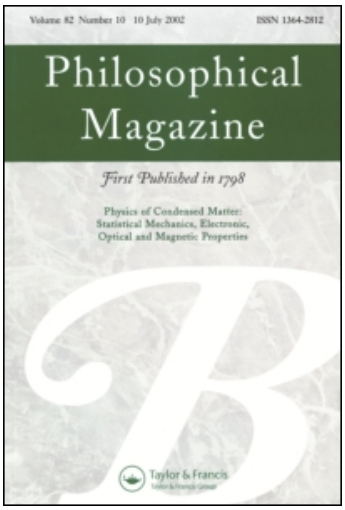

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Small-polaron variable-range hopping in quasi-two- dimensional materials: Application to $PrBa_2Cu_{3-x}Ga_xO_{7-y}$

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Small-polaron variable-range hopping in quasi-two-dimensional materials: application to $PrBa_2Cu_{3-x}Ga_xO_{7-y}$

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ABSTRACT

We have developed a theory for variable-range hopping (VRH) due to small polarons in quasi-two-dimensional systems at high temperatures. We included the effects of temperature, electric fields, magnetic fields and scattering in the derivation of the conductivity. We found that the conductivity for quasi-two-dimensional systems depends on these factors differently from three-dimensional systems. We applied the theory to explain the resistivity data of $PrBa_2Cu_{3-x}Ga_xO_{7-y}$ at high temperatures ($T > 150\,K$). To explain the low-temperature data ($T < 150\,K$), we used the pure electron VRH mechanisms. Good agreement between theory and experiment was found.

§ 1. INTRODUCTION

Since the discovery of high-temperature superconductivity, there has been considerable interest in the transport properties of the 123 compound $PrBa_2Cu_3O_{7-y}$ (PBCO) (Kabasawa *et al.* 1992, 1993, Xu and Guan 1993, Triberis *et al.* 1994, Singh *et al.* 1994 a,b, van Ancum *et al.* 1995 a,b, Singh and Thompson 1996, Thompson and Singh 1997). It is very similar to the popular $YBa_2Cu_3O_{7-y}$ superconductor but remains non-superconducting at all temperatures. This makes it very useful in superconducting junction technologies such as superconductor–normal metal–superconductor junctions. Also, the unique non-superconducting property of PBCO among the 123 oxide compounds lends insight into the nature of high-temperature conductivity. For these reasons, a thorough understanding of the transport properties of PBCO is essential for both technological and scientific reasons.

Recently Xu and Guan (1993) measured the resistivity of a PBCO polycrystalline ceramic material doped with Ga. They replaced Cu^{2+} by Ga^{3+} in PBCO samples and found a compound which is denoted as $PrBa_2Ca_{3-x}Ga_xO_{7-y}$ (PBCGO). The Ga concentration x was varied from 0.0 to 0.6. They found that the resistivity of PBCGO increases with increase in the doping parameter x. The resistivity is very sensitive to the Ga concentration at low temperatures ($T < 150\,K$) and is less sensitive to doping at high temperatures ($T > 150\,K$). At constant temperature the resistivity increases monotonically with increasing doping of Ga. This is in contrast with conventional doped semiconductors whose resistivity decreases with increase in the impurity concentration. They considered the PBCGO compound as a compensated semiconductor and tried to fit their low-temperature data by using the Mott type (Mott and Davis 1971) of variable-range hopping (VRH) mechanism. According to Mott, the logarithm of resistivity has a $T^{-1/4}$ power law. On the other hand, they

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tried to fit their high-temperature data by using the nearest-neighbour hopping mechanism which gives a T^{-1} power law for the resistivity. They had problems fitting their experiments with these mechanisms especially at high temperatures. They suggested that the conduction of carriers in these compounds at high temperatures may be due to band conduction, next-neighbour hopping or a more complicated form of VRH.

Triberis *et al.* (1994) have tried to explain the experimental data of Xu and Guan by using their three-dimensional small-polaron hopping model. They assumed that small polarons are formed in the PBCGO compounds owing to strong electron–phonon interactions. The polarons hop from one localized state to another by emitting and absorbing phonons. They derived an expression for the resistivity using percolation arguments. They found that at low temperatures the logarithm of conductivity has a $T^{-1/4}$ power law dependence whereas the logarithm of conductivity has a $T^{-2/5}$ power law for high temperatures. Their low-temperature expression of conductivity has the same form as the Mott expression for electron hopping. They tried to fit the high-temperature data by using the $T^{-2/5}$ power law and the low-temperature data by the $T^{-1/4}$ power law. They concluded that polaron hopping is responsible for both the low- and the high-temperature resistivity. Since polarons and electrons have the same power-law dependence for the resistivity at low temperatures, it is difficult to say that polaron hopping is responsible for the resistivity in PBCO materials at those temperatures.

Note that Mott derived his VRH conductivity formula for three-dimensional systems. Therefore, when Xu and Guan used the Mott expression to explain their data, they automatically assumed that the electron conduction in their PBCGO compound is three dimensional in nature. Triberis *et al.* have also derived their expression of conductivity for three-dimensional systems. Recently, Kabasawa *et al.* (1992, 1993) and others (van Ancum *et al.* 1995 a,b) have measured the temperature-, electric-field- and magnetic-field-dependent conductivity of PBCO compounds. Their data suggests that the conduction in these compounds is due to VRH, and that PBCO compounds behave as quasi-two-dimensional (QTD) systems rather than three-dimensional systems (Singh *et al.* 1994 a,b, 1996, Singh and Thompson 1996). Hence, the three-dimensional theories of Mott and Triberis *et al.* may not be suitable for explaining the experimental data of Xu and Guan.

Triberis *et al.* (1994) have derived the expressions for three-dimensional conductivity due to small-polaron hopping using the percolation model in a series of papers. Similar three-dimensional polaron VRH conducivity calculations based on the percolation model have also been used by other workers to interpret the behaviour of the high-temperature conductivity of different amorphous materials (Meaudre *et al.* 1983, Triberis 1986, Mohan and Rao 1993, Ruscher *et al.* 1988, Selvaraj and Rao 1988, Brahma and Chakrovorty 1990, Brahma *et al.* 1991), doped single crystals and Pr–Re–Ba–Cu–O compounds (Triberis *et al.* 1992). The aim of the present paper is to develop a theory of VRH due to small polarons for QTD systems at high temperatures. We have used the method of Singh *et al.* (1994 a,b, 1996, Singh and Thompson 1996) to derive an expression for the conductivity. According to this method, we considered that polaron localized states are randomly distributed in the energy and spatial coordinates. The polarons hop from one localized state to another with the help of the absorption and emissions of phonons. The mobility and the hopping range are calculated as functions of energy with respect to the Fermi level. The conductivity is then

calculated from the mobility by integrating over energy. The small-polaron energy consists of a site-dependent local electron energy e_i and a site-dependent electron–phonon interaction binding energy λ_i. Triberis *et al.* have neglected the contribution of energy e_i in their calculations whereas we have included its effect in our calculations. We have also included the effect of electric fields, magnetic fields and scattering in the derivation of the conductivity. Triberis considered the three-dimensional electric field dependence in a previous work (Triberis 1987, 1988).

We found that the logarithm of the conductivity has a $T^{-1/2}$ power law dependence, which is different from that of the three-dimensional case. In the presence of an electric field, we found that the logarithm of conductivity has a $(1-\beta^2)^{3/8}$ dependence for $\beta < 1$, where $\beta = qF/2\alpha k_B T$. Here, F is the electric field, q is the charge of a carrier, α is the inverse of the localization length and k_B is Boltzmann's constant. For weak magnetic fields, without scattering, we found an H^2 dependence for the logarithm of the conductivity, where H is the magnetic field. For strong fields, again without scattering, we found an $H^{1/3}$ dependence. We also found a more complicated magnetic field expression in the presence of scattering.

We applied the present theory to explain the high-temperature experimental data of Xu and Guan. To explain the low-temperature data of Xu and Guan, we used the QTD theory of Thompson and Singh (1997, 1998) which is based on the pure electron VRH mechanism. The recent experimental data on PBCO (Kabasawa *et al.* 1992, 1993, van Ancum *et al.* 1995 a,b) also show that pure electron VRH theory is sufficient to explain the experimental data at low temperatures ($T < 150$ K). We found good agreement between theory and experiment at low and high temperatures. We found that the density of states varies from $D_0 = 5.5 \times 10^{34}\,\mathrm{J^{-1}\,m^{-2}}$ to $D_0 = 6.4 \times 10^{32}\,\mathrm{J^{-1}\,m^{-2}}$ as the doping concentration changes from $x = 0.05$ to $x = 0.4$. Similarly, the concentration of polaron localized sites changes from $N_0 = 2.3 \times 10^{16}\,\mathrm{m^{-2}}$ to $N_0 = 2.0 \times 10^{13}\,\mathrm{m^{-2}}$ when the doping concentration changes from $x = 0.05$ to $x = 0.4$.

§2. Variable-range hopping due to polarons

To include small polarons in a model of hopping conductivity, one must include the electron–phonon interaction. Holstein (1959 a,b) presented such a model which consists of a system of n identical diatomic molecules of natural frequency ω_0 whose orientations and centres of gravity are fixed, but whose internuclear separations may vary. This model has been called the molecular crystal model. This model was expanded by Triberis and Friedman (1981), and they found that the energies of localized polaronic states in the presence of the electron–phonon interaction are given as $E_i = e_i - \lambda_i$, where e_i is the site-dependent local electronic energy and λ_i is the binding energy due to the site-dependent electron–phonon interaction. The energy λ_i is measured with respect to e_i. In the absence of electron–phonon interactions, $E_i = e_i$.

According to Emin (1975) Triberis and Friedman (1981) and Triberis *et al.* (1994), the polaron transition rate from site i to site j in the high-temperature regime, $k_B T > \hbar\omega_0$ is written as

$$\gamma_{ij} = \begin{cases} \gamma_0 \exp(-2\alpha R_{ij}) \exp\left(-\dfrac{\lambda_i + \lambda_j}{4k_B T}\right) \exp\left(-\dfrac{E_j - E_i}{2k_B T}\right), & E_j > E_i, \\ \gamma_0 \exp(-2\alpha R_{ij}) \exp\left(-\dfrac{\lambda_i + \lambda_j}{4k_B T}\right) \exp\left(\dfrac{E_i - E_j}{2k_B T}\right), & E_j < E_i. \end{cases} \tag{1}$$

The first expression above corresponds to the absorption of phonons whereas the second corresponds to the emission of phonons. In these expressions, R_{ij} is the spatial distance between the sites i and j in QTD space and γ_0 is a constant factor. In the rest of paper we shall express energies and spatial coordinates in reduced coordinates, where $\varepsilon \equiv (e_i - 2\lambda_i)/2_B T$, $\omega \equiv e_j/2k_B T$, $\epsilon \equiv (\lambda_i + \lambda_j)/2k_B T$, $\lambda \equiv \lambda_i/2k_B T$ and $x \equiv 2\alpha R_{ij}$.

To calculate the conductivity, we have used the method given by Singh *et al.* (1994 a,b, 1996) and Singh and Thompson (1996). We assume that the localized polaron states are randomly distributed in the two-dimensional coordinate space x, and in the two-dimensional energy coordinates ϵ and ω. This four-dimensional space is called the hopping space. The distance between the initial site and the final site in the hopping space is denoted by the range R. Polarons hop from one site to another through the emission and absorption of phonons in this space. In the reduced coordinates, equation (1) can be written as

$$\gamma_{ij} = \gamma_0 \exp(-R)$$
$$R = x - \frac{\epsilon}{2} + \omega - \varepsilon. \tag{2}$$

First we have to calculate the number N of states available for hopping in the hopping space; the expressions of mobility and conductivity are obtained using the value of N. The expression for N given by Singh *et al.* (1994 a,b 1996) and Singh and Thompson (1996) is for a three-dimensional hopping space (i.e. two spatial and one energy coordinates) but, in the present case, our hopping space is four dimensional. Therefore the expression of Singh *et al.* for N is modified and is written as

$$N = \frac{(k_B T)^2}{\alpha^2} \int_0^{2\pi} d\theta \int_0^{x_{max}} x\,dx \int_\lambda^{\epsilon_{max}} d\epsilon \int_{-\infty}^{\omega_{max}} \frac{D(\omega)^2}{N_0} [1 - f(2\omega - 2\epsilon + 2\lambda)]\,d\omega, \tag{3}$$

where $f(E_j/k_B T) \equiv 1/[1 + \exp(E_j/k_B T)] = f(2\omega - 2\epsilon + 2\lambda)$ is the Fermi distribution, N_0 is the two-dimensional spatial concentration of polaron sites and $D(\omega)$ is a two dimensional density of states (DOS).

We shall assume that the DOS is constant: $D(\omega) = D_0$. Energies are measured from the Fermi level, which is taken to be at zero. The integration limits in the above expression are obtained from equation (2) by fixing the value of R. For a given value of x and ϵ, the upper limit of ω is $\omega_{max} = (R + \varepsilon) - x + \epsilon/2$. The lower limit of ω can be taken as $\epsilon - \lambda$ if one assumes that $f(2\omega - 2\epsilon + 2\lambda) = 1$ for a negative argument of the Fermi distribution and $f(2\omega - 2\epsilon + 2\lambda) = 0$ for a positive argument. Similarly equation (2) gives the maximum value of ϵ as a function of x when $\omega = \epsilon - \lambda$. The minimum value of ϵ is λ. The spatial coordinate in the hopping space has the minimum value $x = 0$. The maximum value of x is obtained from equation (2) by putting $\lambda_j = 0$ and $\omega = \epsilon - \lambda$. After some mathematical manipulation, the value for N finally arrived at is

$$N = \left(\frac{T}{T_p}\right)^2 \left(R + \varepsilon + \frac{\lambda}{2}\right)^4, \tag{4}$$

where $T_p = (2N_0\alpha^2/D_0^2 k_B^2 \pi)^{1/2}$. Here, the subscript p stands for polaron.

§ 3. Electric fields

In the presence of an electric field, the energy difference $E_j - E_i$ changes to $E_j - \epsilon_i + qFR_{ij}\cos\theta$ (Singh *et al.* 1994 a,b, 1996, Singh and Thompson 1996). Here, θ is the angle between the electric field F and the hopping direction R_{ij}. Therefore the equation for the range in the presence of an electric field is

$$R = x(1 + \beta\cos\theta) - \frac{\epsilon}{2} + \omega - \varepsilon. \tag{5}$$

For a fixed value of R in the hopping space, the expression for N becomes

$$N = \left(\frac{T}{T_p}\right)^2 \left(R + \varepsilon + \frac{\lambda}{2}\right)^4 (1 - \beta^2)^{3/2} \tag{6}$$

for $\beta < 1$. Note that, if we put $\beta = 0$, equation (6) reduces to equation (4). Therefore, we shall use equation (6) to calculate the expression for the conductivity; to get the non-electric field results, we put $\beta = 0$ in our formulations.

Following the method of Singh *et al.* and using the value of N given in equation (6), we can calculate the average nearest-neighbour range. This is found to be

$$R_{nn}^p = \left(\frac{T_p}{T}\right)^{1/2} (1 - \beta^2)^{3/8} - \varepsilon - \frac{\lambda}{2}. \tag{7}$$

Note that R_{nn}^p is proportional to $(T/T_p)^{-1/2}$ for constant electric fields.

The mobility is expressed in terms of R_{nn}^p as (Singh *et al.* 1994 a,b)

$$\mu(\varepsilon) = \frac{v_p x_f}{2\alpha F} \exp\left[-R_{nn}^p(\varepsilon)\right], \tag{8}$$

where v_p is the hopping attack frequency, taken to be a constant phonon frequency, and x_f is the average forward hopping distance. The expression for x_f given by Singh (1994 a,b) is modified for the present case and is written as

$$x_f = \frac{\displaystyle\int_\lambda^{2(\varepsilon + R_{nn}^p + \lambda/2)} d\epsilon \int_0^\pi d\theta \cos\theta \int_{-\infty}^{\varepsilon + R_{nn}^p + \epsilon/2} d\omega \frac{D(\omega)^2}{N_0} [1 - f(2\omega - 2\epsilon + 2\lambda)] x^2}{\displaystyle\int_\lambda^{2(\varepsilon + R_{nn}^p + \lambda/2)} d\epsilon \int_0^\pi d\theta \int_{-\infty}^{\varepsilon + R_{nn}^p + \epsilon/2} d\omega \frac{D(\omega)^2}{N_0} [1 - f(2\omega - 2\epsilon + 2\lambda)] x}. \tag{9}$$

After some mathematical manipulation, equation (9) reduces to

$$x_f = \frac{\beta}{2(1 - \beta^3)^{5/8}} \left(\frac{T_p}{T}\right)^{1/2}. \tag{10}$$

From the mobility, we can calculate the conductivity as follows:

$$\sigma = \frac{q(k_B T)^2 D_0^2}{N_0} \int_0^\infty \int_{-\infty}^{\lambda_i} \mu(e_i, \lambda_i)\, de_i\, d\lambda_i. \tag{11}$$

Equation (11) is a modified version of the conductivity expression found by Singh *et al.* (1994 a,b). Putting equation (8) into equation (11), we get the following expression for the conductivity:

$$\sigma = c_p T \left(\frac{T_p}{T}\right)^{1/2} (1 - \beta^2)^{-5/8} \exp\left[-\left(\frac{T_p}{T}\right)^{1/2} (1 - \beta^2)^{3/8}\right] \tag{12}$$

for $\beta < 1$, where $c_p = q^2 k_B D_0^2 \nu_p / 4 N_0 \alpha^2$. Note that, in the present case, the logarithm of conductivity is proportional to $(T/T_p)^{-1/2}$ whereas for three-dimensional systems, the logarithm of the conductivity obeys a $(T/T_p)^{-2/5}$ power law (Triberis and Friedman 1981, Triberis *et al.* 1994). The above expression includes also the effect of an electric field. According to this equation, the logarithm of the conductivity obeys a $(1-\beta^2)^{3/8}$ power law for $\beta < 1$.

§4. Magnetic fields

In the previous section, we calculated the expression for the conductivity in the presence of an electric field. In this section we include the effect of magnetic fields on the conductivity. Recently, Thompson and Singh (1998) have developed a theory for the magnetoconductivity for strong magnetic fields (i.e. $\lambda \ll \alpha^{-1}$) and weak magnetic fields (i.e. $\lambda \gg \alpha^{-1}$), where $\lambda = (\hbar/qH)^{1/2}$, α^{-1} is the localization length in the absence of a magnetic field, q is the charge of a carrier and H is the magnetic field. For general magnetic fields, the analytical expression for the conductivity cannot be obtained (Thompson and Singh 1998).

Thompson and Singh considered that, for QTD materials in the presence of a weak magnetic field ($\lambda \gg \alpha^{-1}$), one can replace the function $\exp(-2\alpha R_{ij})$ appearing in the hopping probability by a function $\exp[-(2\alpha R_{ij} + [(R_{ij}^3)/(24\alpha\lambda^4)])]$. Note that the first term has the same form as in the absence of a magnetic field. The entire effect of the magnetic field is contained in the second term which is much smaller than the first. Making this replacement in the present problem, the expression for the range given in equation (5) becomes

$$R = x(1 + \beta\cos\theta) + \gamma x^3 - \frac{\epsilon}{2} + \omega - \varepsilon, \tag{13}$$

where $\gamma = 1/96\alpha^4\lambda^4$.

With the help of equation (13), and following the method of the previous sections and of Thompson and Singh, we have derived expression for the hopping range and the conductivity. The hopping range is written as

$$R_{nn}^p = \left(\frac{T_p}{T}\right)^{1/2} (1-\beta^2)^{3/8} \left(1 + \frac{\gamma(3\beta^4 + 24\beta^2 + 8)}{5(1-\beta^2)^{9/4}} \frac{T_p}{T}\right) - \varepsilon - \frac{\lambda}{2}, \tag{14}$$

where T_p is the same as in §2. The expression for the magnetoconductivity for weak magnetic fields is written as

$$\sigma = c_p T \left(\frac{T_p}{T}\right)^{1/2} (1-\beta^2)^{-5/8} \left(1 + \frac{2\gamma}{(1-\beta^2)^{9/4}} \frac{T_p}{T} \left(\tfrac{3}{10}\beta^4 + \tfrac{15}{8}\beta^2 - \tfrac{1}{20}\right)\right)$$
$$\times \exp\left[-\left(\frac{T_p}{T}\right)^{1/2} (1-\beta^2)^{3/8} \left(1 + \frac{\gamma(3\beta^4 + 24\beta^2 + 8)}{5(1-\beta^2)^{9/4}} \frac{T_p}{T}\right)\right] \tag{15}$$

for $\beta < 1$, where c_p is the same as in §3. Note that, if we consider only the magnetic field dependence, the logarithm of the conductivity is proportional to H^2 for weak magnetic fields.

In the case of high magnetic fields ($\lambda \ll \alpha^{-1}$) for QTD materials, Thompson and Singh have replaced the function $\exp(-2\alpha R_{ij})$ appearing in the hopping probability

by a function $\exp(-R_{ij}^2/4\lambda^2)$ to calculate the conductivity. Making this replacement in the present problem, the expression for the range given in equation (5) becomes

$$R = \gamma x^2 + x\beta\cos\theta - \frac{\epsilon}{2} + \omega - \varepsilon, \tag{16}$$

where now $\gamma = 1/8\lambda^2\alpha^2$.

With the help of equation (16), the previous sections, and the work of Thompson and Singh (1998), we have derived the expressions for the hopping range and the conductivity. The hopping range is given as

$$R_{nn}^{p} = \left(\frac{T_p}{T}\right)^{2/3}\left(\frac{\gamma}{2}\right)^{1/3} - \frac{\beta^2}{4\gamma} - \varepsilon - \frac{\lambda}{2}, \tag{17}$$

where T_p is still the same as in § 2. The expression for the magnetoconductivity for strong magnetic fields is written as

$$\sigma = \frac{c_p T}{\gamma}\exp\left[-\left(\frac{T_p}{T}\right)^{2/3}\left(\frac{\gamma}{2}\right)^{1/3} + \frac{\beta^2}{4\gamma}\right]. \tag{18}$$

Equation (18) is valid for $\beta < 1$ to second order in β. Note that, if we consider only the magnetic field dependence, the logarithm of the conductivity for strong magnetic fields is proportional to $H^{1/3}$.

§ 5. Scattering

Recently, we have shown that scattering plays an important role in understanding the magnetoconductivity of PBCO materials for electron VRH conduction (Thompson and Singh 1998). Therefore, in this section, we shall include the effect of scattering on the calculation of the polaron VRH conductivity. Shklovskii (1983 a,b) has shown that, when the average hopping length much exceeds the mean distance between the impurities, the hopping carrier meets many other impurities and scattering takes place. He included the effect of scattering in the calculation of the hopping probability in the presence of a magnetic field. He found that in the presence of scattering the spatial function appearing in the hopping probability changes as follows;

$$\begin{aligned}
&\exp(-2\alpha R_{ij}) \rightarrow \exp\left(-\frac{2R_{ij}}{b}\right),\\
&b = \frac{1}{\alpha}\left[1 - \left(\frac{1}{\alpha\lambda}\right)^{4/3} L\right], \qquad \lambda \gg N_0^{-1/2},\\
&b = \frac{1}{\alpha}\left[1 - q'\left(\frac{1}{N_0^{1/2}\alpha\lambda^2}\right)^{4/3}\right], \qquad (\alpha N_0^{1/2})^{-1/2} \ll \lambda \ll N_0^{-1/2},\\
&b = s(\lambda^2 N_0^{1/2}), \qquad \lambda \ll (\alpha N_0^{1/2})^{-1/2},
\end{aligned} \tag{19}$$

where b is called the scattering length, which includes the effects of scattering and the magnetic field. In equation (19), L is a logarithmic factor, s and q' are numerical factors, N_0 is the two-dimensional concentration of donor sites, and λ is the magnetic length defined as $\lambda = (\hbar/qH)^{1/2}$. Therefore, one can include the effect of scattering in the calculation of the polaron hopping probability by making the

replacement given in equation (19). The range given by equation (1) remains the same except the definition of x changes from $2\alpha R_{ij}$ to $2R_{ij}/b$.

In this case, the expression for conductivity has a similar form as given in equation (12) which is written as

$$\sigma = c_p^H T \left(\frac{T_p^H}{T}\right)^{1/2} (1-\beta_H^2)^{-5/8} \exp\left[-\left(\frac{T_p^H}{T}\right)^{1/2} (1-\beta_H^2)^{3/8}\right], \tag{20}$$

where c_p^H, T_p^H, and β_H have the following forms:

$$c_p^H = \frac{q^2 k_B D_0^2 v_p b^2}{4N_0}, \quad \beta_H = \frac{qFb}{2k_B T}, \quad T_p^H = \left(\frac{2N_0}{D_0^2 k_B^2 \pi b^2}\right)^{1/2}. \tag{21}$$

Note that the magnetic field and scattering dependencies in the above expressions come through the parameter b. Equation (20) is valid only for temperatures, electric fields and magnetic fields for which $\beta_H < 1$.

§6. Results and discussion

Recent experimental and theoretical studies in PBCO (Kabasawa *et al.* 1992, 1993, Singh *et al.* 1994 a,b, 1996, van Ancum *et al.* 1995 a,b, Singh and Thompson 1996, Thompson and Singh 1997, 1998) indicate that this compound behaves as a QTD system rather than as a three-dimensional system. The electron conduction takes place mainly in the CuO_2 planes. Therefore, we can apply our present theory to explain the high temperature ($T > 150$ K) data of Xu and Guan. In our calculations, we used only one fitting parameter, T_p. The theoretical and experimental data are presented in figure 1. One can see that there is a good agreement between theory and experiment for all concentrations. In our calculations we varied T_p with the concen-

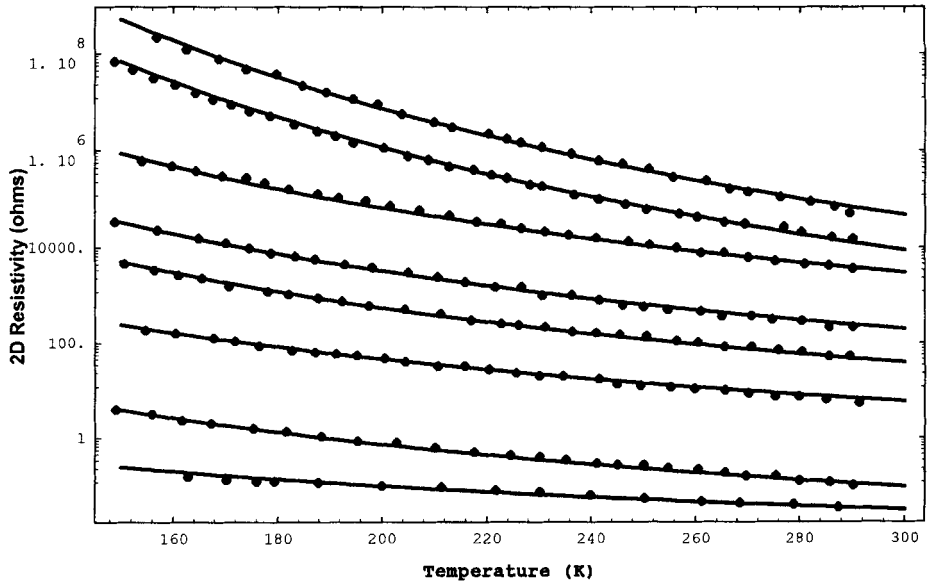

Figure 1. Conductivity against temperature at high temperatures. Equation (12) used with $\beta = 0$ to fit the data of Xu and Guan (1993).

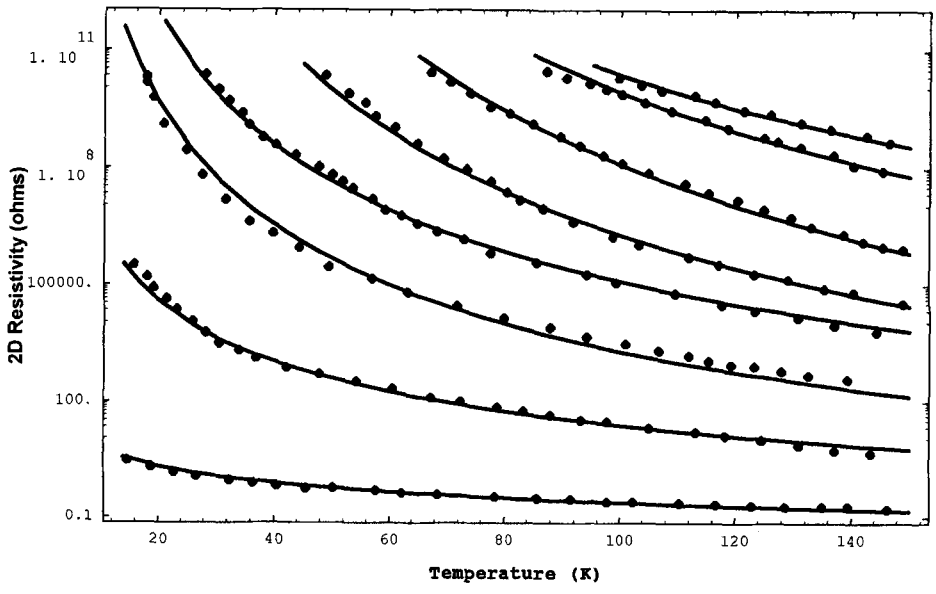

Figure 2. Conductivity against temperature at low temperatures. The solid curves are the theoretical predictions from Thompson and Singh (1997).

tration. (There is a multiplicative constant involved in converting the three-dimensional resistivity units of the experiment to the two-dimensional units of the theory.)

Recently, Singh and Thompson and others have established that the low-temperature conductivity data of PBCO can be explained using a QTD electron VRH mechanism. Therefore, we shall try to explain the low-temperature ($T < 150\,\mathrm{K}$) data of Xu and Guan by using the electron VRH theory for QTD systems given by Thompson and Singh (1997). Using this conductivity expression, we fitted the experimental data using one fitting parameter, T_0. The theoretical and experimental data are presented in figure 2 for all concentrations. Good agreement between theory and experiment is found. The same data were fitted by Triberis using the three-dimensional polaron VRH mechanism. Their formulation of conductivity due to polarons at low temperatures has a $T^{-1/4}$ power law which is the same as the Mott power law for localized electrons. Therefore fitting the data of Xu and Guan by this power law does not necessarily prove that polarons are responsible for hopping in PBCO materials at low temperatures. On the other hand our theory gives a $T^{-1/3}$ power law and our theoretical fitting with these data is consistent with other work in the literature (Kabasawa *et al.* 1992, 1993, Singh *et al.* 1994 a,b, 1996, van Ancum *et al.* 1995 a,b, Singh and Thompson 1996, Thompson and Singh 1997, 1998).

From the parameter $T_0 = \Gamma(\frac{4}{3})^3(12\alpha^2/D_0 k_B \pi)$ we can calculate the DOS. Taking the value of $\alpha^{-1} = 8\,\mathrm{nm}$ from the work of Thompson and Singh (1997), we get D_0 as a function of Ga concentration. Here we have neglected the concentration dependence of α^{-1}. The results are shown in figure 3 for doping concentrations from $x = 0.05$ to $x = 0.4$. One can see that the DOS decreases with increase in the Ga concentration. The magnitude of the DOS near $x = 0$ has the same order of magnitude as reported in the literature (Kabasawa *et al.* 1992, 1993, Singh *et al.* 1994 a,b, 1996, van Ancum *et al.* 1995 a,b, Singh and Thompson 1996, Thompson and Singh 1997, 1998). Note that D_0 is very sensitive to the concentration. For example, $D_0 = 5.5 \times 10^{34}\,\mathrm{J^{-1}\,m^{-2}}$ for $x = 0.05$ and $D_0 = 6.4 \times 10^{32}\,\mathrm{J^{-1}\,m^{-2}}$ for $x = 0.4$.

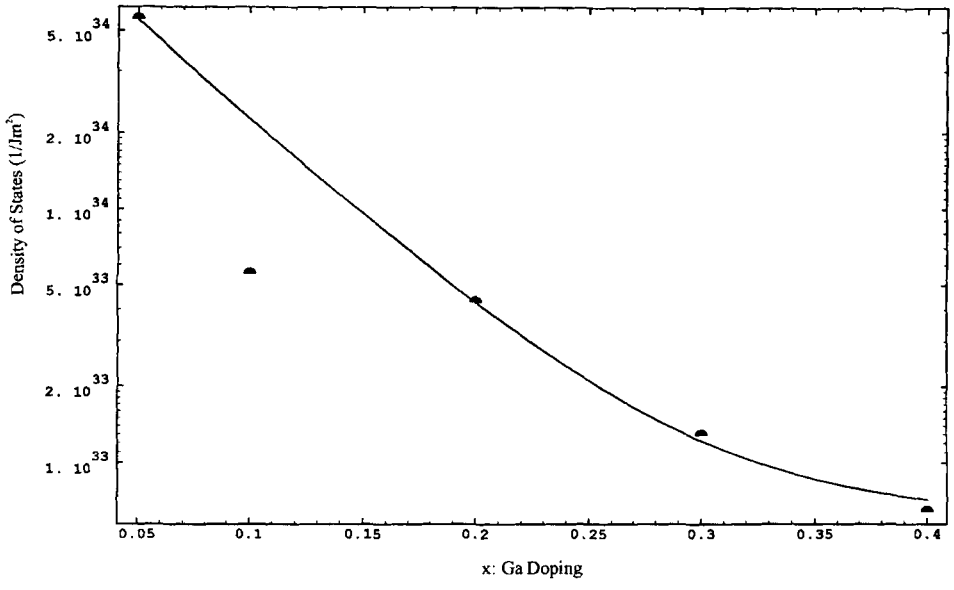

Figure 3. D_0 against Ga doping. The solid curve shows an exponential decrease.

From the high-temperature data, we found the values of T_p as a function of the Ga doping concentration x. From the fitting parameters $T_p = (2N_0\alpha^2/D_0^2k_B^2\pi)^{1/2}$ and $T_0 = \Gamma(\frac{4}{3})^3(12\alpha^2/D_0k_B\pi)$ we can find the spatial concentration of localized polaron sites N_0. Assuming that the DOSs appearing in these two expressions are almost the same, we can say that $N_0 = \Gamma(\frac{4}{3})^6 144\alpha^2T_p^2/\pi T_0^2$. Using the experimental values of T_p and T_0, we have calculated N_0 as a function of x. The results are shown in figure 4. For values of x near zero, we get a concentration of localized states consistent with previous work (Kabasawa 1993, Thompson and Singh 1998). One

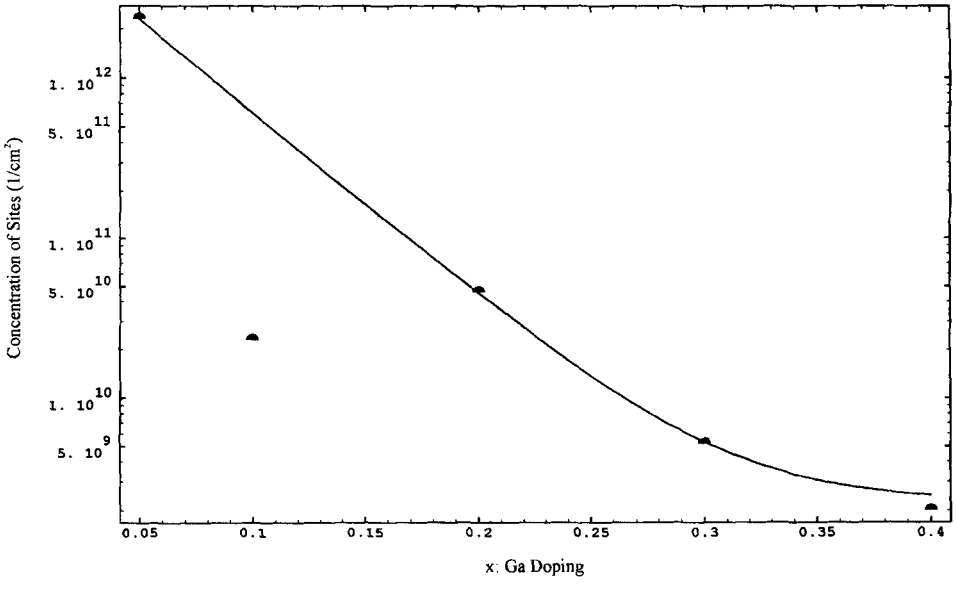

Figure 4. N_0 against Ga doping. The solid curve shows an exponential decrease.

can see from the figure that, as the Ga concentration increases, the number of hopping sites generally decreases. In other words, the substitution of Cu^{+2} by Ga^{+3} results in the filling of holes and diminishes the number of sites between which the polarons hop. Note that N_0 is more sensitive to concentration than D_0. For example, when x changes from $x = 0.05$ to $x = 0.4$, N_0 changes by a factor of 1000 whereas D_0 changes by a factor of only 100.

The sensitivity of the resistivity with the concentration can also be understood as follows. In our theory, the doping dependence of the resistivity comes through the doping dependence of the DOS $D_0(x)$ and the concentration $N_0(x)$ of localized sites. One can express the resistivity ρ in terms of $D_0(x)$ and $N_0(x)$ as $\ln \rho \approx [D_0^2(x)/N_0(x)]^{1/2}$ for high temperatures and $\ln \rho \approx [D_0(x)]^{1/3}$ for low temperatures. Note that, in the first expression, there are two quantities $D_0(x)$ and $N_0(x)$ which vary with doping, whereas, in the second equation, only one quantity, $D_0(x)$, depends on the doping level. Since N_0 is a factor of ten more sensitive to the doping level than is D_0, the effect of $D_0^2(x)$ is largely cancelled by $N_0(x)$ at high temperatures, and the resistivity is less affected by the variation of the Ga concentration. On the other hand, at low temperatures there is no cancellation and the resistivity is very sensitive to the doping concentration.

It is interesting to note that the temperature-dependent data of Xu and Guan can be fitted by two different mechanisms: both QTD and three-dimensional VRH hopping. Therefore, we propose electric- and magnetic-field-dependent conductivity measurements to clarify the above ambiguity. According to our theory the logarithm

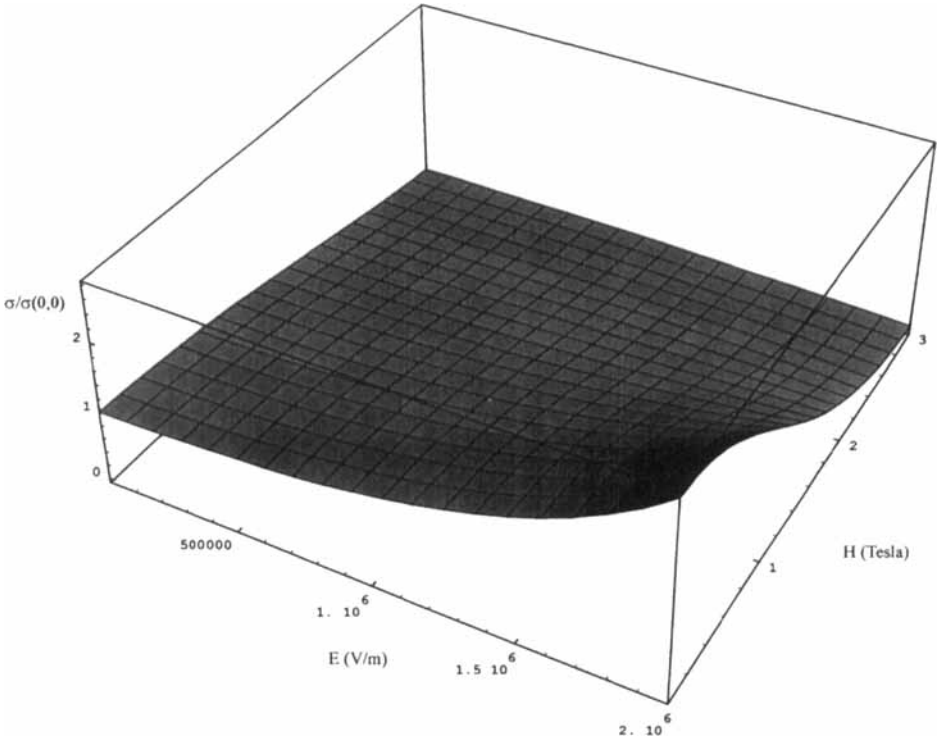

Figure 5. High-temperature small-polaron VRH conductivity against electric field and magnetic field for the non-scattering case.

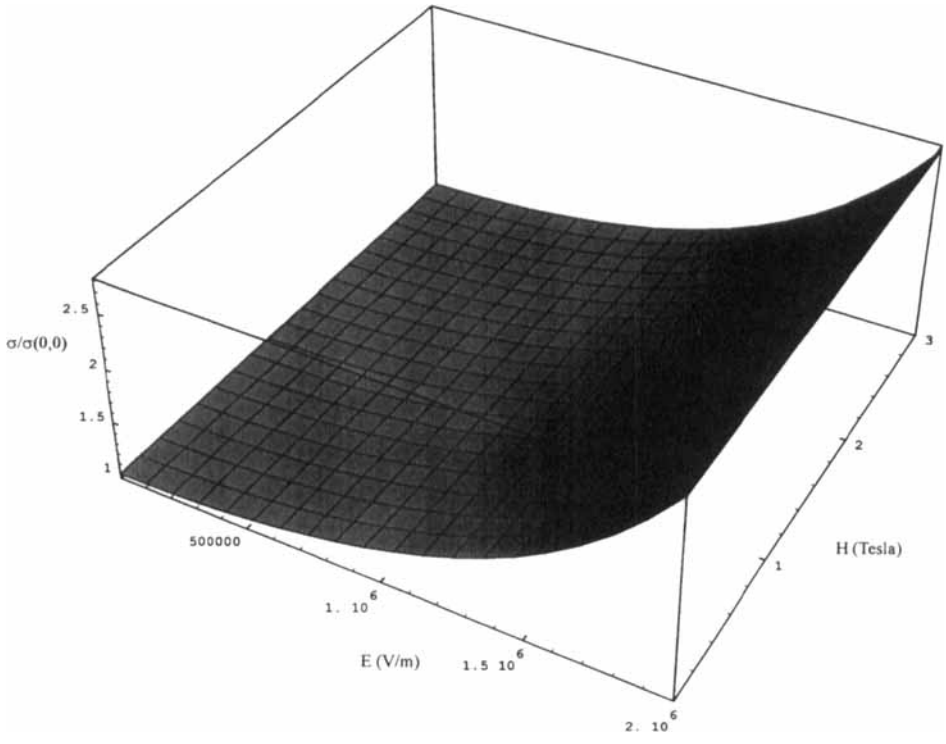

Figure 6. High-temperature small-polaron VRH conductivity against electric field and magnetic field for the scattering case.

of conductivity varies with electric fields as $(1-\beta^2)^{3/8}$ for high temperatures. It varies with weak and strong magnetic fields as H^2 and $H^{1/3}$ respectively in the absence of scattering. With scattering, the conductivity varies in a more complicated fashion, depending on the applied magnetic field strength and the concentration N_0. Predictions based on our equations (15) and (20) can be found in figures 5 and 6 which plot the high-temperature small-polaron VRH conductivity with electric and magnetic fields, for the non-scattering and scattering cases respectively. One can clearly see that the magnetic field affects the electric field dependence in the former case, unlike the latter. These figures can be compared with similar predictions made for the low-temperature electron VRH case, shown by Thompson and Singh (1998). Such a comparison shows that the effect of scattering on the electric field dependence is qualitatively the same for both the low and high temperature cases.

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