$

in which  $\vec{d}(\vec{r}')$  is the relative displacement of an ion pair,  $N_0$  being the ion pair density, and  $M$  stands for the reduced mass of an ion pair. Now  $\vec{d}(\vec{r}')$  relates to the polarization field  $\vec{F}(\vec{r}')$  by

$$\vec{F}(\vec{r}') = N_0 \bar{e}^* \vec{d}(\vec{r}') \quad 006399 \quad (1.30)$$

which defines  $\bar{e}^*$  as an effective ionic charge. In Fröhlich's simply theory,  $\vec{F}(\vec{r}')$  takes the form:

$$\vec{F}(\vec{r}') = \begin{cases} \frac{1}{4\pi\bar{e}} \bar{D} & ; \quad |\vec{r}' - \vec{r}_1| > l_i, \\ 0 & ; \quad |\vec{r}' - \vec{r}_1| < l_i. \end{cases} \quad (1.31)$$

Substitution of the electric displacement  $\bar{D} = -e \nabla_{\vec{r}'} \left( \frac{1}{|\vec{r}' - \vec{r}_1|} \right)$  into Eq. (1.31) and using Eq. (1.30) gives  $\vec{d}(\vec{r}')$  as a function of  $\vec{r}'$ :

$$\vec{d}(\vec{r}') = -\frac{e}{4\pi\bar{e}N_0\bar{e}^*} \nabla_{\vec{r}'} \left( \frac{1}{|\vec{r}' - \vec{r}_1|} \right), \quad |\vec{r}' - \vec{r}_1| > l_i \quad (1.32)$$

Imposing the identity  $\frac{\partial}{\partial \vec{r}'} \frac{\partial}{\partial t} \left( \frac{1}{|\vec{r}' - \vec{r}|} \right) = - \frac{\partial}{\partial \vec{R}} \left( \frac{\vec{R} \cdot \dot{\vec{U}}}{R^3} \right) = \frac{3(\vec{R} \cdot \dot{\vec{U}})\vec{R} - R^2 \dot{\vec{U}}}{R^5}$ ,

where  $\vec{R} = \vec{r}' - \vec{r}$  and  $\dot{\vec{R}} = -\dot{\vec{r}} = -\dot{\vec{U}}$ , on  $\dot{\vec{d}}(\vec{r}')$  gives explicitly.

$$\left( \dot{\vec{d}}(\vec{r}') \right)^2 = \begin{cases} \frac{1}{16 \pi^2 \bar{\epsilon}^2 N_0^2} \left( \frac{e}{e^*} \right)^2 \left( \frac{3(\vec{R} \cdot \dot{\vec{U}})^2 + R^2 \dot{\vec{U}}^2}{R^6} \right), & R > l_i \\ 0, & R < l_i \end{cases} \quad (1.33)$$

Evaluation of  $T_{ion}$  using Eq. (1.33) and Eq. (1.29) is then straightforward, the result is

$$T_{ion} = \frac{1}{3} \frac{M}{4 \pi (\bar{\epsilon}^*)^2 N_0} \frac{e^2}{\bar{\epsilon}} \frac{v^2}{l_i^3}. \quad (1.34)$$

$N_0$ ,  $e^*$  and  $M$  are related to  $\epsilon$  and  $\epsilon_\infty$  according to the Szigetel relation, viz.,

$$\epsilon - \epsilon_\infty = \frac{\epsilon}{\epsilon_\infty} \left( \frac{\epsilon_\infty + 2}{3} \right)^2 \frac{4 \pi (e^*)^2 N_0}{M \omega_L^2} = \frac{\epsilon \epsilon_\infty}{\bar{\epsilon}}. \quad (1.35)$$

Rewriting Eq. (1.34) as

$$T_{ion} = \frac{1}{3} \left( \frac{\epsilon_\infty + 2}{3 \epsilon_\infty} \right)^2 \frac{e^2}{\bar{\epsilon} \omega_L^2} \frac{v^2}{l_i^3}, \quad (1.36)$$

and substituting this into Eq. (1.28), we finally obtain

$$\frac{m_{Fr}^*}{m_{eff}} - 1 = \frac{2 T_{ion}}{m_{eff} v^2} = \frac{2}{3} \left( \frac{\epsilon_\infty + 2}{\epsilon_\infty} \right)^2 \frac{e^2}{\bar{\epsilon} m_{Fr}^* \omega_L^2} \cdot \frac{1}{l_i^3}. \quad (1.37)$$

Inserting the polaron radii  $l_1$  and  $l_2$  for the two cases of approximation, Eq. (1.37) becomes, in terms of  $\alpha$ ,

$$\frac{m_{Fr}^*}{m_{eff}} - 1 = \begin{cases} c_1 \alpha^4 & , \text{static case} \\ c_2 \alpha & , \text{dynamic case,} \end{cases} \quad (1.38)$$

where  $c_1$  and  $c_2$  are constants.

Eq. (1.38) manifests that  $m_{Fr}^* \geq m_{eff}$ ; as  $\alpha$  tends to zero, the polaron mass  $m_{Fr}^*$  approaches the electron effective mass  $m_{eff}$ .



In the static case  $m_{F_n}^*$  is extremely sensitive to  $\alpha$ . Later we shall visualize that the static and dynamic cases in the simple models correspond to the strong and weak coupling limits respectively.