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# A study of the polaronic band width and the small-to-large-polaron transition in a many-polaron system

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**Abstract.** A short-range electron–phonon (e–ph) interaction is considered in a many-electron narrow-band system where electron hopping is comparable with the phonon frequency. The behaviour of the polarons as a function of the e–ph interaction strength and the electron concentration is studied within the framework of the mean-field theory using a modified Lang–Firsov transformation and two-phonon coherent states of the phonon subsystem. The small-to-large-polaron transition and the effect of the two-phonon coherent state are discussed.

## 1. Introduction

In the presence of an electron–phonon (e–ph) interaction an electron couples with phonons to form a polaron, composed of the original electron dressed with the phonon cloud that moves along with the electron [1, 2]. The nature of polarons, for short-range e–ph coupling, depends mainly on three quantities: the intersite transfer energy of the electron, the e–ph coupling energy and the frequency of the phonons. In the adiabatic case (the phonon frequency  $\omega_0$  is small compared with the electronic band width) a small polaron with a thick phonon cloud is formed for large e–ph coupling. The band width of the small polaron is reduced exponentially by the Lang–Firsov [2] factor, and thus the polarons appear to be very heavy. For weak e–ph coupling the electron is almost bare with only a very thin phonon cloud extending over a wide region [3, 4]. Within the adiabatic limit, Toyozawa [3], Shinozuka and Toyozawa [4] and Emin [5] obtained a discontinuous jump in the polaronic effective mass at a critical e–ph coupling strength [3–5]. However, Löwen [6] showed that there is no abrupt (discontinuous) phase transition in the ground state of an e–ph system, described by a generalized Holstein Hamiltonian, for a finite phonon frequency as the e–ph coupling increases. In the non-adiabatic limit (very large  $\omega_0$ ) the phonons can follow the electron instantaneously and the corresponding polaron is a small polaron with no mass enhancement [7]. Both in the adiabatic and in the non-adiabatic limit a number of investigations [3–5, 7, 8] have been carried out; however, in the intermediate regime (finite phonon frequency), where quantum lattice fluctuations may play an important role, a few studies have been made, particularly for a many-polaron system [7–9].

The study of many-polaron systems has attracted renewed interest in the context of the high- $T_c$  oxide superconductors [10–15]. For a many-polaron system, Hang [16] pointed out that a two-phonon coherent state for the phonon subsystem corresponds to the ground state of the system and has an important effect in reducing the effective mass of polarons. We studied the significance of the two-phonon coherent state in the strong-correlation limit and its implication in understanding the properties of the high- $T_c$  systems [14]. In [14, 16] the Lang–Firsov transformation, which diagonalizes the e–ph interaction terms completely, has

been used. However, in that method the lattice deformations, which may be produced at different sites around the charge carrier, cannot be treated as variational parameters and this restricts study of the nature of the polarons.

The present work aims to study the nature of polarons in a many-polaron system as a function of the e-ph coupling strength and the electron density for the intermediate regime (finite phonon frequency). We consider a short-range e-ph interaction, but the lattice deformations at different sites around the electron are treated as variational parameters. The role of the two-phonon coherent state is also studied. We observe that the lattice deformation may spread over a wider region in a suitable parameter space even for a short-range interaction. In a narrow region of e-ph coupling an interesting variation in the polaronic effective mass with the electron concentration is observed. The polaronic effective mass is very high for both a nearly empty and an almost filled band, whereas it is much lower in the intermediate electron concentrations. In section 2 the variational ground-state energy of a many-polaron system is determined using suitable phonon states and the mean-field approximation. The results of the numerical calculations and its implication are discussed in section 3.

## 2. Formulation

To describe a many-polaron system we consider a tight-binding Hamiltonian in the presence of a (local) e-ph interaction which is expected to capture the main features of the physics of lattice fermions coupling with a boson mode. The corresponding Hamiltonian includes the nearest-neighbour hopping  $t_{ij}$ , e-ph interaction  $g_1$  and an on-site repulsion  $U$  between electrons of different spins. The model Hamiltonian for such an interacting system is written

$$H = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + g_1 \sum_{i,\sigma} n_{i\sigma} (b_i + b_i^+) + \omega_0 \sum_i b_i^+ b_i \quad (1)$$

where  $c_{i\sigma}^+$  and  $c_{i\sigma}$  are the creation and annihilation operators, respectively, for an electron at site  $i$  with spin  $\sigma$ ,  $b_i^+$  and  $b_i$  are the creation and annihilation operators, respectively, for the phonons which are assumed to be dispersionless, and  $\omega_0$  represents the frequency of the phonon system.

In the presence of large e-ph coupling, the lattice would be deformed around an electron, forming a polaron. To study the spread and the depth of the lattice deformations around the electron we apply the modified Lang-Firsov transformation [3-5] to the Hamiltonian  $H$ :

$$\begin{aligned} \tilde{H} = \exp(R) H \exp(-R) = & - \sum_{i,j,\sigma} t_{ij} \exp(Y_i - Y_j) c_{i\sigma}^+ c_{j\sigma} - \epsilon_p \sum_{i,\sigma} n_{i\sigma} - V_1 \sum_{i,j} n_i n_j \\ & + V_2 \sum_{i,\delta+\delta' \neq 0} n_{i+\delta} n_{i+\delta'} + U_{\text{eff}} \sum_i n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_i b_i^+ b_i + V_{\text{pol-ph}} \end{aligned} \quad (2)$$

where

$$R = \sum_i \left( \bar{\lambda}_1 n_i (b_i^+ - b_i) + \bar{\lambda}_2 \sum_{\delta} n_i (b_{i+\delta}^+ - b_{i+\delta}) \right) \quad \bar{\lambda}_1 = \lambda_1/\omega_0 \quad \bar{\lambda}_2 = \lambda_2/\omega_0 \quad (3)$$

$\delta$  is a nearest-neighbour vector,

$$Y_i = \bar{\lambda}_1(b_i^+ - b_i) + \bar{\lambda}_2 \sum_{\delta} (b_{i+\delta}^+ - b_{i+\delta}) \tag{4}$$

$$\varepsilon_P = (2g_1 - \lambda_1)\bar{\lambda}_1 - z\lambda_2\bar{\lambda}_2 \quad (z \text{ is the coordination number}) \tag{5}$$

$$V_1 = 2(g_1 - \lambda_1)\bar{\lambda}_2 \tag{6}$$

$$U_{\text{eff}} = U - 2[(2g_1 - \lambda_1)\bar{\lambda}_1 - z\lambda_2\bar{\lambda}_2] \tag{7}$$

$$V_2 = \lambda_2\bar{\lambda}_2 \tag{8}$$

$$V_{\text{pol-ph}} = \sum_i (g_1 - \lambda_1)(b_i + b_i^+)n_i - \sum_{i,\delta} \lambda_2(b_{i+\delta} + b_{i+\delta}^+)n_i \tag{9}$$

Here  $\varepsilon_P$  is the polaron self-energy,  $V_1$  is the attractive interaction between nearest-neighbour polarons, induced by the e-ph coupling,  $V_2$  is the interaction between next-nearest-neighbour polarons,  $U_{\text{eff}}$  is the effective on-site interaction and  $V_{\text{pol-ph}}$  represents the polaron-phonon interaction.

$\bar{\lambda}_1 (= \lambda_1/\omega_0)$  and  $\bar{\lambda}_2 (= \lambda_2/\omega_0)$  are the lattice displacements, created around an electron at the same site and nearest-neighbour sites, respectively, which move along with the electron. When  $\lambda_1 = g_1$  and  $\lambda_2 = 0$ , the transformation  $\exp(-R)$  is exactly the Lang-Firsov [2] transformation. In this transformation, one diagonalizes the terms corresponding to the e-ph interaction but hopping terms are treated as perturbation [17]. If the hopping part is not sufficiently small, one would look for a better phonon wavefunction. Here we treat  $\lambda_1$  and  $\lambda_2$  as variational parameters and use a two-phonon coherent state  $|\psi_{\text{ph}}\rangle = \exp[\alpha \sum_i (b_i b_i - b_i^+ b_i^+)]|0\rangle$  as a trial wavefunction for the new phonon (the equilibrium position is displaced with respect to the original phonons) state.  $\alpha$  is a variational parameter. To obtain an effective polaronic Hamiltonian we take the average of  $\tilde{H}$  over the two-phonon coherent state:

$$H_{\text{eff}} = \langle \psi_{\text{ph}} | \tilde{H} | \psi_{\text{ph}} \rangle \tag{10}$$

$$\begin{aligned} &= -t \sum_{i,j,\sigma} c_{i\sigma}^+ c_{j\sigma} \exp[-\bar{\lambda}^2 \exp(-4\alpha)] - \varepsilon_P \sum_i n_i - V_1 \sum_{i,j} n_i n_j \\ &+ V_2 \sum_{i,\delta+\delta' \neq 0} n_{i+\delta} n_{i+\delta'} + U_{\text{eff}} \sum_i n_{i\uparrow} n_{i\downarrow} + N\omega_0 \sinh^2 \alpha \end{aligned} \tag{11}$$

where

$$\begin{aligned} t &= t_{ij} \\ \bar{\lambda}^2 &= (\bar{\lambda}_1 - \bar{\lambda}_2)^2 + (z-1)\bar{\lambda}_2^2 \end{aligned} \tag{12}$$

and  $N$  is the total number of sites in the system. As  $\alpha$  increases, the energy of the phonon subsystem increases; however, the polaronic narrowing effect in the band width is reduced and, consequently, the kinetic energy of the polaron increases [14, 16]. So a proper choice of  $\alpha$  can minimize the ground-state energy of the system. Now we calculate the ground-state energy of the many-polaron system (11) in the framework of the mean-field theory. Within the mean-field approximation the Hamiltonian (11) shows different kinds of ordering, e.g. a charge-density wave (CDW), a spin-density wave or superconductivity, depending on the

values of  $V_1$ ,  $V_2$  and  $U_{\text{eff}}$  and the number of the polarons in the system [9–15]. However, a CDW appears in the system for  $U_{\text{eff}} < 0$ , i.e. when the effective on-site interaction is attractive. Here we shall restrict our considerations to the case of a positive but small  $U_{\text{eff}}$ . Therefore our system does not provide any CDW ordering. A detailed study of the magnetic phase diagram for a single-band Hubbard model (with positive  $U$ ) has been made by several groups within the framework of mean-field theory [18–20]. It is found that the magnetic state appears in the neighbourhood of  $n = 1$  and, for a large region of electron concentrations  $0 < n < 0.75$  and  $1.25 < n < 2$ , the state is paramagnetic. In this study we focus our attention on the effect of the e-ph interactions in a Hubbard system for electron concentrations away from  $n = 1$ , where the ground state is paramagnetic. We shall evaluate the ground-state energy in the absence of any ordering. In the framework of the Hartree-Fock approximation the terms corresponding to  $n_{i\uparrow}n_{i\downarrow}$  and  $n_i n_j$  are approximated as

$$\begin{aligned} n_{i\uparrow}n_{i\downarrow} &= n_{i\uparrow}\langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle n_{i\downarrow} - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \\ n_i n_j &= n_i \langle n_j \rangle + \langle n_i \rangle n_j - \langle n_i \rangle \langle n_j \rangle \end{aligned} \quad (13)$$

and the ground-state energy per site is, then, obtained as

$$(1/N)E_g = -2t_c z p - \varepsilon_p n - V_1 z n^2 - V_2 z' n^2 + \frac{1}{4}U_{\text{eff}}n^2 + \omega_0 \sinh^2(2\alpha) \quad (14)$$

where

$$t_c = t \exp[-\bar{\lambda}^2 \exp(-4\alpha)] \quad (15)$$

$n = (1/N) \sum_i \langle n_i \rangle$  is the number of electrons per site in the system

$$p = \langle c_{i\sigma}^+ c_{j\sigma} \rangle = \frac{1}{Nz} \sum_q \gamma_q \langle c_{q\sigma}^+ c_{q\sigma} \rangle \quad (16)$$

$$\begin{aligned} z' &= \sum_{\delta+\delta' \neq 0} 1 \\ \gamma_q &= \sum_j \exp[iq \cdot (R_i - R_j)] \end{aligned} \quad (17)$$

and

$$\langle c_{q\sigma}^+ c_{q\sigma} \rangle = 1 / \{ \exp[\beta(\xi_q - \mu)] + 1 \} \quad (18)$$

where  $\xi_q (= -t\gamma_q)$  is the quasi-particle energy,  $\mu$  is the chemical potential and  $\beta = 1/k_B T$ . At  $T = 0$ ,

$$\langle c_{q\sigma}^+ c_{q\sigma} \rangle = \theta(\mu - \xi_q).$$

Hence

$$p = \frac{1}{Nz} \sum_q \gamma_q \theta(\mu - \xi_q). \quad (19)$$

For simplicity we shall calculate  $p$  using a square density of states:

$$\rho(\xi_q) = \begin{cases} 1/2W & \text{if } -W < \xi_q < W \\ 0 & \text{otherwise.} \end{cases} \quad (20)$$

$W(=zt)$  is the band half-width. The hopping energy at  $T=0$  is then obtained as

$$p = \frac{1}{4}(2n - n^2). \quad (21)$$

Substituting the value of  $p$  in equation (14) the ground-state energy of the system with a square density of states is obtained as

$$E_g/N = -\frac{1}{2}(2n - n^2)zt_c - \varepsilon_p n - V_1 z n^2 + V_2 z' n^2 + \frac{1}{4}U_{\text{eff}} n^2 + \omega_0 \sinh^2(2\alpha). \quad (22)$$

The variational parameters  $\lambda_1$ ,  $\lambda_2$  and  $\alpha$  are determined from the minimization conditions of the ground-state energy. For numerical calculations we consider a square lattice with  $z=4$  and  $z'=12$ .

### 3. Results and discussion

In this section we discuss the results of our numerical calculations. It emerges that the variational parameters  $\lambda_1$  and  $\lambda_2$ , characterizing the deformations around the charge carrier, and  $\alpha$ , the two-phonon coherent state parameter, have a marked dependence on the hopping parameter  $t$ , the e-ph coupling  $g_1$  and the electron density  $n$ . We present the results for two values of the hopping parameter  $\bar{t} = t/\omega_0 = 2$  and 0.5 which are in the crossover region between the adiabatic (small- $\omega_0$ ) limit and the non-adiabatic (large- $\omega_0$ ) limit. For  $\bar{t} = 2.0$ , the variations in the quantities  $\lambda_1$ ,  $\lambda_2$  and  $t_c$  with  $\bar{g}_1 (= g_1/\omega_0)$  are shown in figures 1, 2 and 3, respectively, for two different electron concentrations  $n = 0.3$  and 0.05. It is clear from figures 1–3 that a sharp transition occurs from small polarons to large polarons at  $g_1 = g_c$  as  $g_1$  decreases from a large value. When  $g_1 > g_c$  we find that  $\lambda_1/g_1 = 1$  and  $\lambda_2 = 0$  which indicates that the phonon cloud around the charge carrier is confined to a single site where the electron resides; thus the polarons are small polarons. In this region the squeezing parameter  $\alpha = 0$  and a large Holstein reduction factor makes the effective polaronic hopping very small ( $t_e \leq 10^{-6}t$ ). At  $g_1 = g_c$ ,  $\lambda_1/g_1$  reduces drastically from 1 and  $\lambda_2/\lambda_1$  develops abruptly, which indicate that the phonon cloud becomes thin and spreads over a wider region as  $g_1$  decreases from  $g_c$ . For  $g_1 < g_c$  the corresponding polaronic hopping ( $t_e$ ) is of the order of the bare hopping ( $t$ ). It is evident from figures 1–3 that  $g_c$ , the small-to-large-polaron transition point, shifts towards smaller values as the electron concentration  $n$  decreases from 0.3 to 0.05. In figures 4, 5 and 6 we plot the variations in  $\lambda_1$ ,  $\lambda_2$  and  $t_c$ , respectively, with  $\bar{g}_1$  for  $\bar{t} = 0.5$  and for electron concentrations  $n = 0.3$  and 0.05. For  $\bar{t} = 0.5$ , a transition from small polarons to large polarons is also observed as  $g_1$  decreases from a large value. However, the transition occurs at a lower value of  $g_1$  and is not as sharp as for  $\bar{t} = 2$ . In fact the transition for  $\bar{t} = 0.5$  is continuous. It is seen that the abrupt changes in  $\lambda_1$ ,  $\lambda_2$  and  $\alpha$ , as observed for large  $\bar{t}$ -values, are reduced with decreasing  $\bar{t}$  and the transition becomes continuous below a certain value of  $\bar{t}$ . Similar conclusions have also been obtained in some previous studies [3–5, 7].

In figure 7 we plot the variation in the two-phonon coherent state parameter  $\alpha$  with  $g_1$  for different  $\bar{t}$ -values of 2.0 and 0.5 and electron concentrations  $n = 0.3$  and 0.05. It is seen from figure 7 that  $\alpha$ , which is zero for  $g_1 = 0$ , increases with increasing  $g_1$ , reaches a

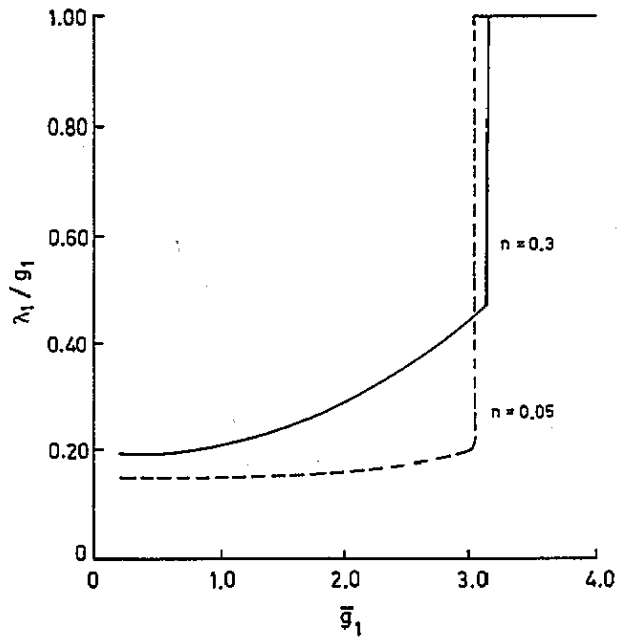


Figure 1. Variation in  $\lambda_1/g_1$  with the e-ph coupling strength  $\bar{g}_1$  ( $= g_1/\omega_0$ ) for electron concentrations  $n = 0.3$  (—) and  $0.05$  (----).  $\bar{\tau} = t/\omega_0 = 2.0$ .

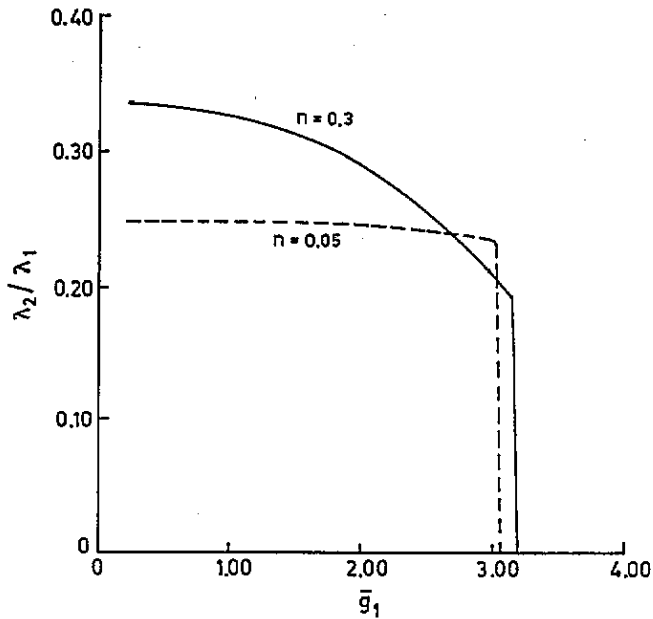


Figure 2. Variation in  $\lambda_2/\lambda_1$  with e-ph coupling strength  $\bar{g}_1$  ( $= g_1/\omega_0$ ) for electron concentrations  $n = 0.3$  (—) and  $n = 0.05$  (----).  $\bar{\tau} = t/\omega_0 = 2.0$ .

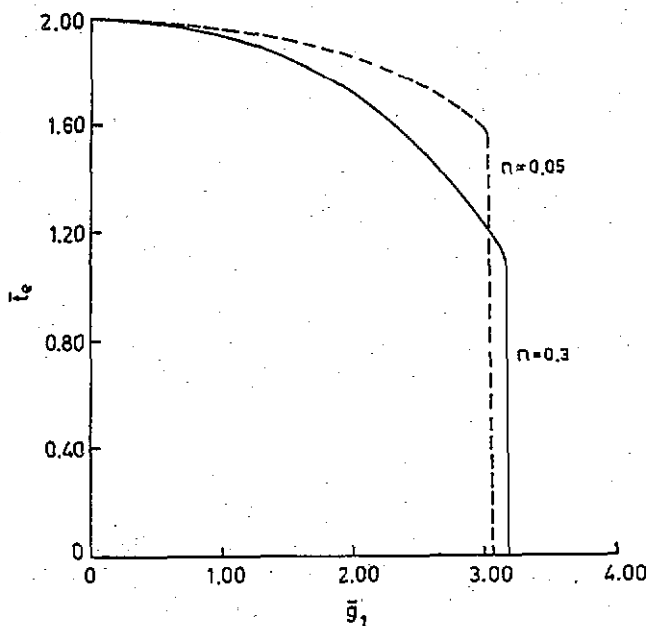


Figure 3. Variation in  $\bar{t}_e$  ( $= t_e/\omega_0$ ) with e-ph coupling strength  $\bar{g}_1$  ( $= g_1/\omega_0$ ) for electron concentrations  $n = 0.3$  (—) and  $n = 0.05$  (----).  $\bar{t} = t/\omega_0 = 2.0$ .

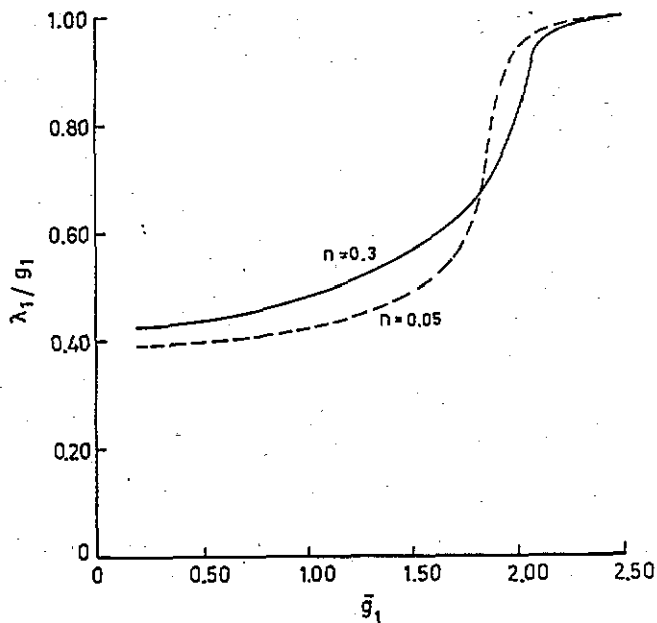


Figure 4. Variation in  $\lambda_1/g_1$  with  $\bar{g}_1$  ( $= g_1/\omega_0$ ) for  $n = 0.3$  (—) and  $0.05$  (----).  $\bar{t} = t/\omega_0 = 0.5$ .



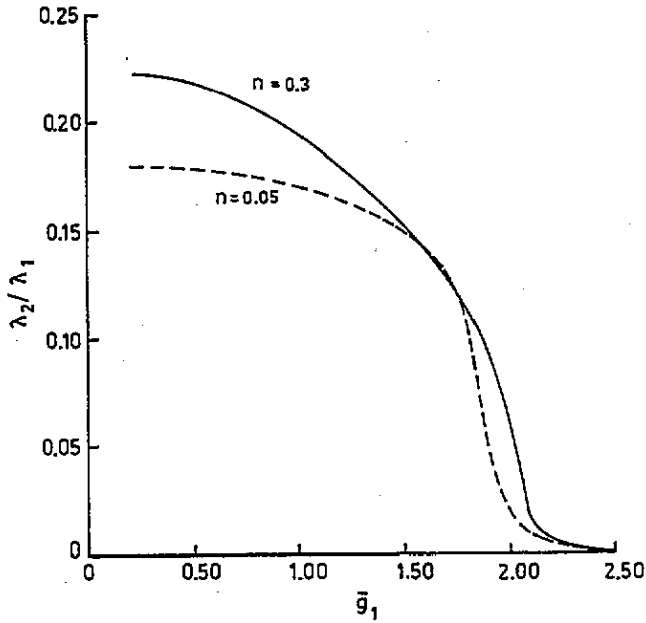


Figure 5. Variation in  $\lambda_2/\lambda_1$  with  $\bar{g}_1$  ( $= g_1/\omega_0$ ) for  $n = 0.3$  (—) and  $0.05$  (---).  $\bar{t} = t/\omega_0 = 0.5$ .

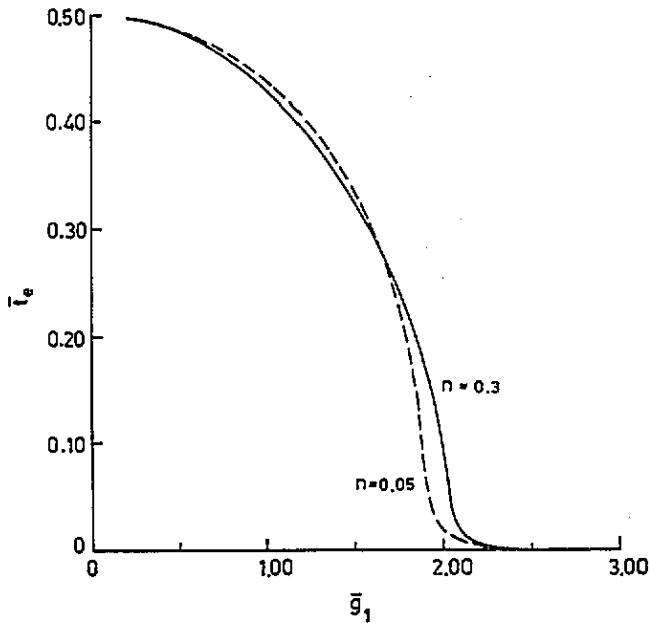


Figure 6. Variation in  $\bar{t}_e$  ( $= t_e/\omega_0$ ) with  $\bar{g}_1$  ( $= g_1/\omega_0$ ) for  $n = 0.3$  (—) and  $0.05$  (---).  $\bar{t} = t/\omega_0 = 0.5$ .

maximum and then decreases rapidly as the transition from large polarons to small polarons occurs. For  $\bar{t} = 2.0$  the transition is discontinuous and  $\alpha$  goes abruptly to zero in the small-polaron regime; for  $\bar{t} = 0.5$ ,  $\alpha$  decreases continuously and becomes zero for large  $g_1$ .  $\alpha$  is smaller for  $n = 0.05$  than for  $n = 0.3$  (figure 7). To investigate the role of the two-phonon coherent state we compare the results for two variational states of the phonon subsystem: one of these is just the displaced oscillator state,  $\exp(-R)|0\rangle$  and the other is the squeezed phonon state defined as  $\exp(-R)\exp(-S)|0\rangle$ . The variation in  $\lambda_1/g_1$  and  $t_e/t$  with  $g_1$  for the above-mentioned two variational states of the phonon subsystem ( $\alpha = 0$  and  $\alpha \neq 0$ ) are shown in figure 8 for  $n = 0.3$  and  $\bar{t} = 0.5$ . It is evident from figure 8 that the effect of the two-phonon coherent state is negligible for strong as well as weak e-ph couplings but the role of the two-phonon coherent state becomes significant in the intermediate range of  $g_1$ . It is also seen from figure 8 that consideration of the two-phonon coherent state shifts the value of  $g_c$  to a higher value. For  $n = 0.05$  the distinction between the  $\alpha = 0$  and  $\alpha \neq 0$  curves is very small (not shown in figure), implying that the effect of the two-phonon coherent state is not appreciable for smaller numbers of electrons.

We have also investigated the variation in the quantities  $\lambda_1$ ,  $\lambda_2$  and  $t_e$  with fermion concentration  $n$  for a constant value of  $g_1$ . In figure 9 we present plots of  $\lambda_1/g_1$  and  $\lambda_2/\lambda_1$  and in figure 10 of  $t_e/t$  versus  $n$  for  $\bar{t} = 0.5$  and  $\bar{g}_1 = 2.0$ .  $\lambda_1/g_1$  is about 1 and  $\lambda_2/\lambda_1$  is very small for low as well as high densities of electrons. As the electron concentration increases from  $n = 0$ ,  $\lambda_1$  decreases while  $\lambda_2$  increases; thus the phonon cloud around the electron becomes thinner while its size becomes larger with increasing number of electrons. In the intermediate range of electron concentrations ( $0.4 < n < 1.6$ ),  $\lambda_1$  and  $\lambda_2$  show an almost constant value and then, at higher values of  $n$ ,  $\lambda_1$  increases while  $\lambda_2$  decreases with increasing  $n$ . The curves are symmetric around  $n = 1$ . Correspondingly the effective polaron hopping is very small ( $t_e/t = 0.03$ ) for very low and high densities of electrons while it has a value an order of magnitude higher in the intermediate range of electron concentrations (figure 10). It is also seen from figures 9 and 10 that  $\lambda_1$ ,  $\lambda_2$  and  $t_e$  change rapidly in a narrow range of electron concentrations (around  $n \simeq 0.25$ ). It should be mentioned, however, that such a rapid change in  $\lambda_1$ ,  $\lambda_2$  and  $t_e$  with electron concentration occurs only for a narrow range of  $g_1$ . In figure 10 we also plot the variation in  $t_e$  with  $n$  for different  $g_1$ -values for  $\bar{t} = 0.5$ . It is seen that the curves for  $\bar{g}_1 = 2.0$  and 2.1 are of a similar nature. With increasing value of  $g_1$  the narrow band region spreads at the expense of the wide region. For  $\bar{g}_1 = 2.2$  the whole region of  $n$  corresponds to a narrow band while for  $\bar{g}_1 = 1.8$  the whole region of  $n$  corresponds to a wide band. For these values of  $g_1$  no abrupt change in  $t_e$  is observed. Thus a rapid change in  $t_e$  with electron concentration may be experimentally observed if the e-ph interaction strength lies in a narrow region. In this narrow range of e-ph couplings, the effective mass of the polarons is very high for low and high electron densities whereas the effective mass is much lighter for an intermediate electron concentration.

It may be mentioned that in figures 9 and 10 we have plotted the curves in the electron concentration range  $0.75 < n < 1.25$  also. For this region of electron concentrations a single-band Hubbard model may exhibit magnetic ordering and our results obtained using a paramagnetic state may not be valid for general values of  $U$ ,  $t$  and  $g_1$ . However, our main interest is the occurrence of sudden changes in the polaronic properties. For  $\bar{g}_1 = 2.0$  and 2.1 the transition from small polarons to large polarons occurs at carrier concentrations which lie away from the range  $0.75 < n < 1.25$ . Thus our main results would not be affected by possible magnetic ordering in the system. Furthermore in this range of electron concentrations the polarons are large polarons (for  $\bar{g}_1 < 2.1$ ) and a small range of bare  $U$ -values exists for which  $U_{\text{eff}} < t_{\text{eff}}$  and the paramagnetic state prevails almost in the entire

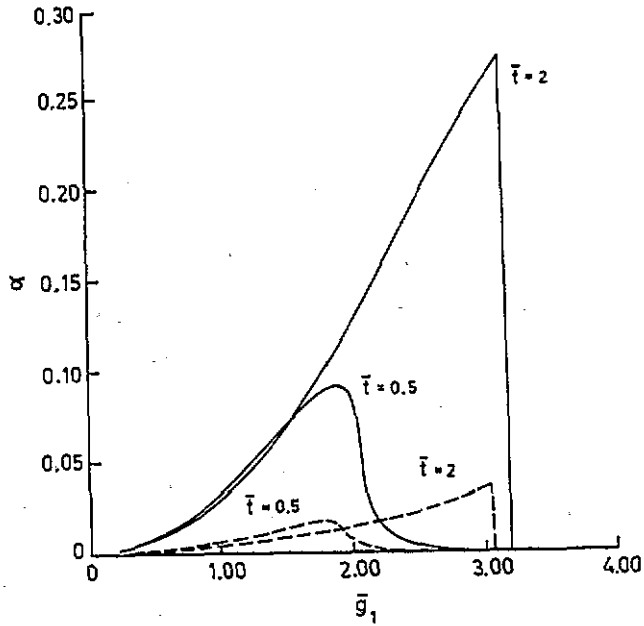


Figure 7. Variation in the two-phonon coherent state parameter  $\alpha$  with  $\bar{g}_1 (= g_1/\omega_0)$  for different hopping  $\bar{i} (= t/\omega_0) = 2.0$  and  $0.5$  and electron concentrations  $n = 0.3$  (—) and  $0.05$  (---).

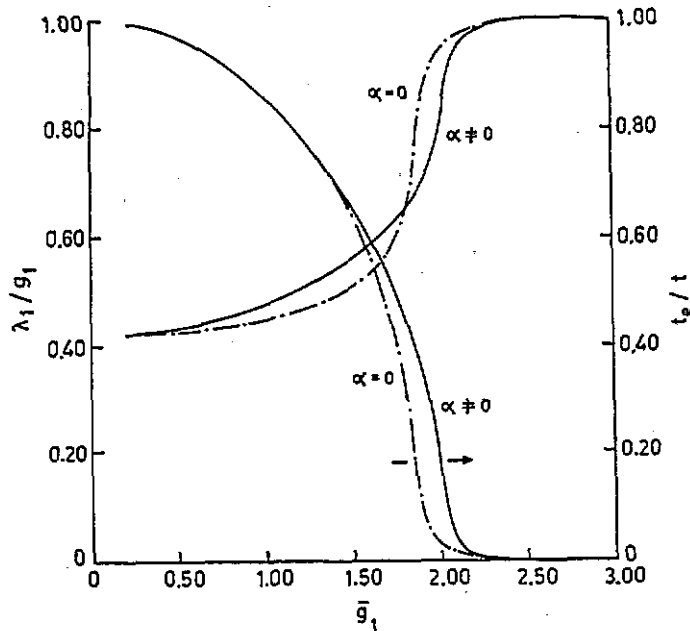


Figure 8. Variation in  $\lambda_1/g_1$  and  $t_e/t$  with  $\bar{g}_1 (= g_1/\omega_0)$  for two different phonon states: one with  $\alpha = 0$  (---) and, for the other,  $\alpha$  is solved self-consistently (—).

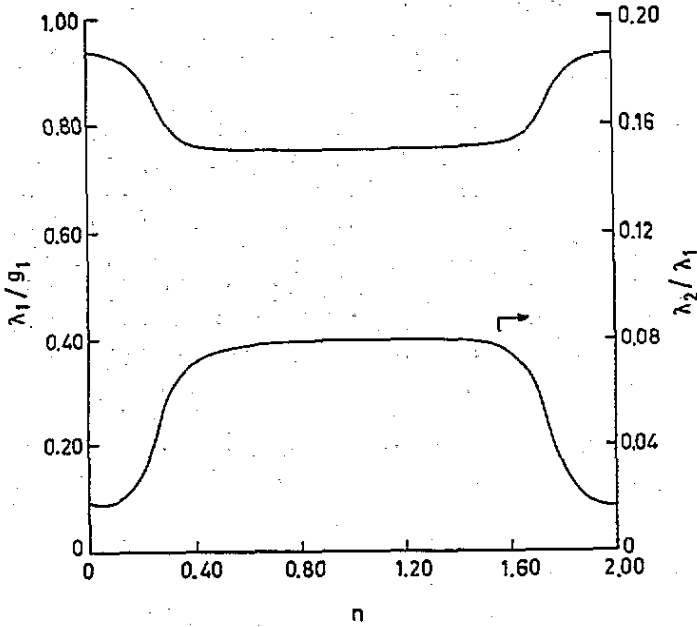


Figure 9. Variation in  $\lambda_1/g_1$  and  $\lambda_2/\lambda_1$  with  $n$  for  $\bar{g}_1 (= g_1/\omega_0) = 2.0$  and  $\bar{r} = t/\omega_0 = 0.5$ .

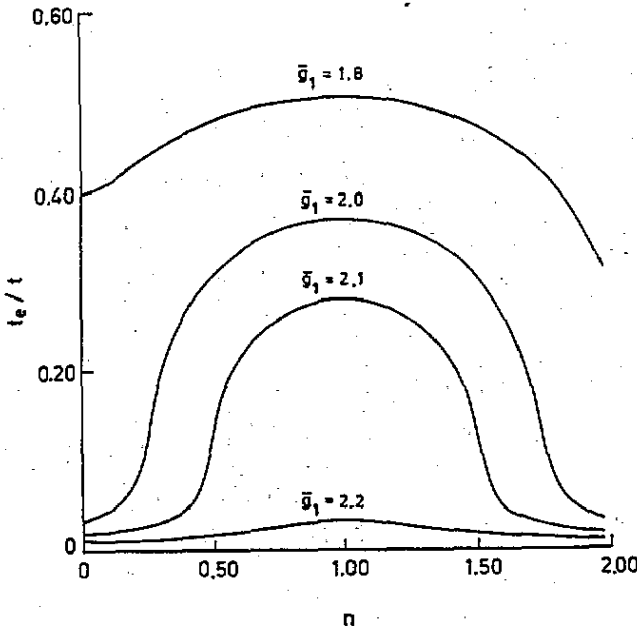


Figure 10. Variation in  $t_e/t$  with  $n$  for different  $\bar{g}_1 (= g_1/\omega_0)$  and  $\bar{r} = t/\omega_0 = 0.5$ .

range of electron concentrations excluding  $n = 1$ . For this restricted range of  $U$  the results in figures 9 and 10 would be valid in almost the entire range of  $n$ .

Finally we should mention some limitations of our calculation. We have considered lattice distortions only up to the nearest-neighbour site of the charge carrier. Although for large polarons the lattice distortion may extend up to distant neighbouring sites such as second, third and fourth, even the e-ph interaction has a very short range (confined to within the electron residing site). Considerations of such distant neighbour lattice distortions as variational parameters should reduce the amount of discontinuity in  $\lambda_1$ ,  $\lambda_2$  or  $\alpha$ , as observed for large  $t$ -values at  $g_c$ . In fact, Löwen [6] showed that the ground state of an e-ph system does not exhibit a discontinuous transition for finite  $\omega_0$  as e-ph coupling increases. He pointed out that the discontinuous transition beyond a critical e-ph coupling as obtained in previous mean-field studies [3–5] are due to the approximations involved and are directly connected with the adiabatic limit. The abrupt or discontinuous jump observed in the present study in a certain parameter space may be a consequence of an insufficient number of variational parameters used.

For small  $t$ -values we obtain continuous transitions. In this parameter region the inclusion of distant lattice distortions would not change the qualitative behaviour of the results and the corresponding quantitative corrections would be very small as long as  $\lambda_2/\lambda_1$  is small.

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