

## Polarons in a polar crystal slab at finite temperatures

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1989 J. Phys.: Condens. Matter 1 3201

(<http://iopscience.iop.org/0953-8984/1/20/003>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 94.79.44.176

The article was downloaded on 10/05/2010 at 18:11

Please note that [terms and conditions apply](#).

## Polarons in a polar crystal slab at finite temperatures

You-Cheng Li†‡ and Shi-Wei Gu§

† Institute of Theoretical Physics, Hebei Normal University, Shijiazhuang, Hebei, People's Republic of China

§ Centre of Theoretical Physics, Chinese Centre of Advanced Science and Technology (World Laboratory), Beijing, and Department of Physics, Jiao Tong University, Shanghai, People's Republic of China

Received 3 June 1988, in final form 17 October 1988

**Abstract.** With both the electron–longitudinal optical phonon and the electron–surface optical (SO) phonon interaction included, the temperature dependence of the effective mass and self-energy of a polaron in a polar crystal slab is investigated by means of the Lee–Low–Pines variation method. These quantities are calculated for GaAs as an example. It is found that both the effective mass and the self-energy will decrease with increasing temperature. In particular, for a very thin slab, the temperature dependence of the effective mass is nearly entirely determined by the SO phonon effect.

### 1. Introduction

Fröhlich polarons have been the subject of continuous interest for several decades. In the past, most work has been devoted to the study of the ground-state energy and the effective mass of polarons at zero temperature. Recently, there has been renewed interest in the temperature behaviour of the properties of these polarons [1–8].

The different assumptions about the mechanism of the electron–phonon interaction and the different methods applied in theoretical investigations have led to significantly different dependences of the polaron mass on temperature. In [9] the polaron energies were approximately calculated using the Hartree method and the conclusion was that the polaron mass would decrease with increasing temperature. However, using the Gurari variation method, the contrary result was reached in [10]. Until now, even though more factors have been taken into account and more perfect methods have been used, the conclusions have not been yet identical. For sufficiently low lattice temperatures, some theories [1–3] predicted a polaron mass that would decrease with increasing temperature, while other theories [4, 5] led to a polaron mass that would increase with increasing temperature.

The effective mass of the charge carriers in a crystal is usually determined by cyclotron resonance experiments. The experimental data for silver halides at low magnetic fields [11] showed that the polaron mass increases with increase in the lattice or carrier

‡ Present address: Department of Physics, University of North Iowa, Cedar Falls, IA 50614, USA. Permanent address: Centre of Theoretical Physics, Chinese Centre of Advanced Science and Technology (World Laboratory), Beijing, and Institute of Theoretical Physics, Hebei Normal University, Shijiazhuang, Hebei, People's Republic of China.

temperature. For cyclotron resonance measurements on GaAs-Ga<sub>1-x</sub>Al<sub>x</sub>As heterojunctions, it was reported in [12] that the effective mass of the polaron showed an anomalous increase with increasing temperature, i.e. the mass increased with increased temperature up to about 100 K and started to decrease for higher temperatures. It is obvious that different experiments also gave different results.

Electron-optical phonon coupling plays an important role in determining the temperature characteristic of polarons [13]. With the wide application of heterojunctions and superlattices to technology, the electron-phonon interaction has been theoretically investigated in 3D systems [14, 15] as well as in 2D systems [7, 16, 17]. However, to the best of our knowledge, only the temperature dependence of the virtual coupling of a quasi-free electron with bulk longitudinal optical (LO) phonons has been discussed.

In [12], the magnetophonon resonance results yielded phonon frequencies significantly below the bulk LO values, which suggested that the dominant interaction of electrons would not be with the bulk LO phonons. Therefore the electron interaction with other phonon modes associated with the presence of the interface should also be taken into account.

The first deduction of the Hamiltonian operators of the Fröhlich polaron in a polar slab with the electron-surface optical (SO) phonon interaction included was given in [18]. Then, in the zero-temperature limit, we and our collaborators [19] investigated the influence of the SO mode effect on the polaron in a polar slab and found that the SO mode effect would enhance the effective mass and self-energy of the polaron just as the LO mode would do.

The purpose of this present paper is to study how the electron-phonon interactions affect the temperature dependence of the properties of a polaron in a polar crystal slab. In particular, for the first time, the electron-SO phonon interaction is taken into account at finite temperatures. The effective mass and self-energy of the polaron as functions of temperature are derived by means of the Lee-Low-Pines [20] variation technique. Taking GaAs as an example, for an arbitrary slab thickness, we calculate the polaron's mass and self-energy at various finite temperatures. The results show that the effective mass and self-energy will both decrease with increasing temperature. At any determined temperature, the electron coupling with SO phonons will make contributions to the enhancement of the effective mass and self-energy and, with the slab getting thinner, such an effect will become more pronounced. In the 2D limit, the temperature dependence of the effective mass will be determined entirely by the SO mode effect and not by the LO mode effect.

The results deduced in this paper will be suitable for weakly and intermediately coupled polarons.

## 2. Hamiltonian

Consider a polar crystal slab with thickness  $2d$ ; the space at  $|z| \leq d$  is occupied by the crystal and at  $|z| > d$  is a vacuum. The slab is very thin and the size of the  $x$ - $y$  plane is much larger than  $2d$ . For simplicity, we assume that the effective-mass approximation is valid and the potential barrier at the slab surface is approximately infinite, i.e. the tunnelling of electrons through the surface is neglected. Then, we formulate the problem as the motion of an electron of mass  $m^*$  in an infinite square-well potential of width  $2d$  and have the Hamiltonian of the electron-phonon system as

$$H = H_e + H_{\text{ph}} + H_{\text{e-LO}} + H_{\text{e-SO}} \quad (1)$$

The first term  $H_e$  is the Hamiltonian of the electron in the slab and given by

$$H_e = -(\hbar^2/2m^*)\partial^2/\partial z^2 + (\hbar^2/2m^*)K_\rho^2 \quad |z| \leq d \quad (2)$$

where  $m^*$  is the band mass of the electron,  $\rho$  and  $K_\rho$  respectively represent the position vector and the wavevector in the  $x$ - $y$  plane for the electron.

The second term in (1) is the phonon field Hamiltonian and is written as

$$H_{\text{ph}} = H_{\text{LO}} + H_{\text{SO}} \quad (3)$$

$$H_{\text{LO}} = \sum_{k,m,p} a_{m,p}^+(\mathbf{k})a_{m,p}(\mathbf{k})\hbar\omega_{\text{LO}} \quad (3a)$$

$$H_{\text{SO}} = \sum_{q,p} b_p^+(q)b_p(q)\hbar\omega_{\text{Sp}} \quad (3b)$$

where  $a_{m,p}^+(\mathbf{k})$  is the creation operator,  $a_{m,p}(\mathbf{k})$  is the annihilation operator for the bulk LO phonon with frequency  $\omega_{\text{LO}}$  and the two-dimensional wavevector  $\mathbf{k}$ ,  $b_p(q)$  and  $b_p^+(q)$  are the corresponding operators for the SO phonon with frequency  $\omega_{\text{Sp}}$  and wavevector  $q$ . The phonon modes are specified by subscripts  $p$  and  $m$ . The parity index  $p$ , taking the value + and -, refers to the mirror symmetry with respect to the plane  $z = 0$ . The index  $m$  is the quantum number denoting the  $z$  component of the LO phonon wavevector. For even parity ( $p$  takes +),  $m$  is odd and, for odd parity ( $p$  takes -),  $m$  is even. We take  $N$  as the slab thickness in the unit of the lattice spacing constant  $a$ , i.e. set  $2d = Na$ . From the Brillouin zone boundary limitation:  $m\pi/2d \leq \pi/2a$ ,  $m$  can be any integer within the range  $1 \leq m \leq N/2$ .

In the above equations, the phonon frequencies can be expressed in terms of the transverse optical (TO) phonon frequency  $\omega_{\text{TO}}$  by

$$\omega_{\text{LO}}^2 = \omega_{\text{TO}}^2(\varepsilon_0/\varepsilon_\infty) \quad (4a)$$

$$\omega_{\text{S}\pm}^2 = \omega_{\text{TO}}^2[(\varepsilon_0 + 1) \mp (\varepsilon_0 - 1) \exp(-2qd)]/[(\varepsilon_\infty + 1) \mp (\varepsilon_\infty - 1) \exp(-2qd)] \quad (4b)$$

where  $\varepsilon_0$  is the static dielectric constant,  $\varepsilon_\infty$  is the optical dielectric constant and  $\omega_{\text{S}\pm}$  represents the phonon frequency  $\omega_{\text{Sp}}$  as  $p$  takes + or -.

The last two terms in (1) represent, respectively, the electron-LO phonon and the electron-SO phonon interaction Hamiltonian and they are directly given in [18]:

$$H_{\text{e-LO}} = \sum_{\mathbf{k}} \left[ B \exp(-i\mathbf{k} \cdot \boldsymbol{\rho}) \left( \sum_{m=1,3,\dots}^{N/2} \frac{\cos[(m\pi/2d)z]}{[k^2 + (m\pi/2d)^2]^{1/2}} a_{m,+}^+(\mathbf{k}) + \sum_{m=2,4,\dots}^{N/2} \frac{\sin[(m\pi/2d)z]}{[k^2 + (m\pi/2d)^2]^{1/2}} a_{m,-}^+(\mathbf{k}) \right) + \text{HC} \right] \quad (5a)$$

$$H_{\text{e-SO}} = \sum_q \left( \frac{\sinh(2qd)}{q} \right)^{1/2} \exp(-qd) \times \{ C \exp(-i\mathbf{q} \cdot \boldsymbol{\rho}) [G_+(q, z)b_\mp^\dagger(q) + G_-(q, z)b_\pm^\dagger(q)] + \text{HC} \} \quad (5b)$$

where

$$B^* = i[(4\pi e^2/V)\hbar\omega_{\text{LO}}(1/\varepsilon_\infty - 1/\varepsilon_0)]^{1/2} \quad (5c)$$

$$C^* = i[(2\pi e^2/A)\hbar\omega_{\text{TO}}(\varepsilon_0 - \varepsilon_\infty)]^{1/2} \quad (5d)$$

$$G_+ = \frac{\cosh(qz)/\cosh(qd)}{(\epsilon_\infty + 1) - (\epsilon_\infty - 1) \exp(-2qd)} \left( \frac{(\epsilon_\infty + 1) - (\epsilon_\infty - 1) \exp(-2qd)}{(\epsilon_0 + 1) - (\epsilon_0 - 1) \exp(-2qd)} \right)^{1/4} \quad (5e)$$

$$G_- = \frac{\sinh(qz)/\sinh(qd)}{(\epsilon_\infty + 1) + (\epsilon_\infty - 1) \exp(-2qd)} \left( \frac{(\epsilon_\infty + 1) + (\epsilon_\infty - 1) \exp(-2qd)}{(\epsilon_0 + 1) + (\epsilon_0 - 1) \exp(-2qd)} \right)^{1/4}. \quad (5f)$$

In the above equations,  $A$  and  $V$  are the surface area and the volume of the slab, respectively.

To simplify the calculations, we first perform the unitary transformations twice to Hamiltonian (1) with

$$U_1 = \exp \left[ -i \left( \sum_{k,m,p} a_{m,p}^+(\mathbf{k}) a_{m,p}(\mathbf{k}) \mathbf{k} \cdot \boldsymbol{\rho} + \sum_{q,p} b_p^+(\mathbf{q}) b_p(\mathbf{q}) \mathbf{q} \cdot \boldsymbol{\rho} \right) \right] \quad (6a)$$

$$U_2 = \exp \left( \sum_{k,m,p} [a_{m,p}^+(\mathbf{k}) f_{m,p}(\mathbf{k}) - a_{m,p}(\mathbf{k}) f_{m,p}^*(\mathbf{k})] + \sum_{q,p} [b_p^+(\mathbf{q}) g_p(\mathbf{q}) - b_p(\mathbf{q}) g_p^*(\mathbf{q})] \right). \quad (6b)$$

After tedious but direct calculations, we obtain the transformed Hamiltonian  $H^*$

$$H^* = U_2^{-1} U_1^{-1} H U_1 U_2. \quad (7)$$

We still assume that, at finite temperatures, the successive virtual phonons in the field around the electron are emitted individually, i.e. there is no interaction between different phonons. Therefore, we omit those terms including the factor  $[a_{m,p}^+ a_{m,p} b_p^+ b_p]$  in  $H^*$ .

As shown in [12], the phonon frequencies will decrease with increasing temperature but, if the temperature is restricted to the range lower than the room temperature ( $T < 300$  K), the relative change  $|\Delta\omega|/\omega$  in the frequency is only 1%. Then, we can take the phonon frequencies as approximately constants. In addition, because the electron-phonon interaction energies are much smaller than  $\omega_{LO}\hbar$  and  $\omega_{Sp}\hbar$ , we also omit them from the total energy of the phonons. With the considerations mentioned above, we assume that the eigenvalues of  $a^+a$  and  $b^+b$  in the phonon state at a finite temperature are given by the Planck distribution functions

$$N_1 = \langle a_{m,p}^+(\mathbf{k}) a_{m,p}(\mathbf{k}) \rangle = [\exp(\omega_{LO}\hbar/k_B T) - 1]^{-1} \quad (8a)$$

$$N_2 = \langle b_p^+(\mathbf{q}) b_p(\mathbf{q}) \rangle = [\exp(\omega_{Sp}\hbar/k_B T) - 1]^{-1} \quad (8b)$$

where  $k_B$  is the Boltzmann constant.

At finite temperatures, the wavefunction of the phonon state can be chosen as  $|\{N_{m,p}(\mathbf{k})\}, \{N_{Sp}(\mathbf{q})\}\rangle$ , in which  $\{N_{m,p}(\mathbf{k})\}$  and  $\{N_{Sp}(\mathbf{q})\}$ , respectively, represent the numbers of LO and so phonons. At last, the expected value of  $H^*$  (equation (7)) referring to the phonon state is easily obtained:

$$\overline{H^*} = \langle \{N_{m,p}(\mathbf{k})\}, \{N_{Sp}(\mathbf{q})\} | H^* | \{N_{Sp}(\mathbf{q})\}, \{N_{m,p}(\mathbf{k})\} \rangle. \quad (9)$$

### 3. Variation method

According to the Lee–Low–Pines variation technique, if it is noted that the only preferred direction in the  $x$ – $y$  plane is the direction of  $\mathbf{K}_\rho$ , we can introduce two parameters  $\eta_1$  and  $\eta_2$  given by

$$\sum_{\mathbf{k}, m, p} |f_{m,p}(\mathbf{k})|^2 \mathbf{k} = \eta_1 \mathbf{K}_\rho \quad \sum_{\mathbf{q}, p} |g_p(\mathbf{q})|^2 \mathbf{q} = \eta_2 \mathbf{K}_\rho. \quad (10)$$

Inserting equation (10) into equation (9) and from

$$\delta \overline{H^*} / \delta f_{m,p} = \delta \overline{H^*} / \delta f_{m,p}^* = \delta \overline{H^*} / \delta g_p = \delta \overline{H^*} / \delta g_p^* = 0$$

we determine the variation parameters  $f_{m,p}^*$  and  $g_p^*$  as

$$f_{m,+}^* = \{-B \cos[(m\pi/2d)z] / [\mathbf{k}^2 + (m\pi/2d)^2]^{1/2}\} / [\hbar\omega_{LO} + (\hbar^2/2m^*)] \\ \times (2N_1 + 1) |\mathbf{k}|^2 - (\hbar^2/m^*)(1 - \eta_1) \mathbf{K}_\rho \cdot \mathbf{k} \quad (11a)$$

$$f_{m,-}^* = \{-B \sin[(m\pi/2d)z] / [\mathbf{k}^2 + (m\pi/2d)^2]^{1/2}\} / [\hbar\omega_{LO} + (\hbar^2/2m^*)] \\ \times (2N_1 + 1) |\mathbf{k}|^2 - (\hbar^2/m^*)(1 - \eta_1) \mathbf{K}_\rho \cdot \mathbf{k} \quad (11b)$$

$$g_+^* = -C [\sinh(2qd)/q]^{1/2} \exp(-qd) G_+ / [\hbar\omega_{s+} + (\hbar^2|\mathbf{q}|^2/2m^*)] \\ \times (2N_{2+} + 1) - (\hbar^2/m^*)(1 - \eta_2) \mathbf{K}_\rho \cdot \mathbf{q} \quad (11c)$$

$$g_-^* = -C [\sinh(2qd)/q]^{1/2} \exp(-qd) G_- / [\hbar\omega_{s-} + (\hbar^2|\mathbf{q}|^2/2m^*)] \\ \times (2N_{2-} + 1) - (\hbar^2/m^*)(1 - \eta_2) \mathbf{K}_\rho \cdot \mathbf{q} \quad (11d)$$

where  $N_{2+}$  and  $N_{2-}$  represent the values of  $N_2$  in (8b) corresponding to even parity (+) and odd parity (-), respectively. The parameters  $f_{m,\pm}$  and  $g_\pm$  can be easily expressed as the corresponding conjugate formulae of equations (11a)–(11d).

In this paper, since we are interested only in slow electrons just as observed in experiments, we then set  $\mathbf{K}_\rho \approx 0$ . Inserting equations (11a)–(11d) and their conjugate formulae into equation (10), we calculate  $\eta_1$  and  $\eta_2$  by expanding the relevant formulae to the first power of  $\mathbf{K}_\rho$  and obtain

$$\eta_1 = \alpha F_B(z) / [1 + \alpha F_B(z)] \quad (12)$$

where

$$F_B(z) = \frac{8}{Nau_l} \left[ \sum_{(m=1,3,\dots)}^{N/2} \cos^2\left(\frac{m\pi}{2d}z\right) I_m + \sum_{(m=2,4,\dots)}^{N/2} \sin^2\left(\frac{m\pi}{2d}z\right) I_m \right] \quad (12a)$$

and

$$I_m = \int_0^\infty \frac{x^3 dx}{[1 + (2N_1 + 1)x^2]^3 [x^2 + (m\pi/Nau_l)^2]}. \quad (12b)$$

We also obtain

$$\eta_2 = \alpha F_S(z) / [1 + \alpha F_S(z)] \quad (13)$$

where

$$F_S(z) = 4\epsilon_0^{1/2} \epsilon_\infty^{3/2} (Nau_l)^3 (I_{Q1} + I_{Q2}) \quad (13a)$$

and

$$\begin{aligned}
 I_{Q1} &= \int_0^{N\pi/2} \frac{x^2 \exp(-x) \sinh x [\cosh(xz/2d)/\cosh(x/2)]^2}{[(Nau_{S+})^2 + x^2(2N_{2+} + 1)]^3 [(\varepsilon_\infty + 1) - (\varepsilon_\infty - 1) \exp(-x)]^{3/2}} \\
 &\quad \times [(\varepsilon_0 + 1) - (\varepsilon_0 - 1) \exp(-x)]^{-1/2} dx \quad (13b) \\
 I_{Q2} &= \int_0^{N\pi/2} \frac{x^2 \exp(-x) \sinh x [\sinh(xz/2d)/\sinh(x/2)]^2}{[(Nau_{S-})^2 + x^2(2N_{2-} + 1)]^3 [(\varepsilon_\infty + 1) + (\varepsilon_\infty - 1) \exp(-x)]^{3/2}} \\
 &\quad \times [(\varepsilon_0 + 1) + (\varepsilon_0 - 1) \exp(-x)]^{-1/2} dx.
 \end{aligned}$$

In the above equations, the dimensionless  $\alpha$  is the coupling constant for the electron-LO phonon interaction and is given by

$$\alpha = (m^* e^2 / \hbar^2 u_l) (1/\varepsilon_\infty - 1/\varepsilon_0) \quad (14)$$

and the polaron wavevector  $u_l$  and  $u_{S\pm}$  are defined by

$$u_l^2 = 2m^* \omega_{LO} / \hbar \quad u_{S\pm}^2 = 2m^* \omega_{S\pm} / \hbar. \quad (15)$$

In equation (13b), we also define the variable  $x = 2qd$ .

#### 4. Effective mass and self-energy

At finite temperatures the variation minimum of  $\overline{H^*}$  (equation (9)) is just the effective Hamiltonian of the free polaron in a polar slab. Substituting equations (10)–(13) into equation (9) and considering  $\eta_1 \ll 1$  and  $\eta_2 \ll 1$  as shown in our calculations, we get the effective Hamiltonian as

$$\begin{aligned}
 H_{\text{eff}} = \text{Min } \overline{H^*} &\simeq -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} + \frac{\hbar^2 K_\rho^2}{2m^*} [1 - \alpha F_B(z) - \alpha F_S(z)] + V_I^{(B)}(z) + V_I^{(S)}(z) \\
 &+ \frac{\hbar^2}{2m^*} \left[ \left( \sum_{k,m,p} N_1 \mathbf{k} \right)^2 + \left( \sum_{q,p} N_2 \mathbf{q} \right)^2 \right] + \sum_{k,m,p} N_1 \hbar \omega_{LO} + \sum_{q,p} N_2 \hbar \omega_{Sp}. \quad (16)
 \end{aligned}$$

On the basis of the expansion of the self-energy correction of the polaron with respect to the small wavevector  $\mathbf{K}_\rho$ , we give a standard definition [21] for the polaron's effective mass, i.e. in equation (16) let

$$\hbar^2 K_\rho^2 / 2M^* = (\hbar^2 K_\rho^2 / 2m^*) [1 - \alpha F_B(z) - \alpha F_S(z)].$$

Then, we obtain the effective mass as

$$M^* = m^* [1 - \alpha F_B(z) - \alpha F_S(z)]^{-1} \simeq m^* [1 + \alpha F_B(z) + \alpha F_S(z)]. \quad (17)$$

In the zero-temperature limit,  $N_1$  and  $N_2$  (equations (8a) and (8b)) will obviously tend to zero and then  $F_B(z)$  and  $F_S(z)$  will also approach the values at zero temperature. So, such a definition of the temperature-dependent effective mass is adequate because there is no discrepancy between the two mass expressions at zero and finite temperatures [8].

In equation (16),  $V_I^{(B)}(z)$  and  $V_I^{(S)}(z)$  are the effective potentials induced respectively by the electron-LO phonon and the electron-SO phonon interaction. After straightforward calculations, we obtain

$$V_I^{(B)} = -\frac{4\alpha\hbar\omega_{LO}u_l}{Na} \left[ \sum_{(m=1,3,\dots)}^{N/2} \frac{\cos^2[(m\pi/2d)z]}{(m\pi/2d)^2 - u_l^2} \ln\left(\frac{m\pi\sqrt{2N_1+1}}{Nau_l}\right) + \sum_{(m=2,4,\dots)}^{N/2} \frac{\sin^2[(m\pi/2d)z]}{(m\pi/2d)^2 - u_l^2} \ln\left(\frac{m\pi\sqrt{2N_1+1}}{Nau_l}\right) \right] \quad (18a)$$

$$V_I^{(S)} = -2\alpha\hbar\omega_{LO}\epsilon_0^{1/2}\epsilon_\infty^{3/2}(Nau_l)(I_{P1} + I_{P2}) \quad (18b)$$

where

$$I_{P1} = \int_0^{N\pi/2} \frac{\exp(-x) \sinh x [\cosh(xz/Na)/\cosh(x/2)]^2}{[(Nau_{S+})^2 + x^2(2N_{2+} + 1)][(\epsilon_\infty + 1) - (\epsilon_\infty - 1) \exp(-x)]^{3/2}} \times [(\epsilon_0 + 1) - (\epsilon_0 - 1) \exp(-x)]^{-1/2} dx \quad (18c)$$

$$I_{P2} = \int_0^{N\pi/2} \frac{\exp(-x) \sinh x [\sinh(xz/Na)/\sinh(x/2)]^2}{[(Nau_{S-})^2 + x^2(2N_{2-} + 1)][(\epsilon_\infty + 1) + (\epsilon_\infty - 1) \exp(-x)]^{3/2}} \times [(\epsilon_0 + 1) + (\epsilon_0 - 1) \exp(-x)]^{-1/2} dx.$$

In order to calculate the average values of the effective mass and the self-energy in the slab, it is necessary to obtain the approximate wavefunction in the  $z$  direction. For this purpose, first we separate  $H_{\text{eff}}$  (equation (16)) into two parts:

$$H_{\text{eff}} = H_z + H_1$$

where

$$H_z = -(\hbar^2/2m^*)(\partial^2/\partial z^2) + V_I^{(B)}(z) + V_I^{(S)}(z) \quad (19)$$

and  $H_1$  includes the other terms in  $H_{\text{eff}}$  (equation (16)). In  $H_1$ , only the effective mass  $M^*$  relates to the coordinate  $z$ , but its change with  $z$  is so small that we can approximately take it as a constant independent of  $z$ . Therefore, the motion in the  $x$ - $y$  plane can be separated from the motion along the  $z$  direction and  $H_z$  (equation (19)) will represent the Hamiltonian of the electron-phonon system in the  $z$  direction. In addition, for the III-V compounds such as GaAs, the effective potentials  $V_I^{(B)}(z)$  and  $V_I^{(S)}(z)$  in  $H_z$  (equation (19)) are also very small; consequently they can be neglected compared with the kinetic energy of the electron along the  $z$  direction. Hence, we still consider the electron moving approximately in an infinite square-well potential along the  $z$  direction and the corresponding eigen-equation can be expressed as

$$-(\hbar^2/2m^*)(\partial^2/\partial z^2)\varphi_l(z) = E_l\varphi_l(z) \quad |z| \leq d. \quad (20)$$

From the well known solution of equation (20), we have the wavefunction  $\varphi_l(z)$  of the electron along the  $z$  direction as

$$\varphi_l(z) = \begin{cases} (1/\sqrt{d}) \sin[(l\pi/2d)(z + d)] & |z| \leq d \\ 0 & |z| > d \end{cases} \quad (21)$$

where  $l$  is the quantum number and is taken as a positive integer. For the conduction electron,  $l$  will be limited by the band width:

$$E_l = l^2\hbar^2\pi^2/8m^*d^2 \leq \pi^2\hbar^2/2m^*a^2, \quad \text{i.e. } l \leq 2d/a = N.$$

Thus the expected value of the effective mass  $M^*$  is expressed by



$$\begin{aligned} \overline{M^*} &= \langle \varphi_l(z) | M^*(z) | \varphi_l(z) \rangle \\ &= m^* [1 + \langle \varphi_l(z) | \alpha F_B(z) | \varphi_l(z) \rangle + \langle \varphi_l(z) | \alpha F_S(z) | \varphi_l(z) \rangle] \end{aligned} \tag{22}$$

where

$$\langle \varphi_l(z) | F_B(z) | \varphi_l(z) \rangle = \frac{4}{Nau_l} \left( \sum_{m=1}^{N/2} I_m + \frac{1}{2} I_l \right) \tag{22a}$$

in which

$$\begin{aligned} I_m &= \int_0^\infty \frac{x^3 dx}{[1 + (2N_1 + 1)x^2]^3 [x^2 + (m\pi/Nau_l)^2]} \\ &= 1 - (2N_1 + 1)^2 (m\pi/Nau_l)^4 + 2(2N_1 + 1) \\ &\quad \times (m\pi/Nau_l)^2 \ln[(2N_1 + 1)(m\pi/Nau_l)^2] \\ &\quad \times \{4(2N_1 + 1)[1 - (2N_1 + 1)(m\pi/Nau_l)^2]^3\}^{-1} \end{aligned} \tag{22b}$$

$$I_l = I_m |_{m=l}$$

and

$$\langle \varphi_l(z) | F_S(z) | \varphi_l(z) \rangle = 4\varepsilon_0^{1/2} \varepsilon_\infty^{3/2} (Nau_l)^3 [\langle I_{Q1} \rangle + \langle I_{Q2} \rangle] \tag{22c}$$

in which

$$\begin{aligned} \langle I_{Q1} \rangle &= \frac{1}{2} \int_0^{N\pi/2} \frac{x^2 \exp(-x) \sinh x}{[(Nau_{S+})^2 + (2N_{2+} + 1)x^2]^3} \frac{1}{[\cosh(x/2)]^2} \\ &\quad \times \frac{1 + (l^2 \pi^2 \sinh x)/[x(x^2 + l^2 \pi^2)]}{[(\varepsilon_\infty + 1) - (\varepsilon_\infty - 1) \exp(-x)]^{3/2} [(\varepsilon_0 + 1) - (\varepsilon_0 - 1) \exp(-x)]^{1/2}} dx \\ \langle I_{Q2} \rangle &= \frac{1}{2} \int_0^{N\pi/2} \frac{x^2 \exp(-x) \sinh x}{[(Nau_{S-})^2 + (2N_{2-} + 1)x^2]^3} \frac{1}{[\sinh(x/2)]^2} \\ &\quad \times \frac{-1 + (l^2 \pi^2 \sinh x)/[x(x^2 + l^2 \pi^2)]}{[(\varepsilon_\infty + 1) + (\varepsilon_\infty - 1) \exp(-x)]^{3/2} [(\varepsilon_0 + 1) + (\varepsilon_0 - 1) \exp(-x)]^{1/2}} dx. \end{aligned} \tag{22d}$$

By calculating the expected values of the induced potentials  $V_I^{(B)}$  and  $V_I^{(S)}$  referring to  $|\varphi_l(z)\rangle$ , we obtain the self-energies  $E_s^B$  and  $E_s^S$  which come, respectively, from the bulk LO and so phonon contributions. The results are

$$\begin{aligned} E_s^B &= \langle \varphi_l(z) | V_I^{(B)}(z) | \varphi_l(z) \rangle \\ &= -2\alpha\hbar\omega_{LO} Nau_l \left[ \sum_{m=1}^{N/2} \frac{1}{(m\pi)^2 (2N_1 + 1) - (Nau_l)^2} \ln\left(\frac{m\pi\sqrt{2N_1 + 1}}{Nau_l}\right) \right. \\ &\quad \left. + \frac{1}{2(l\pi)^2 (2N_1 + 1) - (Nau_l)^2} \ln\left(\frac{l\pi\sqrt{2N_1 + 1}}{Nau_l}\right) \right] \end{aligned} \tag{23a}$$

$$E_s^S = \langle \varphi_l(z) | V_I^{(S)}(z) | \varphi_l(z) \rangle = -2\alpha\hbar\omega_{LO} Nau_l \varepsilon_0^{1/2} \varepsilon_\infty^{3/2} (\langle I_{P1} \rangle + \langle I_{P2} \rangle) \tag{23b}$$

where

**Table 1.** Characteristic parameters of crystal GaAs. All the parameters are taken from [22] except for the lattice constant  $a$  which is taken from [23].  $m_0$  is the free-electron rest mass.

$\alpha$	$\hbar\omega_{\text{LO}}$ (meV)	$\hbar\omega_{\text{TO}}$ (meV)	$m^*/m_0$	$a$ (Å)	$\epsilon_0$	$\epsilon_\infty$
0.0681	36.70	33.83	0.0657	5.654	12.83	10.9

$$\begin{aligned}
 \langle I_{\text{P1}} \rangle &= \frac{1}{2} \int_0^{N\pi/2} \frac{\exp(-x) \sinh x}{[(Nau_{\text{S}+})^2 + x^2(2N_{2+} + 1)]} \frac{1}{\cosh^2(x/2)} \left( \frac{l^2 \pi^2 \sinh x}{x(x^2 + l^2 \pi^2)} + 1 \right) \\
 &\quad \times \frac{1}{[(\epsilon_\infty + 1) - (\epsilon_\infty - 1) \exp(-x)]^{3/2} [(\epsilon_0 + 1) - (\epsilon_0 - 1) \exp(-x)]^{1/2}} dx \\
 \langle I_{\text{P2}} \rangle &= \frac{1}{2} \int_0^{N\pi/2} \frac{\exp(-x) \sinh x}{[(Nau_{\text{S}-})^2 + x^2(2N_{2-} + 1)]} \frac{1}{\sinh^2(x/2)} \left( \frac{l^2 \pi^2 \sinh x}{x(x^2 + l^2 \pi^2)} - 1 \right) \\
 &\quad \times \frac{1}{[(\epsilon_\infty + 1) + (\epsilon_\infty - 1) \exp(-x)]^{3/2} [(\epsilon_0 + 1) + (\epsilon_0 - 1) \exp(-x)]^{1/2}} dx.
 \end{aligned} \tag{23c}$$

In these equations,  $\alpha$ ,  $u_l$  and  $u_{\text{S}\pm}$  are defined, respectively, by equations (14) and (15).

## 5. Results and discussion

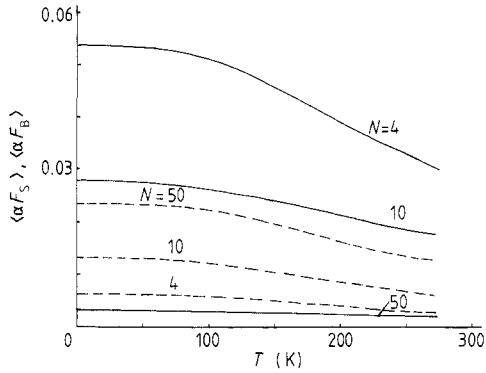
According to the equations deduced in § 4 and taking GaAs as an example, for the ground state ( $l = 1$ ) at different temperatures, we calculate the effective mass and the self-energies of the polaron in a polar slab with arbitrary thickness. For slow electrons which are usually observed in experiments, we set  $\mathbf{K}_p \approx 0$ . The crystal characteristic parameters are related to the temperature [22], but within the temperature range (less than room temperature) considered in this paper their changes with temperature are very small. Therefore, in our calculations, we assume these parameters are constant and take their values approximately as those at low temperatures. Table 1 gives the characteristic parameters of crystal GaAs.

In this paper, we obtain the effective mass of the polaron defined as

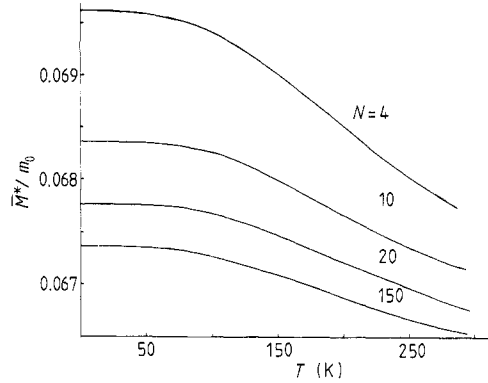
$$\overline{M}^* = m^*[1 + \langle \alpha F_{\text{B}} \rangle + \langle \alpha F_{\text{S}} \rangle]$$

where  $\langle \alpha F_{\text{B}} \rangle$  and  $\langle \alpha F_{\text{S}} \rangle$  are due to interactions of the electron with bulk LO and so phonons, respectively. For different slab thicknesses, the variations in  $\langle \alpha F_{\text{B}} \rangle$  and  $\langle \alpha F_{\text{S}} \rangle$  with increasing temperature are shown in figure 1. Only when the slab is very thin would the so phonon effect  $\langle \alpha F_{\text{S}} \rangle$  be much stronger than the LO phonon effect and become the primary factor in determining the effective mass. With increase in the slab thickness, the so mode contribution will decrease rapidly and the LO phonon effect  $\langle \alpha F_{\text{B}} \rangle$  will become stronger and give the dominant contribution to the mass as the slab is relatively thick ( $N > 50$ ).

Both  $\langle \alpha F_{\text{B}} \rangle$  and  $\langle \alpha F_{\text{S}} \rangle$  will decrease with increasing temperature. It is well worth noting that, the thinner the slab is, the more marked the change in the so phonon effect with the temperature will be. As  $N$  becomes relatively large, such a change in  $\langle \alpha F_{\text{S}} \rangle$  will



**Figure 1.**  $\langle \alpha F_B \rangle$  (---) and  $\langle \alpha F_S \rangle$  (—) as functions of temperature  $T$  for different slab thicknesses  $N$ .



**Figure 2.** Temperature dependence of the effective mass  $\bar{M}^*/m_0$  ( $m_0$  is the free-electron rest mass).

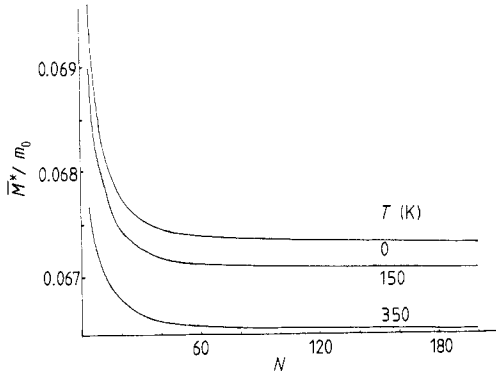
nearly disappear. However, for the LO phonon effect the result turns out to be contrary to the SO mode effect; as the slab becomes thicker the change in  $\langle \alpha F_B \rangle$  with temperature will become increasingly marked.

Being determined by the sum of  $\langle \alpha F_S \rangle$  and  $\langle \alpha F_B \rangle$ , as described in figure 2, the effective mass  $\bar{M}^*/m_0$  monotonically decreases with increase in temperature. In particular, the most obvious change in the mass will appear within the temperature range 100–250 K. On increase in the temperature, the uncorrelated motion of phonons becomes an important factor and the coherence between the electron motion and the phonon motion gets weaker. It results in the weakness of the electron–phonon interactions, i.e. in a decrease in the effective mass with increasing temperature.

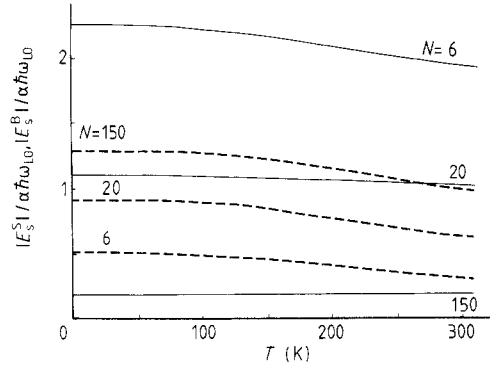
In [12] an anomalous increase in the polaron mass with temperature was obtained and it was also interpreted as being caused by the temperature dependence of the screening of the electron–phonon interaction. From an explicit calculation of the polaron mass for an arbitrary temperature with the inclusion of full dynamical screening, in [7] a temperature behaviour was theoretically obtained which agreed qualitatively with the data in [12] but the results at 100 K are quantitatively a factor of almost 2 smaller than observed experimentally.

The experiment results in [12] also suggested that the dominant interaction of electrons would be not with the bulk LO phonons, and some phonon modes associated with the presence of the interface should be considered. With the SO mode included in this paper, we find that, for a very thin slab, the SO mode effect is much greater than the bulk LO mode effect (compare the curves for  $N = 4$  in figure 1), i.e. the temperature dependence of the effective mass is really attributed to the attractive action of SO phonons. In the 2D limit (see the curve for  $N = 4$  in figure 2), we quantitatively obtain the same result as that reported in [12] but, since we have not taken the strong screening of the electron–phonon interaction into account, there will be no anomalous increase in the effective mass at low temperatures in our results.

Figure 3 depicts how the effective mass changes with the slab thickness at finite temperatures. As  $N$  tends to zero, the SO phonon effect enhances the mass greatly and, with a slight increase in  $N$ , such an effect is weakened rapidly and the mass also decreases swiftly. For further increase in  $N$ , the effective mass will gently approach a stable value determined by the LO phonon effect. Owing to the temperature dependence of the LO



**Figure 3.** Effective mass  $\bar{M}^*/m_0$  against the slab thickness  $N$  at different finite temperatures.



**Figure 4.** LO and SO self-energies against temperature  $T$  for different slab thicknesses: —,  $|E_s^S|/\alpha\hbar\omega_{LO}$ ; ---,  $|E_s^B|/\alpha\hbar\omega_{LO}$ .

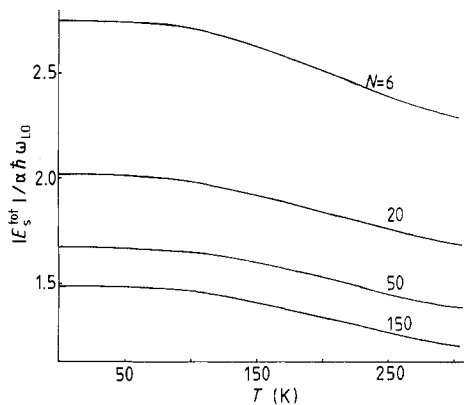
mode action, for infinite  $N$ , the higher the finite temperature is, the lower the stable bulk value will be.

The polaron self-energy consists of two parts:  $E_s^B$  and  $E_s^S$ , which are induced respectively by the electron–LO phonon interaction and the electron–SO phonon interaction. When the temperature increases, the irregular motion of the ions in crystals will become more violent; consequently the number of polar phonons will decrease greatly and therefore the interactions between electrons and phonons will be weakened. Therefore, the absolute values of both  $E_s^B$  and  $E_s^S$  will decrease with increase in temperature. Figure 4 shows a comparison of the temperature behaviour of  $|E_s^S|$  (full curves) and  $|E_s^B|$  (broken curves). For a very thin slab, the changes in  $|E_s^S|$  and  $|E_s^B|$  with temperature have the same orders of magnitude. However, when the slab becomes thick, the change in  $|E_s^S|$  with temperature will disappear rapidly and for  $|E_s^B|$  there will be no obvious difference in the temperature behaviour between the different slabs. So, only for a very thin slab will the SO phonon action make a large contribution to the temperature dependence of the self-energy and for a thick slab the temperature behaviour will mainly depend on the LO phonon effect. Therefore, just as shown in figure 5, it is obvious that the variation in the total self-energy  $|E_s^B| + |E_s^S|$  with temperature will be greater in a thin slab than in a thick slab.

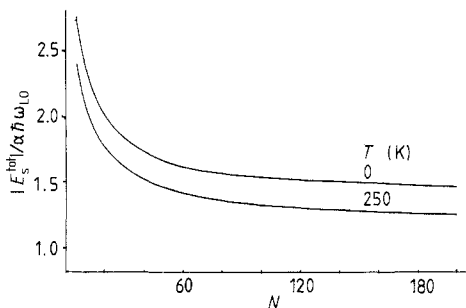
Figure 6 describes the total self-energy as functions of the slab thickness at different temperatures. In the limit when  $N$  approaches zero, the self-energy increases quickly owing to the enhancement action of SO phonons. When  $N$  becomes large, the self-energy will decrease swiftly with rapid weakening of the SO phonon effect. As  $N$  tends to infinity, the self-energy will approach the value of  $|E_s^B|$  at finite temperatures.

### Acknowledgments

One of us (S W Gu) wishes to acknowledge the support by the Science Foundation of the Chinese Academy of Science. Y C Li thanks Professor G Intemann for his warm help.



**Figure 5.** Temperature dependence of the total self-energy  $|E_s^{\text{tot}}|$ .



**Figure 6.** Total self-energy as a function of slab thickness  $N$  at different finite temperatures.

## References

- [1] Saitoh M 1980 *J. Phys. Soc. Japan* **49** 878
- [2] Saitoh M and Arisawa K 1980 *J. Phys. Soc. Japan Suppl. A* **49** 675
- [3] Arisawa K and Saitoh M 1981 *Phys. Lett.* **82A** 462
- [4] Peeters F M and Devreese J T 1982 *Phys. Rev. B* **25** 7302; 1985 *Phys. Rev. B* **31** 5500
- [5] Fedyanin V K and Rodriguez C 1982 *Phys. Status Solidi b* **110** 105
- [6] Peeters F M and Devreese J T 1983 *Phys. Status Solidi b* **115** 285
- [7] Wu X, Peeters F M and Devreese J T 1987 *Phys. Rev. B* **36** 9765
- [8] Khandekar D C, Bhagwat K V and Lawande S V 1988 *Phys. Rev. B* **37** 3085
- [9] Yokota T 1953 *Busseiron-kenkyu* **69** 137
- [10] Fulton T 1956 *Phys. Rev.* **103** 1712
- [11] Masumi T 1984 *Polarons and Excitons in Polar Semiconductors and Ionic Crystals* ed. J T Devreese and F M Peeters (New York: Plenum) p 99
- [12] Barter J E, Ascarelli G and Rodriguez S 1971 *Phys. Rev. Lett.* **27** 100
- [13] Brummell M A, Nicholas R J, Hopkins M A, Harris J J and Foxon C T 1987 *Phys. Rev. Lett.* **58** 77
- [13] Sarma Das and Mason B A 1985 *Phys. Rev. B* **31** 5536
- Lei X L 1985 *J. Phys. C: Solid State Phys.* **18** L731
- [14] Lindemann G, Lassnig R, Seidenbusch W and Gornik E 1983 *Phys. Rev. B* **28** 4693
- [15] Sigg H, Bluysen H J A and Wyder P 1983 *Solid State Commun.* **48** 897
- [16] Larsen D M 1984 *Phys. Rev. B* **30** 4595
- [17] Sarma Das 1984 *Phys. Rev. Lett.* **52** 859
- [18] Licari J J and Evrard R 1977 *Phys. Rev. B* **15** 2254
- [19] Liang X-X, Gu S-W and Lin D-L 1986 *Phys. Rev. B* **34** 2807
- Li Y-C, Zheng L-F and Gu S-W 1988 *Phys. Rev. B* **38** 4096
- [20] Lee T D, Low F E and Pines D 1953 *Phys. Rev.* **90** 297
- [21] Peeters F M, Wu X and Devreese J T 1988 *Phys. Rev. B* **37** 933
- [22] Kartheuser E 1972 *Polarons in Ionic Crystals and Polar Semiconductors* ed. J T Devreese (Amsterdam: North-Holland) p 727
- [23] O'Keefe M and Hyde B G 1978 *Acta Crystallogr. B* **34** 3519