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# The temperature dependence of the $N$ -dimensional polaron

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**Abstract.** The Lee–Low–Pines-like intermediate method is adopted to study the properties of a slow-moving optical polaron in an  $N$ -dimensional polar crystal at a finite temperature. The analytical expressions for the internal energy and effective mass of the polaron for a certain momentum  $K_p$  are derived using the approximation that the thermophonon number is independent of the wavevector. The numerical results obtained by considering the dependence of the thermophonon number on the wavevector are also obtained. It is shown that the temperature effect of the polaron diminishes with increasing dimensionality.

## 1. Introduction

The dimensional dependence of the polaron properties has attracted considerable interest during the last few years. Peeters *et al* [1] have studied the problem of the  $N$ -dimensional polaron with the path integral approach and found that the polaron effects diminish drastically with increasing dimensionality. Also, many workers [2–6] have discussed theoretically the polaron ground-state energy, effective mass, mobility, etc.

Chatterjee [7] has discussed the  $N$ -dimensional bound polaron with a variational method and path integral formulation. We [8] have studied the internal excitation states of the  $N$ -dimensional polaron with the improved Huybrechts [9] linear combination method. The results also show that the polaron effects become weaker with increasing dimensionality.

Most work in this field, to our knowledge, has been carried out at the zero-temperature limit. The temperature dependence of the polaron effect on the dimensionality is very interesting because experiments are performed at a non-zero temperature. This gives us the impetus to study the properties of an  $N$ -dimensional optical polaron at a finite temperature. In this paper, an improved Lee–Low–Pines (LLP) [10] intermediate-coupling theory is adopted from the work of Yokota [11], who studied the 3D polaron problem in the 1950s. The analytical expressions for the internal energy and effective mass of the polaron are derived by using the approximation that the thermophonon number is independent of the phonon wavevector. The numerical results are also computed taking into account the fact that the thermophonon number is dependent on the wavevector. It is shown that the polaron has an increasing temperature effect with decreasing dimensionality.

## 2. The variational method

The Hamiltonian of an electron–phonon interaction system in an  $N$ -dimensional polar crystal can be written as [1]

$$H = \frac{1}{2}p^2 + \sum_q b_q^\dagger b_q + \sum_q [\xi_q \exp(-iq \cdot r) b_q + \text{HC}] \quad (1)$$

where

$$\xi_q = i \left[ \Gamma\left[\frac{1}{2}(N-1)\right] 2^{N-3/2} \pi^{(N-1)/2} / V q^{N-1} \alpha \right]^{1/2}. \quad (2)$$

In equation (1),  $p$  and  $r$  are the  $N$ -dimensional momentum and coordinate of an electron, respectively.  $b_q^+$  and  $b_q$  are the creation and annihilation operators respectively of a longitudinal optical phonon with wavevector  $q$ .  $\alpha$  is the dimensionless electron-phonon coupling constant. For convenience, we have chosen the natural units  $\hbar = m = \omega = 1$ , where  $\hbar$ ,  $m$  and  $\omega$  are the Planck constant, the band mass of the electron and the dispersionless frequency of the phonons, respectively.  $V$  is the volume of the  $N$ -dimensional polar crystal.  $\Gamma[\frac{1}{2}(N-1)]$  denotes the gamma function.

The non-interaction eigenstates of the electron-phonon system can be chosen as [11, 12]

$$|P, \{n(q)\}\rangle = \exp(s_1) \exp(s_2) \exp(-s_1) \exp \left[ i \left( P - \sum_q n(q) q \right) \cdot r \right] \prod_q \frac{(b_q^+)^{n(q)}}{[n(q)!]^{1/2}} |0\rangle \quad (3)$$

with

$$s_1 = -i \sum_q b_q^+ b_q q \cdot r \quad \text{and} \quad s_2 = - \sum_q (f_q b_q^+ - f_q^* b_q).$$

In equation (3),  $|0\rangle$  is the vacuum phonon state.  $\{n(q)\} = n(q_1), n(q_2), \dots, n(q_i), \dots$  are the thermophonon numbers corresponding to different wavevectors  $q$ .  $P$  is the total momentum of the system and  $f_q$  the variational parameter.  $\exp(s_1) \exp(s_2) \exp(-s_1) = \exp[-\sum_q \{f_q b_q \exp(iq \cdot r) - f_q^* b_q^+ \exp(-iq \cdot r)\}]$  is the operator of the displacement oscillator. If we adopt the orthogonal and complete set of the non-interaction eigenstates (3), the partition function of the system can be determined using Peierls' variational principle:

$$Z = \text{Tr} \left[ \exp \left( -\frac{H}{T} \right) \right] \geq \sum_n \exp \left( -\frac{\langle n|H|n\rangle}{T} \right) \quad (4)$$

where  $|n\rangle$  denotes the eigenstate of the non-interaction system. The unit of  $T$  is  $\hbar\omega/k$ , where  $k$  is the Boltzmann constant.

The polaron energy corresponding to the eigenstate is given by

$$\begin{aligned} E[P, \{n(q)\}] &= \langle P, \{n(q)\} | H | P, \{n(q)\} \rangle \\ &= \frac{1}{2} \left( P - \sum_q q n(q) \right)^2 + \sum_q (\xi_q^* f_q + \xi_q f_q^*) + \sum_q |\xi_q|^2 (1 - P \cdot q + \frac{1}{2} q^2) \\ &\quad + \frac{1}{2} \left| \sum_q |f_q|^2 q \right|^2 + \sum_q n(q) \left( 1 + q \cdot \sum_{q'} q' |f_{q'}|^2 \right) + \sum_q |f_q|^2 q^2 n(q) \end{aligned} \quad (5)$$

where  $\sum_q q n(q)$  is the momentum summation of the phonons with different frequencies emitted by the electron. The variational parameter  $f_q$  should be determined by the maximization of the partition function because the free energy of the system has a minimum at the equilibrium state.

Since the total momentum  $p - \sum_q b_q^+ b_q q$  of the system commutes with the Hamiltonian (1), it is a constant of motion. In the present representation, the total momentum becomes a  $C$ -number which has been replaced by its eigenvalue  $P$ . We are now interested in the properties of a single polaron with a given momentum. The corresponding partition function can be obtained by fixing the polaron momentum  $K_p = P - \sum_q n(q) q$  as Yokota [11] did:

$$Z_p = \sum_{P, \{n(q)\}} \exp \left( -\frac{E(P, \{n(q)\})}{T} \right) \delta \left( P - \sum_q q n(q) - K_p \right)$$

$$= \exp \left[ -\frac{1}{T} \left( \frac{1}{2} K_p^2 + \sum_q (\xi_q^* f_q + \xi_q f_q^*) + \sum_q |f_q|^2 (1 - K_p \cdot q + \frac{1}{2} q^2) + \frac{1}{2} \left| \sum_q |f_q|^2 q \right|^2 \right) \right] \sum_{\{n(q)\}} \exp \left( -\sum_q \frac{n(q)(1 + q^2 |f_q|^2)}{T} \right) \quad (6)$$

where

$$\sum_{\{n(q)\}} \exp \left( -\sum_q \frac{n(q)(1 + q^2 |f_q|^2)}{T} \right) = \prod_q \frac{1}{1 - \exp[-(1 + q^2 |f_q|^2)/T]}$$

The free energy of the system can be written as

$$E_p = -T \ln Z_p = \frac{1}{2} K_p^2 + \sum_q (\xi_q^* f_q + \xi_q f_q^*) + \frac{1}{2} \left| \sum_q |f_q|^2 q \right|^2 - \sum_q |f_q|^2 (K_p \cdot q + \frac{1}{2} q^2) + \sum_q (|f_q|^2 - 1) + T \sum_q \ln \left[ \exp \left( \frac{1 + q^2 |f_q|^2}{T} \right) - 1 \right]. \quad (7)$$

Putting

$$n(q) = 1 / \{ \exp[(1 + q^2 |f_q|^2)/T] - 1 \} \quad (8)$$

and

$$\eta K_p = \sum_q q |f_q|^2 \quad (9)$$

from minimization of the free energy with respect to  $f_q^*$ , we obtain

$$f_q = -\xi_q / \{ 1 - (1 - \eta) q \cdot K_p + \frac{1}{2} [2n(q) + 1] q^2 \}. \quad (10)$$

It should be pointed out that  $n(q)$  deviates from the Bose distribution by  $q^2 |f_q|^2$  which is caused by the interaction between the electron and phonons. Inserting equation (10) into equation (9) and multiplying both sides by  $K_p$ , we derive

$$\eta K_p^2 = \frac{q \cdot K_p |\xi_q|^2}{[1 - (1 - \eta) q \cdot K_p + \frac{1}{2} [2n(q) + 1] q^2]^2} \simeq \sum_q 2 |\xi_q|^2 (K_p \cdot q)^2 (1 - \eta) \frac{1}{\{ 1 + \frac{1}{2} [2n(q) + 1] q^2 \}^3} \quad (11)$$

in which the expansion of the denominator to the second order of small  $K_p$  has been introduced. The summation over  $q$  in (11) can be reduced to the following integral:

$$\sum_q \rightarrow \frac{V}{(2\pi)^N} \int \dots \int dq.$$

By using  $\int d_N x f(x) = \int f(x) r^{N-1} dr \sin^{N-2} \theta_{N-1} d\theta_{N-1} d\theta_{N-2} \dots d\theta_1$ , equation (11) becomes

$$\eta K_p^2 = (1 - \eta) K_p^2 A \quad (12)$$

where

$$A = \frac{\sqrt{2}\alpha}{\pi} \int_0^\infty dq \int_0^\pi d\theta_{N-1} \frac{q^2 (\sin^{N-2} \theta_{N-1} - \sin^N \theta_{N-1})}{\{ 1 + \frac{1}{2} [2n(q) + 1] q^2 \}^3}.$$

This can be solved to give

$$\eta = A / (1 + A). \quad (13)$$

The internal energy of the polaron for a certain momentum  $K_p$  is given by

$$E(N, T) = E_p - T \frac{\partial E_p}{\partial T} = \frac{1}{2}(1 - \eta^2)K_p^2 - \sum_q \frac{|\xi_q|^2}{1 - (1 - \eta)q \cdot K_p + \frac{1}{2}[2n(q) + 1]q^2}. \quad (14)$$

In equation (14), the direct contribution of the thermophonon to the energy has been omitted, which increases the polaron self-energy and destabilizes the polaron. At zero temperature,  $E(N, T)$  becomes the polaron ground-state energy  $E(N, 0)$ . In section 3, we shall make a comparison between these two energies to obtain the temperature effect of the polaron. Repeating the process for obtaining equation (12), we have

$$E(N, T) = -\frac{\alpha}{\sqrt{2\pi}} \int_0^\infty dq \int_0^\pi d\theta_{N-1} \frac{\sin^{N-2}\theta_{N-1}}{1 + \frac{1}{2}[2n(q) + 1]q^2} + K_p^2 \left( \frac{1}{2}(1 - \eta^2) - \frac{\alpha(1 - \eta)^2}{\sqrt{2\pi}} \int_0^\infty dq \int_0^\pi d\theta_{N-1} \frac{q^2(\sin^{N-2}\theta_{N-1} - \sin^N\theta_{N-1})}{\{1 + \frac{1}{2}[2n(q) + 1]q^2\}^3} \right) \quad (15)$$

in which the first term is the self-energy of the polaron. From the second term in equation (15), the effective mass of the polaron can be written as

$$m^*(N, T) = \left[ 2 \left( \frac{1}{2}(1 - \eta^2) - \frac{\alpha(1 - \eta)^2}{\sqrt{2\pi}} \int_0^\infty dq \int_0^\pi d\theta_{N-1} \frac{q^2(\sin^{N-2}\theta_{N-1} - \sin^N\theta_{N-1})}{\{1 + \frac{1}{2}[2n(q) + 1]q^2\}^3} \right) \right]^{-1} = 1 + A. \quad (16)$$

### 3. Discussion and numerical computation

In equations (15) and (16), if we take the thermophonon number approximately as the Bose distribution

$$n(q) \rightarrow n_0 = 1/\{\exp(1/T) - 1\} \quad (17)$$

then the polaron ground-state energy is given by

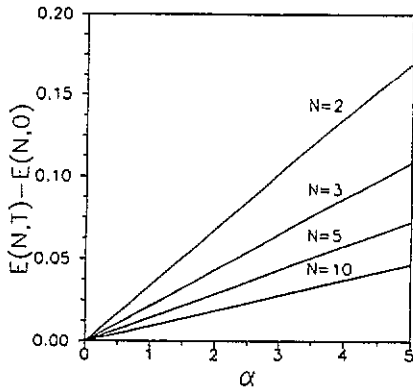
$$E_B(N, T) = -\{\sqrt{\pi}\Gamma[\frac{1}{2}(N - 1)]/2\Gamma(\frac{1}{2}N)\}[\alpha/(2n_0 + 1)^{1/2}] + [1/2m_B^*(N, T)]K_p^2. \quad (18)$$

The polaron effective mass is reduced to

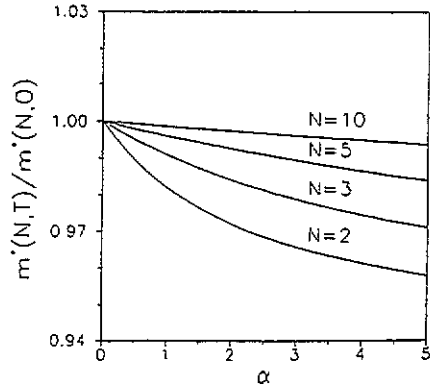
$$m_B^*(N, T) = 1 + \{\sqrt{\pi}\Gamma[\frac{1}{2}(N - 1)]/4N\Gamma(\frac{1}{2}N)\}[\alpha/(2n_0 + 1)^{3/2}]. \quad (19)$$

For the general situation, the thermophonon number can be given by self-consistent computation of equations (8) and (10). Thereby the polaron energy and its effective mass are obtained from equations (15) and (16). We have computed the numerical results within the intermediate-coupling region for different dimensions. Figures 1–4 show the numerical results corresponding to the polaron momentum  $K_p = 0.01$  and the temperature  $T = 100$  K. To perform the numerical computation of the exponential factor in equation (17), we choose the frequency  $\omega$  of the optical phonon to be  $5 \times 10^{13} \text{ s}^{-1}$ . The dimensionless length of the crystal adopted in figures 1–3 is  $5000^{1/2}$ .

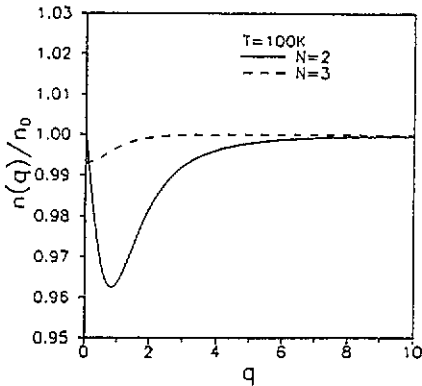
The difference  $E(N, T) - E(N, 0)$  between the polaron energies at a finite temperature and at zero temperature as a function of the electron–phonon coupling constant  $\alpha$  is given in figure 1. The following points are shown.



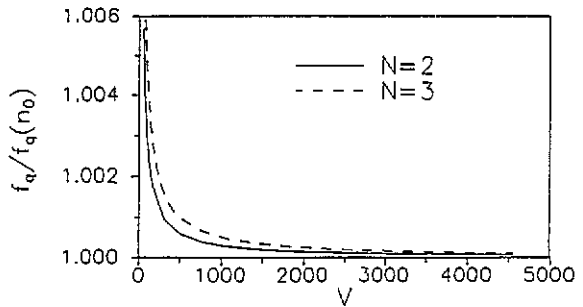
**Figure 1.** The difference  $E(N, T) - E(N, 0)$  between the polaron energy at a finite temperature and that at zero temperature as a function of the electron-phonon coupling constant  $\alpha$ .



**Figure 2.** The ratio  $m^*(N, T)/m^*(N, 0)$  of the polaron effective mass at a finite temperature to that at zero temperature as a function of the electron-phonon coupling constant  $\alpha$ .



**Figure 3.** The ratio  $n(q)/n_0$  of the thermophonon number obtained by numerical computation to that obtained by analytical approximation as a function of the wavevector magnitude  $q$ .



**Figure 4.** Displacement amplitude ratio  $f_q/f_q(n_0)$  of the thermophonon number obtained by numerical computation to that obtained from the analytical expression as a function of the crystal volume  $V$ .

(1) The polaron energy at a finite temperature is higher than that at zero temperature. This is physically obvious because the thermophonons cause the self-trapping of the polaron to become 'shallow'.

(2) The temperature effect of the polaron diminishes with decreasing electron-phonon coupling constant  $\alpha$ .

(3) The difference between the polaron energies at a finite temperature and at zero temperature decreases with increasing dimensionality. This indicates that the temperature effect of the polaron energy with higher dimensions is weaker.

Figure 2 gives the relation between the ratio  $m^*(N, T)/m^*(N, 0)$  of the polaron effective mass at a finite temperature to that at zero temperature as a function of the electron-phonon coupling constant  $\alpha$ . It can be seen that the ratio is much nearer to unity for higher dimensions. The temperature effect on the polaron effective mass also becomes increasingly

weaker with increasing dimensionality. It is shown from the previous results that the temperature effect of the polaron drastically diminishes with increasing dimensionality.

In equation (10), the displacement amplitude  $f_q$  is proportional to  $V^{1/2}$ . We have computed the thermophonon number  $n(q)$  and  $f_q$  for a dimensionless length of the crystal of  $500^{1/2}$  when  $N = 2, 3$  to compare the analytical expressions (18) and (19) with the exact numerical results. Figure 3 gives the ratio of the numerically computed thermophonon number  $n(q)$  to that of the Bose approximation  $n_0$  as a function of the wavevector magnitude  $q$  for  $N = 2, 3$ . The deviation of  $n(q)$  from  $n_0$  can be omitted for lower  $q$ , although a minimum occurs at a certain  $q$ , namely  $q_c$  (for  $N = 2$  and  $3$ ,  $q_c \simeq 0.8$  and  $10^{-4}$ , respectively).

The ratio of the thermophonon displacement amplitude  $f_q$  (the numerical results) to  $f_q(n_0)$  (given by the Bose approximation) as a function of the volume of the crystal is shown in figure 4. On increase in the crystal volume, the deviation decreases so rapidly that it can be neglected at large  $V$ . The size range of the crystal is usually much larger than that of the polaron; therefore it is suitable to describe the polaron properties with the simple expressions (equations (18) and (19)) derived using the Bose approximation.

Comparing  $E_B(N, T)$  and  $m_B^*(N, T)$  with the corresponding values for  $N = 3$ , at a finite temperature, we obtain the same scaling relations as derived by Sil and Chatterjee [5] at zero temperature:

$$E_B^{ND} = \frac{1}{3} N E_B^{3D} \{ \alpha 3 \sqrt{\pi} \Gamma[\frac{1}{2}(N-1)] / 2N \Gamma(\frac{1}{2}N) \}$$

and

$$m_B^{*ND} = m_B^{*3D} \{ \alpha 3 \sqrt{\pi} \Gamma[\frac{1}{2}(N-1)] / 2N \Gamma(\frac{1}{2}N) \}$$

where  $E_B^{ND}$  and  $m_B^{*ND}$  represent the  $N$ -dimensional polaron energy and effective mass, and  $E_B^{3D}$  and  $m_B^{*3D}$  are the corresponding values in three dimensions. The subscript B indicates that the Bose distribution approximation has been adopted. It can be concluded from equations (18) and (19) that the temperature effect of the polaron drastically diminishes on increase in the dimensionality.

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