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# The Temperature Dependence of the Effective Mass of a Two-Dimensional Polaron

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**Abstract**

*The properties of a two-dimensional polaron in the polar crystal are discussed by means of a model which takes account of the atomicity of the lattice. The lattice vibration and the interaction between the electron and the lattice displacement are treated by second quantization method. The self-trapped energy and the effective mass of the two-dimensional polaron are derived.*

## I. Introduction

An electron moving in the polar crystal has an effective mass because of the periodic ion field. If the interaction between the electron and the lattice displacement is taken into account, the electron is surrounded by a cloud of phonons, and the electron will then be called a polaron. A polaron also has an effective mass owing to the interaction between the electron and the lattice displacement. Obviously, the lattice displacement depends on the temperature, therefore the effective mass of the polaron will also change with temperature. Many authors hold contradictory views about the temperature dependence of the polaron effective mass[1]. Some say that the polaron effective mass will decrease with increasing temperature[2–6]. Some say just the opposite[7–9]. Usually, the crystal lattice is regarded as a continuous medium, and treated macroscopically. Thus Fröhlich Hamiltonian is used. But if the atomic structure of the lattice is taken into account, we will come closer to the real structure of the lattice and get more satisfactory result. This work has already been done by Sewell[10] and Gu[11] on the three-dimensional case. With the development and wide application of the superlattice, two-dimensional problems are becoming more and more important.

In this paper, we will discuss the properties of the two-dimensional polaron. In Sec. II, we will give the Hamiltonian of the electron-lattice system, taking into account of the atomic structure of the lattice, treating the lattice vibration by second quantization method. In Secs. III, IV and V, we will derive the self-trapped energy and effective mass of the two-dimensional polaron through TBA method. Finally, in Sec. VI, we discuss the effect of temperature on the effective mass of the 2-D polaron.

## II. Hamiltonian

For simplicity, we assume that there are only one positive and one negative ions in a primitive cell. The equilibrium position of the positive ion is $\vec{\alpha}_s = a(s_1\vec{u}_1 + s_2\vec{u}_2)$, where $s_1$

and $s_2$ are integers, $\vec{u}_1$ and $\vec{u}_2$ are orthogonal unit vectors. The equilibrium position of the negative ion is $\vec{\alpha}'_s = \vec{\alpha}_s + a\vec{\alpha}$. The Hamiltonian of the electron-lattice system is[10]

$$\begin{aligned}
\hat{H} &= \hat{H}(\text{el}) + \hat{H}(\text{lat}) + \hat{H}(\text{int}) \,, \\
\hat{H}(\text{el}) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \vec{x}^2} \,, \\
\hat{H}(\text{lat}) &= -\sum_s \frac{\hbar^2}{2M_0}\frac{\partial^2}{\partial \vec{Y}_s^2} + V_{\text{op}}(\vec{Y}) - \sum_s \frac{\hbar^2}{2M_a}\frac{\partial^2}{\partial \vec{Z}_s^2} + V_{\text{ac}}(\vec{Z}) \,, \\
\hat{H}(\text{int}) &= \sum_s [V(\vec{x} - \vec{\alpha}_s - \vec{X}_s) + V'(\vec{x} - \vec{\alpha}'_s - \vec{X}'_s)] \,,
\end{aligned} \tag{1}$$

where $H(\text{el})$ is the kinetic energy of the electron, $H(\text{lat})$ is the lattice energy, and $H(\text{int})$ is the interaction energy between the electron and the lattice. $m$ is the electron mass. $\vec{x}$ is the position vector of the electron. $M_0$ and $M_a$ are the reduced and total mass of the positive and negative ions. We assume that the potential energy of the lattice vibration can be divided into two parts: $V_{\text{op}}(\vec{Y})$ being the optical branch potential energy and $V_{\text{ac}}(\vec{Z})$ being the acoustic branch potential energy. We will expand $V_{\text{op}}$ and $V_{\text{ac}}$ to the quadratic terms of $\vec{Y}$ and $\vec{Z}$ as usual. $\vec{X}_s$ and $\vec{X}'_s$ denote the displacement from the equilibrium position of the positive and negative ions in the $s$-th primitive cell. They are related to the relative displacement $\vec{Y}_s$ and centre of mass displacement $\vec{Z}_s$ as follows:

$$\vec{Y}_s = \vec{X}_s - \vec{X}'_s \,, \qquad \vec{Z}_s = \frac{M\vec{X}_s + M'\vec{X}'_s}{M + M'} \,, \tag{2}$$

$$\vec{X}_s = \vec{Z}_s + g\vec{Y}_s \,, \qquad \vec{X}'_s = \vec{Z}_s - (1-g)\vec{Y}_s \,, \tag{3}$$

where $g = M'/(M + M')$. $M$ and $M'$ are the masses of the positive and negative ions respectively.

Introducing the following canonical transformation

$$\begin{aligned}
\hat{\vec{Y}}_s &= \sqrt{\frac{1}{NM_0}}\sum_{\vec{q}} \frac{\vec{q}}{q}\hat{Q}_{\vec{q}}\, e^{-i\vec{q}\cdot\vec{\alpha}_s} \,, & \hat{\vec{P}}_s &= \sqrt{\frac{M_0}{N}}\sum_{\vec{q}} \frac{\vec{q}}{q}\hat{P}_{\vec{q}}\, e^{-i\vec{q}\cdot\vec{\alpha}_s} \,, \\
\hat{\vec{Z}}_s &= \sqrt{\frac{1}{NM_a}}\sum_{\vec{q}} \frac{\vec{q}}{q}\hat{Q}'_{\vec{q}}\, e^{-i\vec{q}\cdot\vec{\alpha}_s} \,, & \hat{\vec{P}'}_s &= \sqrt{\frac{M_a}{N}}\sum_{\vec{q}} \frac{\vec{q}}{q}\hat{P}'_{\vec{q}}\, e^{-i\vec{q}\cdot\vec{\alpha}_s} \,,
\end{aligned} \tag{4}$$

the lattice energy is

$$\hat{H}(\text{lat}) = \sum_{\vec{q}} \frac{1}{2}(\hat{P}_{\vec{q}}\hat{P}^*_{\vec{q}} + \omega^2_{\vec{q}}\hat{Q}_{\vec{q}}\hat{Q}^*_{\vec{q}}) + \sum_{\vec{q}} \frac{1}{2}(\hat{P}'_{\vec{q}}\hat{P}'^*_{\vec{q}} + \omega'^2_{\vec{q}}\hat{Q}'_{\vec{q}}\hat{Q}'^*_{\vec{q}}) \,. \tag{5}$$

The first part is the energy of the optical branch vibration. The second part is the energy of the acoustic phonons. In order to quantize secondly the lattice energy, we introduce another transformation

$$\begin{aligned}
\hat{Q}_{\vec{q}} &= \left(\frac{\hbar}{2\omega_{\vec{q}}}\right)^{1/2}\left(\hat{b}_{-\vec{q}} - \hat{b}^\dagger_{\vec{q}}\right) , & \hat{P}_{\vec{q}} &= -i\left(\frac{\hbar\omega_{\vec{q}}}{2}\right)^{1/2}\left(\hat{b}_{-\vec{q}} + \hat{b}^\dagger_{\vec{q}}\right) , \\
\hat{Q}'_{\vec{q}} &= \left(\frac{\hbar}{2\omega'_{\vec{q}}}\right)^{1/2}\left(\hat{b}'_{-\vec{q}} - \hat{b}'^\dagger_{\vec{q}}\right) , & \hat{P}'_{\vec{q}} &= -i\left(\frac{\hbar\omega_{\vec{q}}}{2}\right)^{1/2}\left(\hat{b}'_{-\vec{q}} + \hat{b}'^\dagger_{\vec{q}}\right) , \\
\left[\hat{b}_{\vec{q}}, \hat{b}^\dagger_{\vec{q}'}\right] &= \left[\hat{b}'_{\vec{q}}, \hat{b}'^\dagger_{\vec{q}'}\right] = \delta_{\vec{q}\vec{q}'} \,, & \left[\hat{b}_{\vec{q}}, \hat{b}'^\dagger_{\vec{q}'}\right] &= 0 \,,
\end{aligned} \tag{6}$$

where $\hat{b}_{\vec{q}}$ and $\hat{b}^\dagger_{\vec{q}}$ are annihilation and creation operators of the optical phonons, $\hat{b}'_{\vec{q}}$ and $\hat{b}'^\dagger_{\vec{q}}$ are annihilation and creation operators of the acoustic phonons. The lattice energy can now be written as $\hat{H}(\text{lat}) = \sum_{\vec{q}} \hbar\omega_{\vec{q}}\hat{b}^\dagger_{\vec{q}}\hat{b}_{\vec{q}} + \sum_{\vec{q}} \hbar\omega'_{\vec{q}}\hat{b}'^\dagger_{\vec{q}}\hat{b}'_{\vec{q}}$, and the Hamiltonian of the electron-lattice system is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \vec{x}^2} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} \hat{b}^{\dagger}_{\vec{q}} \hat{b}_{\vec{q}} + \sum_{\vec{q}} \hbar\omega'_{\vec{q}} \hat{b}'^{\dagger}_{\vec{q}} \hat{b}'_{\vec{q}} + \sum_{s} [V(\vec{x} - \vec{\alpha}_s - \vec{X}_s) + V'(\vec{x} - \vec{\alpha}'_s - \vec{X}'_s)] \,. \tag{7}$$

## III. Localized States

Rewrite the Hamiltonian of the electron-lattice system as

$$\hat{H} = \hat{H}_s + \hat{H}'_s \,,$$

$$\begin{aligned} \hat{H}_s = &-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \vec{x}^2} + V(\vec{x} - \vec{\alpha}_s) + \hat{H}(\mathrm{lat}) + \sum_t [V(\vec{x} - \vec{\alpha}_t - \vec{X}_t) - V(\vec{x} - \vec{\alpha}_t)] \\ &+ \sum_t [V'(\vec{x} - \vec{\alpha}'_t - \vec{X}'_t) - V'(\vec{x} - \vec{\alpha}'_t)] \,, \end{aligned} \tag{8}$$

$$\hat{H}'_s = \sum_{t \neq s} V(\vec{x} - \vec{\alpha}_t) + \sum_t V'(\vec{x} - \vec{\alpha}'_t) \,,$$

where $\hat{H}_s$ is the Hamiltonian of the localized states which includes the bounded-state electron energy in the potential field of the $s$-th positive ion, the lattice energy, and the interaction energy between the electron and all the phonons. $\hat{H}'_s$ includes the interaction between the electron and all the undisplaced ions except the $s$-th positive ion. In this section, we will ignore $\hat{H}'_s$.

The wavefunction of the localized state can be written as the product of the electron wavefunction and the lattice wavefunction

$$\psi_s = \phi(\vec{x} - \vec{\alpha}_s)\chi_s(\mathrm{lat}) \,, \tag{9}$$

where $\phi(\vec{x} - \vec{\alpha}_s)$ satisfies the following eigen-value-equation

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \vec{x}^2} + V(\vec{x} - \vec{\alpha}_s)\right]\phi(\vec{x} - \vec{\alpha}_s) = \mathcal{E}_0 \phi(\vec{x} - \vec{\alpha}_s) \,, \tag{10}$$

and $\mathcal{E}_0$ is the eigen-energy corresponding to the atomic state $\phi$. To simplify the discussion, we suppose that $\phi$ is the $s$-state wavefunction. Hence we have

$$\langle \psi_s | \hat{H}_s | \psi_s \rangle = \mathcal{E}_0 + \langle \chi_s | \hat{H}_s(\mathrm{lat}) | \chi_s \rangle \,, \tag{11}$$

where

$$\begin{aligned} \hat{H}_s(\mathrm{lat}) = \hat{H}(\mathrm{lat}) + \int |\phi(\vec{x} - \vec{\alpha}_s)|^2 dx^2 \cdot \Big\{ &\sum_t [V(\vec{x} - \vec{\alpha}_t - \vec{X}_t) - V(\vec{x} - \vec{\alpha}_t)] \\ &+ \sum_t [V'(\vec{x} - \vec{\alpha}'_t - \vec{X}'_t) - V'(\vec{x} - \vec{\alpha}'_t)] \Big\} \,. \end{aligned} \tag{12}$$

Expanding the potential energy in Eq. (12) with respect to the lattice displacement $\vec{X}_t$, $\vec{X}'_t$, and substituting Eq. (3) into Eq. (12), we get

$$\hat{H}_s(\mathrm{lat}) = \hat{H}(\mathrm{lat}) - \sum_t [\vec{Y}_t \cdot \vec{B}(\vec{\alpha}_t - \vec{\alpha}_s) + \vec{Z}_t \cdot \vec{C}(\vec{\alpha}_t - \vec{\alpha}_s)] \,, \tag{13}$$

where

$$\begin{aligned} \vec{B}(\vec{\beta}) &= \int |\phi(\vec{x})|^2 dx^2 \cdot \nabla [gV(\vec{x} - \vec{\beta}) - (1-g)V'(\vec{x} - \vec{\beta} - a\vec{\alpha})] \,, \\ \vec{C}(\vec{\beta}) &= \int |\phi(\vec{x})|^2 dx^2 \cdot \nabla [V(\vec{x} - \vec{\beta}) + V'(\vec{x} - \vec{\beta} - a\vec{\alpha})] \,. \end{aligned} \tag{14}$$

Substituting Eqs. (4) and (6) into Eq. (13), we get

$$\hat{H}_s(\text{lat}) = \sum_{\vec{q}} \hbar\omega_{\vec{q}}\hat{b}^\dagger_{\vec{q}}\hat{b}_{\vec{q}} + \sum_{\vec{q}}(B_{\vec{q}}\hat{b}_{\vec{q}}e^{i\vec{q}\cdot\vec{a}_s} + B^*_{\vec{q}}\hat{b}^\dagger_{\vec{q}}e^{-i\vec{q}\cdot\vec{a}_s}) + \sum_{\vec{q}} \hbar\omega'_{\vec{q}}\hat{b}'^\dagger_{\vec{q}}\hat{b}'_{\vec{q}} + \sum_{\vec{q}}(B'_{\vec{q}}\hat{b}'_{\vec{q}}e^{i\vec{q}\cdot\vec{a}_s} + B^*_{\vec{q}}\hat{b}'^\dagger_{\vec{q}}e^{-i\vec{q}\cdot\vec{a}_s}) , \tag{15}$$

where

$$B_{\vec{q}} = \sum_t \sqrt{\frac{\hbar}{2NM_0\omega_{\vec{q}}}}\frac{\vec{q}}{q}\cdot\vec{B}(\vec{\alpha}_t)e^{i\vec{q}\cdot\vec{\alpha}_t} , \quad B'_{\vec{q}} = \sum_t \sqrt{\frac{\hbar}{2NM_a\omega'_{\vec{q}}}}\frac{\vec{q}}{q}\cdot\vec{C}(\vec{\alpha}_t)e^{i\vec{q}\cdot\vec{\alpha}_t} . \tag{16}$$

Introducing a unitary transformation

$$\hat{U}_s = \exp\Big[\sum_{\vec{q}}(\hat{b}^\dagger_{\vec{q}}f_{\vec{q}s} - \hat{b}_{\vec{q}}f^*_{\vec{q}s}) + \sum_{\vec{q}}(\hat{b}'^\dagger_{\vec{q}}f'_{\vec{q}s} - \hat{b}'_{\vec{q}}f'^*_{\vec{q}s})\Big] ,$$

where

$$f_{\vec{q}s} = -\frac{B^*_{\vec{q}}e^{-i\vec{q}\cdot\vec{a}_s}}{\hbar\omega_{\vec{q}}} , \qquad f'_{\vec{q}s} = -\frac{B^*_{\vec{q}}e^{-i\vec{q}\cdot\vec{a}_s}}{\hbar\omega'_{\vec{q}}} , \tag{17}$$

the Hamiltonian $\hat{H}_s(\text{lat})$ thus becomes

$$\hat{\mathcal{H}}_s(\text{lat}) = \hat{U}_s^{-1}\hat{H}_s(\text{lat})\hat{U}_s = \sum_{\vec{q}}\hbar\omega_{\vec{q}}\hat{b}^\dagger_{\vec{q}}\hat{b}_{\vec{q}} + \sum_{\vec{q}}\hbar\omega'_{\vec{q}}\hat{b}'^\dagger_{\vec{q}}\hat{b}'_{\vec{q}} - \mathcal{E}_1 , \tag{18}$$

where $\mathcal{E}_1 = \sum_{\vec{q}}(B^*_{\vec{q}}B_{\vec{q}}/\hbar\omega_{\vec{q}}) + \sum_{\vec{q}}(B^*_{\vec{q}}B'_{\vec{q}}/\hbar\omega'_{\vec{q}})$. Hence if $\Theta_n$ is the eigen-state of $\hat{H}$ (lat), and by putting $\chi_{sn}(\text{lat}) = \hat{U}_s\Theta_n$, $\psi_s = \psi_{sn} = \phi(\vec{x}-\vec{\alpha}_s)\vec{\chi}_{sn}$, we can see that

$$\langle\chi_s|\hat{H}_s(\text{lat})|\chi_s\rangle = \langle\Theta_n|\hat{\mathcal{H}}_s(\text{lat})|\Theta_s\rangle . \tag{19}$$

The eigenstate $\Theta_n$ is given by the expression $\Theta_n = \prod_{\vec{q}}|n_{\vec{q}}\rangle|n'_{\vec{q}}\rangle$, and $\hat{b}_{\vec{q}}|n_{\vec{q}}\rangle = \sqrt{n_{\vec{q}}}|n_{\vec{q}}-1\rangle$, $\hat{b}^\dagger_{\vec{q}}|n_{\vec{q}}\rangle = \sqrt{n_{\vec{q}}+1}|n_{\vec{q}}+1\rangle$, $\hat{b}'_{\vec{q}}|n'_{\vec{q}}\rangle = \sqrt{n'_{\vec{q}}}|n'_{\vec{q}}-1\rangle$ and $\hat{b}'^\dagger_{\vec{q}}|n'_{\vec{q}}\rangle = \sqrt{n'_{\vec{q}}+1}|n'_{\vec{q}}+1\rangle$, where $n_{\vec{q}}$ and $n'_{\vec{q}}$ are the number of optical phonons and acoustic phonons with wave vector $\vec{q}$ respectively. It follows from Eqs. (11), (18) and (19) that

$$\langle\psi_s|\hat{H}_s|\psi_s\rangle = \mathcal{E}_0 + \sum_{\vec{q}}\hbar\omega_{\vec{q}}n_{\vec{q}} + \sum_{\vec{q}}\hbar\omega'_{\vec{q}}n'_{\vec{q}} - \mathcal{E}_1 , \tag{20}$$

where $\langle\psi_s|\hat{H}_s|\psi_s\rangle$ is the energy of the localized state and $\mathcal{E}_1$ is the self-trapped energy caused by the reaction on the electron by the lattice.

## IV. The Band Structure

For a given distribution of phonons (i.e., $\Theta_n$), there are $N$ states $\psi_{sn}$, one for each positive ion. These states form a degenerate set. The wavefunction of the whole system can be obtained by taking the linear combination of $\psi_{sn}$, $\Psi = \sum_s C_s\psi_{sn}$. It follows from Eq. (8) and the expression of $\Psi$ that $\sum_s\sum_t C^*_sC_t\langle\psi_{sn}|(E - H_s - \hat{H}'_s)|\psi_{tn}\rangle = 0$, where $E$ is the eigenvalue of $\hat{H}_s + \hat{H}'_s$.

By using the variational method, we obtain

$$\sum_t C_t\langle\psi_{sn}|(E - \hat{H}_s - \hat{H}'_s)|\psi_{tn}\rangle = 0 . \tag{21}$$

In order to solve this set of equations, we adopt the tight-binding approximation, and put

$$\langle\psi_{sn}|\psi_{tn}\rangle = \delta_{st} . \tag{22}$$

Thus, if we assume that the states $\psi_{sn}$ are the eigenstates of $H_s$, then

$$\langle\psi_{sn}|\hat{H}_s|\psi_{tn}\rangle = (E_n(\text{lat}) + \mathcal{E}_0 - \mathcal{E}_1)\delta_{st} . \tag{23}$$

We may put

$$\langle\psi_{sn}|\hat{H}'_s|\psi_{tn}\rangle = W_n(\vec{\alpha}_t - \vec{\alpha}_s)\,. \tag{24}$$

By considering Eqs. (21)–(24), we may rewrite Eq. (21) as

$$\sum_t C_t\{[E + \mathcal{E}_1 - \mathcal{E}_0 - E_n(\mathrm{lat})]\delta_{st} - W_n(\vec{\alpha}_t - \vec{\alpha}_s)\} = 0\,.$$

The solution for $E$ and $C$'s of this set of equations is $C_s = \exp(i\vec{K}\cdot\vec{\alpha}_s)$, where $\vec{K} = (K_1,\, K_2)$ is the electron wave vector which lies in the region $-\frac{\pi}{a} \le K_1,\, K_2 \le \frac{\pi}{a}$, and the energy is given by $E = \mathcal{E}_0 - \mathcal{E}_1 + E_n(\mathrm{lat}) + \sum_t W_n(\vec{\alpha}_t)\exp(i\vec{K}\cdot\vec{\alpha}_t)$. The wavefunction and energy levels of the system are respectively $\Psi = \Psi_{\vec{K}n} = \sum_s \exp(i\vec{K}\cdot\vec{\alpha}_s)\psi_{sn}$ and $E = E_{\vec{K}n} = E_n(\mathrm{lat}) + \mathcal{E}_{\vec{K}n}$, where $\mathcal{E}_{\vec{K}n} = \mathcal{E}_0 - \mathcal{E}_1 + \sum_t W_n(\vec{\alpha}_t)\exp(i\vec{K}\cdot\vec{\alpha}_t)$. Since $E_n$ (lat) is the lattice energy, $\mathcal{E}_{\vec{K}n}$ may be regarded as the polaron energy for wave vector $\vec{K}$ when the lattice state is $\Theta_n$.

By using Eqs. (8), (9) and (24), $W_n$ can be expressed as $W_n(\vec{\alpha}_t - \vec{\alpha}_s) = \langle\chi_{sn}|W_{st}|\chi_{tn}\rangle$, where $W_{st} = \int\phi^*(\vec{x} - \vec{\alpha}_s)H'_s\phi(x - \vec{\alpha}_t)dx^2 = W^0(\vec{\alpha}_t - \vec{\alpha}_s)$. Consequently, the polaron energy is given by $\mathcal{E}_{\vec{K}n} = \langle\Theta_n|\hat{\mathcal{E}}_{\mathrm{op}}(\vec{K})|\Theta_n\rangle$, where $\hat{\mathcal{E}}_{\mathrm{op}}(\vec{K}) = \mathcal{E}_0 - \mathcal{E}_1 + \sum_t W_n^0(\vec{\alpha}_t)\hat{U}_0^\dagger\hat{U}_t\exp(i\vec{K}\cdot\vec{\alpha}_t)$. We see that if the lattice state is $\Theta_n$, the polaron energy is the expectation value of the operator $\hat{\mathcal{E}}_{\mathrm{op}}(\vec{K})$ for the lattice state. Therefore the polaron energy for the wave vector $\vec{K}$ at temperature $T$ is the statistical average over all the lattice states of $\hat{\mathcal{E}}_{\mathrm{op}}(\vec{K})$:

$$\mathcal{E}(\vec{K}) = \frac{\mathrm{Tr}\,[\hat{\mathcal{E}}_{\mathrm{op}}(\vec{K})\cdot\exp(-\beta\hat{H}(\mathrm{lat}))]}{\mathrm{Tr}\,[\exp(-\beta H(\mathrm{lat}))]} = \mathcal{E}_0 - \mathcal{E}_1 + \sum_t W(\vec{\alpha}_t)\exp(i\vec{K}\cdot\vec{\alpha}_t)\,, \tag{25}$$

where

$$W(\vec{\alpha}_t) = W^0(\vec{\alpha}_t)F(\vec{\alpha}_t)\,, \qquad F(\vec{\alpha}_t) = \frac{\mathrm{Tr}\,[\hat{U}_0^\dagger\exp(-\beta\hat{H}(\mathrm{lat}))\hat{U}_t]}{\mathrm{Tr}\,[\exp(-\beta\hat{H}(\mathrm{lat}))]}\,. \tag{26}$$

It can be proved that $W^*(\vec{\alpha}_t) = W(\vec{\alpha}_t) = W(-\vec{\alpha}_t)$[10]. So equation (25) becomes

$$\mathcal{E}(\vec{K}) = \mathcal{E}_0 - \mathcal{E}_1 + W(0) + 2\sum_t{}' W(\vec{\alpha}_t)\cos(\vec{K}\cdot\vec{\alpha}_t)\,,$$

and the summation applied to $\vec{\alpha}_t \neq 0$ and $\vec{\alpha}_t$ whose components are all positive. Since in the case of tight-binding approximation, the summation takes over nearest neighbouring lattice points only, we then obtain

$$\mathcal{E}(\vec{K}) = \mathcal{E}_0 - \mathcal{E}_1 + W(0) + 2\sum_{l=1}^{2} W_l\cos(K_l a)\,. \tag{27}$$

If we consider only the small values of $K$, the energy of the polaron can be written as

$$\mathcal{E}(\vec{K}) = \mathcal{E}(0) - \sum_{l=1}^{2} W_l a^2 K_l^2 + O(K^4) \cong \mathcal{E}(0) + \sum_l \frac{\hbar^2 K_l^2}{2m_1}\,, \tag{28}$$

where $\mathcal{E}(\vec{K}) = \mathcal{E}_0 - \mathcal{E}_1 + W(0) + 2\sum_{l=1}^{2} W_l$ and $m_l = -\hbar^2/2W_l a^2$ is the effective mass of the polaron.

## V. Self-Trapped Energy

We only take into account the contribution of the longitudinal optical phonons to the self-trapped energy, which is $\mathcal{E}_1 = \sum_{\vec{q}}(B_{\vec{q}}^* B_{\vec{q}}/\hbar\omega_{\vec{q}})$. To evaluate $\mathcal{E}_1$, we first calculate the factor $\vec{q}\cdot\vec{B}(\vec{\alpha}_t)$ in Eq. (16), where $\vec{B}(\vec{\alpha}_t)$ is given in Eq. (14). Assume $V$ is the Coulomb potential:

$$V(\vec{x} - \vec{\alpha}_t) = -\frac{Ze^2}{|\vec{x} - \vec{\alpha}_t|}\,, \qquad V'(\vec{x} - \vec{\alpha}_t - a\vec{\alpha}) = \frac{Ze^2}{|\vec{x} - \vec{\alpha}_t - a\vec{\alpha}|}\,, \tag{29}$$

where $Ze$ is the charge carried by the positive and negative ions. We then have

$$\vec{q}\cdot\vec{B}(\vec{\alpha}_t) = Ze^2\int|\phi(\vec{x})|^2dx^2\frac{\vec{q}\cdot(\vec{x}-\vec{\alpha}_t)}{|\vec{x}-\vec{\alpha}|^3} . \tag{30}$$

Since $\phi(\vec{x})$ is the localized electron wavefunction, $|\vec{x}| \ll |\vec{\alpha}_t|$, we can expand $1/|\vec{x}-\vec{\alpha}|^3$ to the second order terms

$$\begin{aligned}\frac{1}{|\vec{x}-\vec{\alpha}_t|^3} &= \frac{1}{|\vec{\alpha}_t|^3} - \vec{x}\cdot\nabla_{\vec{\alpha}_t}\frac{1}{|\vec{\alpha}_t|^3} + \frac{1}{2}(\vec{x}\cdot\nabla_{\vec{\alpha}_t})^2\frac{1}{|\vec{\alpha}_t|^3}\\ &= \frac{1}{|\vec{\alpha}_t|^3} + \frac{3}{|\vec{\alpha}_t|^5}(\vec{x}\cdot\vec{\alpha}_t) + \frac{15}{2}\frac{1}{|\vec{\alpha}_t|^7}(x-\alpha_t)^2 - \frac{3}{2}\frac{|\vec{x}|^2}{|\vec{\alpha}_t|^5} .\end{aligned} \tag{31}$$

Substituting Eq. (31) into Eq. (30), we obtain

$$\vec{q}\cdot\vec{B}(\vec{\alpha}_t) = -Ze^2(\vec{q}\cdot\vec{\alpha}_t)\Big[\frac{1}{|\vec{\alpha}_t|^3} + \frac{9}{4}\frac{1}{|\vec{\alpha}_t|^5}\Big]\int|\phi(\vec{x})|^2|\vec{x}|^2dx^2 . \tag{32}$$

We suppose $\phi(\vec{x})$ to be the $3s$ state wavefunction of a two-dimensional hydrogen atom[12], i.e.,

$$\phi(\vec{x}) = \frac{1}{\sqrt{2\pi}}\frac{2}{5\sqrt{5a_0}}\cdot\exp\frac{-2|\vec{x}|}{5a_0}\cdot\Big[2-4\Big(\frac{4|\vec{x}|}{5a_0}\Big)+\Big(\frac{4|\vec{x}|}{5a_0}\Big)^2\Big] , \tag{33}$$

where $a_0$ is the Bohr radius. Substituting Eq. (33) into Eq. (32), we obtain

$$\vec{q}\cdot\vec{B}(\vec{\alpha}_t) = -Ze^2(\vec{q}\cdot\vec{\alpha}_t)\Big[\frac{1}{|\vec{\alpha}_t|^3} + \frac{7425}{32}\cdot\frac{a_0^2}{|\alpha_t|^5}\Big] . \tag{34}$$

Substitute Eq. (34) into Eq. (16), and change the summation to integration $\sum_t \to (1/a^2)\int d\vec{\alpha}_t$,

$$\begin{aligned}B_{\vec{q}} &= -\frac{Ze^2}{q}\sqrt{\frac{\hbar}{2NM_0\omega_{\vec{q}}}}\sum_t\Big[\frac{1}{|\alpha_t|^3}+\frac{7425}{32}\cdot\frac{a_0^2}{|\alpha_t|^5}\Big](\vec{q}\cdot\vec{\alpha}_t)e^{i\vec{q}\cdot\vec{\alpha}_t}\\ &= -\frac{Ze^2}{q}\sqrt{\frac{\hbar}{2NM_0\omega_{\vec{q}}}}\cdot\frac{1}{a^2}\int(\vec{q}\cdot\vec{\beta})\Big[\frac{1}{\beta^3}+\frac{7425}{32}\cdot\frac{a_0^2}{\beta^5}\Big]e^{i\vec{q}\cdot\vec{\beta}}d\beta\\ &= \frac{2\pi}{i}\cdot\frac{Ze^2}{a^2}\cdot\sqrt{\frac{\hbar}{2NM_0\omega_{\vec{q}}}}\cdot\Big[1+\frac{7425}{32}\cdot\frac{q}{a}\cdot a_0^2\Big] .\end{aligned} \tag{35}$$

Suppose $\omega_{\vec{q}}$ would not change with the wave vector $\vec{q}$, and $0 \le q \le \pi/10a$, we have

$$\begin{aligned}\mathcal{E}_1 &= \sum_{\vec{q}}\frac{B^*_{\vec{q}}B_{\vec{q}}}{\hbar\omega_{\vec{q}}} = \frac{1}{\hbar\omega}\sum_{\vec{q}}B^*_{\vec{q}}B_{\vec{q}} = \Big(\frac{2\pi Ze^2}{a^2}\Big)^2\cdot\frac{\hbar}{2NM_0\omega}\cdot\frac{1}{\hbar\omega}\cdot\frac{Na^2}{(2\pi)^2}\\ &\cdot\int_0^{\pi/10a}\Big[1+\frac{7425}{32}\cdot\frac{q}{a}a_0^2\Big]2\pi q dq = \frac{\pi^2Z^2e^4}{200M_0a^4\omega^2}\cdot\Big[1+\frac{495\pi}{32}\cdot\Big(\frac{a_0}{a}\Big)^2\Big] = \lambda\alpha^2\hbar\omega ,\end{aligned} \tag{36}$$

where

$$\lambda = \frac{\pi^3Z^2\hbar^2}{100M_0a^4\omega^2m}\Big[1+\frac{495\pi}{32}\Big(\frac{a_0}{a}\Big)^2\Big]\Big(\frac{1}{\mathcal{E}_\infty}-\frac{1}{\mathcal{E}_s}\Big)^{-2}, \quad \alpha = \frac{1}{2}\Big(\frac{1}{\mathcal{E}_\infty}-\frac{1}{\mathcal{E}_s}\Big)\frac{e^2}{\hbar\omega}\Big(\frac{2m\omega}{\hbar}\Big)^{1/2} . \tag{37}$$

$\alpha$ is the coupling constant of electron-phonon interaction. The self-trapped energy is proportional to $\alpha^2$, which agrees with the result listed in the literature[13].

## VI. Effective Mass

The effective mass of the polaron, according to Eq. (47), is $m_l = m_0/F_l$, $m_0 = -\hbar/2W_l^0a^2$, where $m_0$ is the effective mass due to the periodic potential field.

By Eqs. (26) and (27), we find that

$$F_l = F(a\vec{U}_l) = \frac{\mathrm{Tr}\,[\hat{U}_0^\dagger\exp(-\beta\hat{H}(\mathrm{lat}))\hat{U}_l]}{\mathrm{Tr}\,[\exp(-\beta\hat{H}(\mathrm{lat}))]} . \tag{38}$$

Substituting $\hat{H}(\mathrm{lat})$ and Eqs. (17) into Eq. (38), and since $F_l = \prod_j\prod_{\vec{q}}\mathcal{F}_{\vec{q}jl}$ we get

$$\mathcal{F}_{\vec{q}jl} = \frac{\mathrm{Tr}\,[\exp(\hat{b}_{\vec{q}j}f^*_{\vec{q}0j}-\hat{b}^\dagger_{\vec{q}j}f_{\vec{q}0j})\exp(-\beta\hbar\omega_{\vec{q}j}\hat{b}^\dagger_{\vec{q}j}\hat{b}_{\vec{q}j})\exp(\hat{b}^\dagger_{\vec{q}j}f_{\vec{q}0j}-\hat{b}_{\vec{q}j}f^*_{\vec{q}0j})]}{\mathrm{Tr}\,[\exp(-\beta\hbar\omega_{\vec{q}j}\hat{b}^\dagger_{\vec{q}j}\hat{b}_{\vec{q}j})]} . \tag{39}$$

Here $j = 1$ indicates the terms associated with the optical phonons and $j = 2$ the acoustic phonons. The matrix elements are calculated to the second order of $f$'s as given below:

$$\begin{aligned}\langle n|\exp(\hat{b}_{\vec{q}j} f^*_{\vec{q}0j} - \hat{b}^\dagger_{\vec{q}j} f_{\vec{q}0j})|m\rangle &= \delta_{nm} + \sqrt{m} f^*_{\vec{q}0j}\delta_{n,m-1} - \sqrt{m+1}\, f_{\vec{q}0j}\delta_{n,m+1} \\ &+ \frac{1}{2}\sqrt{m(m-1)}\, f^{*2}_{\vec{q}0j}\delta_{n,m-2} - \frac{1}{2}(2m+1) f^*_{\vec{q}0j} f_{\vec{q}0j}\delta_{nm} + \frac{1}{2}\sqrt{(m+1)(m+2)}\, f^2_{\vec{q}0j}\delta_{n,m+2}\,,\end{aligned} \tag{40}$$

$$\langle n|\exp(-\beta\hbar\omega_{\vec{q}j}\hat{b}^\dagger_{\vec{q}j}\hat{b}_{\vec{q}j})|K\rangle = \exp(-\beta\hbar\omega_{\vec{q}j}\cdot K)\delta_{mK}\,, \tag{41}$$

$$\begin{aligned}\langle K|\exp(\hat{b}^\dagger_{\vec{q}j} f_{\vec{q}lj} - \hat{b}_{\vec{q}j} f^*_{\vec{q}lj})|n\rangle &= \delta_{Kn} - \sqrt{n} f^*_{\vec{q}lj}\delta_{K,n-1} + \sqrt{n+1}\, f_{\vec{q}lj}\delta_{K,n+1} \\ &+ \frac{1}{2}\sqrt{n(n-1)}\, f^{*2}_{\vec{q}lj}\delta_{K,n-2} - \frac{1}{2}(2n+1) f^*_{\vec{q}lj} f_{\vec{q}lj}\delta_{Kn} + \frac{1}{2}\sqrt{(n+1)(n+2)}\, f^2_{\vec{q}lj}\delta_{K,n+2}\,.\end{aligned} \tag{42}$$

Therefore

$$\mathcal{F}_{\vec{q}jl} = \frac{\sum_{n=0}^{\infty}\exp(-\beta\hbar\omega_{\vec{q}j}n)\left[1 + n f_{\vec{q}0j} f^*_{\vec{q}lj} + (n+1) f^*_{\vec{q}0j} f_{\vec{q}lj} - \frac{1}{2}(2n+1)(f^*_{\vec{q}0j} f_{\vec{q}0j} - f^*_{\vec{q}lj} f_{\vec{q}lj})\right]}{\sum_{n=0}^{\infty}\exp(-\beta\hbar\omega_{\vec{q}j}n)}\,. \tag{43}$$

Substituting Eq. (17) into Eq. (43), and ignoring the contribution of the acoustic phonons,

$$F_l = \frac{\sum_{n=0}^{\infty}\exp(-\beta\hbar\omega_{\vec{q}}n)[1-(2n+1)\Delta_1 + n\Delta_2 + (n+1)\Delta_3]}{\sum_{n=0}^{\infty}\exp(-\beta\hbar\omega_{\vec{q}}n)} = 1-(2\bar{n}+1)\Delta_1 + \bar{n}\Delta_2 + (\bar{n}+1)\Delta_3$$

with $\Delta_1 = \sum_{\vec{q}}(B^*_{\vec{q}}B_{\vec{q}}/\hbar^2\omega^2_{\vec{q}})$, $\Delta_2 = \sum_{\vec{q}}(B^*_{\vec{q}}B_{\vec{q}}/\hbar^2\omega^2_{\vec{q}})e^{i\vec{q}\cdot\vec{a}_l}$, $\Delta_3 = \sum_{\vec{q}}(B^*_{\vec{q}}B_{\vec{q}}/\hbar^2\omega^2_{\vec{q}})e^{-i\vec{q}\cdot\vec{a}_l}$, where $\bar{n} = 1/[\exp(\hbar\omega/k_B t) - 1]$ is the average number of optical phonon at temperature $T$. When $qa \ll 1$, we have

$$F_l = 1 - \frac{2\bar{n}+1}{2}\sum_{\vec{q}}\frac{B^*_{\vec{q}}B_{\vec{q}}}{\hbar^2\omega^2}(\vec{q}\cdot\vec{a}_l)^2\,, \tag{44}$$

where

$$\begin{aligned}\sum_{\vec{q}}\frac{B^*_{\vec{q}}B_{\vec{q}}}{\hbar^2\omega^2}(\vec{q}\cdot\vec{a}_l)^2 &= \frac{Z^2e^4a^2}{2M_0a^2\omega^2}\cdot\int_0^{\pi/10a}\left[1+\frac{7425}{32}\cdot\frac{q}{a}\cdot a_0^2\right]q^3dq\int_0^{2\pi}\cos^2\phi d\phi \\ &= \frac{\pi^5Z^2e^4}{80000M_0a^4\omega^2}\left[1+\frac{297\pi}{16}\left(\frac{a_0}{a}\right)^2\right].\end{aligned}$$

Finally, we find that

$$\frac{m_l}{m_0} = \frac{1}{F_l} = \frac{1}{1-(\pi^2/800)\Lambda\alpha^2(2\bar{n}+1)}\,, \tag{45}$$

where

$$\Lambda = \frac{\pi^3Z^2\hbar^2}{100M_0a^4\omega^2m}\cdot\left[1+\frac{297\pi}{16}\left(\frac{a_0}{a}\right)^2\right]\left(\frac{1}{\mathcal{E}_\infty}-\frac{1}{\mathcal{E}_s}\right)^{-2}. \tag{46}$$

As temperature increases, $\bar{n}$ and thus the ratio $m_l/m_0$ also increase. Therefore the effective mass of the two-dimensional polaron will increase with increasing temperature.

## VII. Result and Discussion

According to the result given in Eq. (46), we consider a special case of NaBr. We have $\mathcal{E}_\infty = 2.62$, $\mathcal{E}_s = 5.99$, $Z = 1$, $\hbar = 1.05459\times10^{-27}$ erg·s, $M_0 = 2.964\times10^{-23}$g, $a = 4.21\times10^{-8}$cm, $\omega = 3.9\times10^{13}\text{s}^{-1}$, $a_0 = 0.53\times10^{-8}$cm, $m = 9.1\times10^{-28}$g, $e = 4.8\times10^{-10}$cgse, $\Lambda = 0.11$, $\alpha = 4.93$. The curve of $m_l/m_0$ versus temperature is shown in Fig. 1. We can see that at very low temperatures, the ratio $m_l/m_0$ depends weakly on the temperature. The dependence gradually becomes linear at higher temperatures.

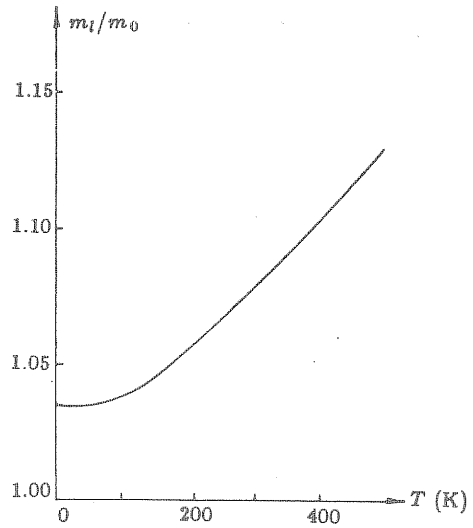


**Fig. 1.** The curve of $m_l/m_0$ versus temperature.

Equation (46) also indicates that the dependence of $m_l/m_0$ on temperature would be enhanced by the coupling constant. At very high temperature, $\bar{n}$ will also be very large. So it is possible that $m_l/m_0$ would change its sign at a certain critical temperature $T_c$. This is however not true, and it follows that our discussion should be restricted to cases at temperatures below $T_c$. The assumption $0 \leq q \leq (\pi/10a)$ is somewhat arbitrary. However we find that if the upper-limit is extended to $\pi/a$, the ratio $m_l/m_0$ changes sign at the higher end. So the range of $\vec{q}$ should also be smaller than a certain value, which we do not know exactly.

We would like to say that, although we have found the temperature dependence of the effective mass of a 2-D polaron under certain conditions, it is mainly a qualitative discussion rather than a quantitative one.

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