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Importance of polaron effects for charge carrier mobility above and below pseudogap temperature in superconducting cuprates

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Abstract. Polaron effects and charge carrier mobility in high-T_c cuprate superconductors (HTSCs) have been investigated theoretically. The appropriate Boltzmann transport equations under relaxation time approximation were used to calculate the mobility of polaronic charge carriers and bosonic Cooper pairs above and below the pseudogap (PG) temperature T^*. It is shown that the scattering of polaronic charge carriers and bosonic Cooper pairs at acoustic and optical phonons are responsible for the charge carrier mobility above and below the PG temperature. We show that the energy scales of the binding energies of large polarons and polaronic Cooper pairs can be identified by PG cross-over temperature on the cuprate phase diagram.

Keywords. High-T_c cuprate superconductors; pseudogap; polaronic charge carriers; bosonic Cooper pairs.

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1. Introduction

High-transition temperature (T_c) superconductivity in copper oxides (cuprates) remains one of the most intriguing phenomena in strongly-correlated electron systems since its discovery by Bednorz and Müller [1,2]. In particular, anomalous charge transport behaviours in the normal state of high-T_c cuprates have provided many challenging issues and stimulated much interest [3–9]. The normal-state gap or pseudogap (PG) is a unique property of this class of superconducting materials, in addition to the unprecedented high superconducting T_c. The term PG was suggested by Mott [10] to name a minimum in the electronic density of states at the Fermi level. The PG in cuprates was first detected by nuclear magnetic resonance and magnetic susceptibility studies [11–13], which measures temperature dependence of the Knight shift and spin-lattice relaxation rate. The Knight shift is proportional to the density of states at the Fermi energy; a gradual depletion was observed below a cross-over temperature T^*, revealing the opening of the PG well above T_c on the underdoped side of the cuprate phase diagram. The origin of the pseudogap was considered to be due to a fluctuating or short-range cross-over phenomenon originating from localized carriers in the form of polarons. Actually, a polaron is defined as a carrier wrapped in both the phonon cloud and the electronic polarization cloud [14]. Therefore, the electronic polarization cloud around a hole carrier can be regarded as a small electron-like pocket on a hole-like Fermi surface of doped cuprates. From a theoretical point of view, the change of the Fermi surface topology from a large surface to small pockets resembles a Lifshitz transition. Although proposed by Lifshitz in noninteracting fermion systems decades ago [15], the Lifshitz transition has only recently begun to be considered as a quantum phase transition in strongly correlated electron systems [16–18]. It has been used to explain experimental data in high-T_c cuprate superconductors (HTSCs) [19,20]. Recently, the Lifshitz transition of the two-dimensional Hubbard model with next-nearest-neighbour hopping, chemical potential and temperature as control parameters is studied by using large-scale dynamical cluster quantum Monte Carlo simulations (see ref. [21]). In the overdoped region, the Fermi surface is complete and electron-like; across the Lifshitz transition, the Fermi surface becomes hole-like and develops a pseudogap. At the Lifshitz transition points, a van Hove singularity in the density of states crosses the Fermi level. The van Hove singularity occurs at finite doping due to correlation effects, and becomes more singular when next-nearest-neighbour hopping becomes more negative. Also note that the van Hove singularity has great impact on the conditions for pairing [21].

Other mechanisms can also be invoked for the reconstruction of the Fermi surface that would result in hole-like and electron-like pockets [22–24]. It seems likely that under certain conditions, holes give negative, and electrons positive, values of the Hall coefficient [25]. If the current carrier is strongly localized in the strong coupling regime, the characteristic relaxation times for hole carriers and electronic polarizations are about $\tau_h \sim 10^{-14}$ s and $\tau_e \sim 10^{-15}$ s, respectively. In this case, the electronic polarization cloud (electron-like pocket) induced by the hole carrier should be taken into account in the polaron transport. At $\tau_h \sim \tau_e$ the current carrier is sufficiently delocalized in the intermediate coupling regime and the electronic polarization becomes unimportant [14]. Such a situation for large hole polarons is probably realized below and above T_c in cuprate superconductors at zero magnetic field. However, in magnetic fields large enough to suppress superconductivity, the situation is completely different for the hole carriers in the underdoped cuprates at sufficiently low temperatures due to the charge carrier localization by strong magnetic fields [26]. A similar explanation of these experiments was recently proposed based on the analysis of the charge carrier mobility [24], which is much reduced at low temperatures due to the small polaron formation. In addition, a small polaron usually moves incoherently by a succession of thermally activated jumps. The predominance of the short-range electron–phonon interaction then ensures that the change of the electronic energy accompanying the nearest-neighbour transfer exceeds its transfer energy [27,28]. The small polaron mobility is generally less than $0.1-1\,\mathrm{cm}^2/(\mathrm{V\,s})$, for example, $\mu \leq 1\,\mathrm{cm}^2/(\mathrm{V\,s})$ at 300 K [29–31]. The mobility rises as the temperature rises, as a small polaron moves by thermally-activated incoherent jumps. By contrast, a large polaron moves very slowly but coherently in concert with atomic vibrations. The predominance of the long-range electron–phonon interaction then ensures that the change of the electronic energy accompanying the nearest-neighbour transfer is less than its transfer energy. However, a huge mass of a large polaron enables it to be only weakly scattered by the phonons it encounters. If the large polarons have thermal energies, then their mobilities must be least of order $1-10\,\mathrm{cm}^2/(\mathrm{V\,s})$. For large polarons, the mobility falls as temperature rises, because scattering by phonons increases. As a result, a large polaron displays a significant mobility at room temperature (e.g. $\mu \geq 1\,\mathrm{cm}^2/(\mathrm{V\,s})$ at 300 K), that falls with rising temperature [28,29].

In the present work, we address the issue of studying the charge carrier mobility in HTSCs. To calculate the mobility of polaronic charge carriers and bosonic Cooper pairs above and below T^*, we use the appropriate Boltzmann transport equations under relaxation time approximation. In particular, we shall address the question of how the scattering of carriers at acoustic and optical lattice vibrations and the Cooper pairing of large polarons proceed in the CuO_2 planes of HTSCs above T_c. In the following, we present a study of the PG state in HTSCs for doping from underdoped and overdoped regions at different temperatures above T_c and discuss the results in the context of the possible origin of the PG state (figure 2).

2. The charge carriers, energy gaps and phase diagram of HTSCs

The undoped cuprates are charge-transfer (CT)-type insulators [32]. Upon doping, the oxygen valence band of these anisotropic three-dimensional (3D) cuprates is occupied by holes. These charge carriers, being placed in a polar crystal, will interact with the acoustic and optical phonons and the ground states of the doped carriers interacting with lattice vibrations are their self-trapped (polaronic) states lying in the CT gap of the cuprates. The polaron concept was introduced by Landau [33] to describe the electronic properties of polar materials and the quasiparticle, which consists of the electron (or hole) together with the lattice distortion (phonon cloud) and electronic polarization induced by it, is called a polaron. Theoretical [34–37] and experimental [38–42] studies show that a polaronic transition from a quasifree state to the self-trapped one occurs in doped cuprates and the electron–phonon interaction is responsible for the enhanced polaron masses $m_p = (2-3)m_e$ [40,41,43] (where m_e is the free electron mass). As the doping (or polaron concentration n_p) grows towards the underdoped region, the Coulomb repulsion between the polarons increases and the binding energy E_p of the polarons decreases, that the polaronic effect weakens with increasing doping and disappears in the overdoped region. Indeed, the binding energies of polarons $E_p = 0.12$ eV and $E_p = 0.06$ eV were observed experimentally in underdoped and optimally doped cuprates, respectively [39]. The radii of polarons in high-T_c cuprates vary from 6 to 10 Å [37,40]. Such polarons having relatively small binding energies, sizes and effective masses are large polarons. According to refs [43,44], the formation of nearly small polarons in the cuprates might also be relevant.

The hole-doped cuprates are inhomogeneous systems (where the charge carriers are distributed inhomogeneously) and the underdoped cuprates are more inhomogeneous than overdoped ones [45]. In these systems the electronic inhomogeneities and electron–phonon interactions play important roles and are responsible for the carrier segregation, which may manifest itself via

local nanoscale phase separation in the form of alternating metallic and insulating domains with mobile and immobile (i.e. localized) carriers, respectively [37]. We believe that the inhomogeneous spatial distribution of charge carriers leads to their aggregation in carrier-rich CuO_2 planes together with charge depletion in spatially separated carrier-poor regions between the CuO_2 planes. The mobile polaronic carriers are confined in thin quasi-two-dimensional (2D) CuO_2 planes (with nonzero thickness) and they have well-defined momentum k at $W_p \gtrsim E_p$ (where W_p and E_p are the bandwidth and binding energy of large polarons, respectively), while the immobile carriers are distributed over the interplane regions and reside between the CuO_2 planes (along the c-axis). In the carrier-rich metallic regions, the normal-state (precursor) Cooper pairing of large polarons may occur in the intermediate coupling regime [37]. As will be discussed below, the formation of incoherent (i.e. nonsuperconducting) polaronic Cooper pairs becomes possible at $T^* > T_c$ in the CuO_2 planes of underdoped to overdoped cuprates. In this case, the unconventional electron–phonon interactions (i.e., the combined and more effective BCS- and Fröhlich-type attractive interactions) are believed to be responsible for the pairing correlation above T_c in these materials. Here we note that Migdal approximation is applied in the extreme adiabatic regime $\hbar\omega_D/E_F \ll 1$, which is valid only for ordinary metals with Fermi energy $E_F \gg 1$ eV. But, the high-T_c cuprates with the low Fermi energy ($E_F \ll 1$ eV) [46] and high-frequency optical phonons ($\hbar\omega_0 = 0.04-0.07$ eV [40,47,48]) are in the nonadiabatic regime (i.e., the ratio $\hbar\omega_0/E_F$ is no longer small).

By applying BCS formalism to the interacting Fermi gas of large polarons, we can write the mean-field Hamiltonian of this system with the pair interaction in the form

$$H_{MF} = \sum_{\vec{k}\sigma} \xi_{\vec{k}} a^+_{\vec{k}\sigma} a_{\vec{k}\sigma} + \sum_{\vec{k}\vec{k}'} V^p_{\vec{k}\vec{k}'} a^+_{\vec{k}\uparrow} a^+_{-\vec{k}\downarrow} a_{-\vec{k}'\downarrow} a_{\vec{k}'\uparrow}, \quad (1)$$

where $a^+_{\vec{k}\sigma}$ ($a_{\vec{k}\sigma}$) is the creation (annihilation) operator for a polaron having momentum $\vec{k}$ and spin projection σ (=↑ or ↓), $V^p_{\vec{k}\vec{k}'}$ is the pair interaction potential (which has both an attractive and a repulsive part) between large polarons. Diagonalizing now the Hamiltonian (1) by using the standard Bogoliubov transformation of Fermi operators, we obtain the ground-state energy of polaronic Cooper pairs. The excited state of these polaronic Cooper pairs is separated from their ground state by BCS-like gap equation $\Delta_{\vec{k}}$ which, at finite temperature is given by

$$\Delta_{\vec{k}}(T) = -\sum_{\vec{k}'} V^p_{\vec{k}\vec{k}'} \frac{\Delta_{\vec{k}'}(T)}{E_{\vec{k}'}(T)} \tanh\left[\frac{E_{\vec{k}'}(T)}{2k_BT}\right]. \quad (2)$$

Further, we use the Bogoliubov-like model potential [49] which may be written as

$$V^p_{\vec{k}\vec{k}'} = \begin{cases} V_c - V_{ph} & \text{for } |\xi_{\vec{k}}|,\ |\xi_{\vec{k}'}| \le \varepsilon_A, \\ V_c & \text{for } \varepsilon_A \le |\xi_{\vec{k}}|,\ |\xi_{\vec{k}'}| < \varepsilon_c, \\ 0 & \text{otherwise,} \end{cases} \quad (3)$$

where $\varepsilon_A = E_p + \hbar\omega_{LO}$, V_{ph} is the phonon-mediated attractive interaction potential between two polarons, V_c is the repulsive Coulomb interaction potential between these carriers, ε_c is the cut-off energy for the Coulomb interaction, ω_{LO} is the longitudinal-optical (LO) phonon frequency.

Using model potential eq. (3) and replacing the sum over $\vec{k}$ by an integral over ξ in eq. (2), we obtain the following BCS-like equation for determining the pairing gap and temperature T^*:

$$\frac{1}{\lambda^p} = \int_0^{\varepsilon_A} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2(T)}} \tanh\left[\frac{\sqrt{\xi^2 + \Delta^2(T)}}{2k_BT}\right], \quad (4)$$

where $\lambda^p = D_p(E_F)\tilde{V}^p$ is the BCS-like coupling constant, $D_p(E_F)$ is the density of states at the polaronic Fermi level, $\tilde{V}^p = V_{ph} - \tilde{V}_c$, $\tilde{V}_c = V_c/[1 + D_p(E_F)V_c \ln(\varepsilon_c/\varepsilon_A)]$ is the screened Coulomb interaction between two polarons.

For $T = T^*$ and $\varepsilon_c = E_F > \varepsilon_A > k_BT^*$, eq. (4) becomes

$$\frac{1}{\lambda^p} = \int_0^{\varepsilon_A} \frac{d\xi}{\xi} \tanh\left[\frac{\xi}{2k_BT^*}\right]. \quad (5)$$

In figure 1, the temperature dependence of the SC gap is shown for different values of BCS-like coupling constant λ^p. As shown in figure 1, the maximal value of the SC gap gets larger and larger when the BCS-like coupling constant λ^p is increased.

When $\varepsilon_A \gg k_BT^*$, we obtain the following general expression for T^*:

$$k_BT^* \simeq 1.134(E_p + \hbar\omega_{LO}) \exp\left[-\frac{1}{\lambda^p}\right]. \quad (6)$$

To determine the doping dependence of Δ and T^*, we can approximate the polaronic density of states in a simple form

$$D_p(E_F) = \begin{cases} 1/E_F & \text{for } \xi < E_F \\ 0 & \text{otherwise.} \end{cases} \quad (7)$$

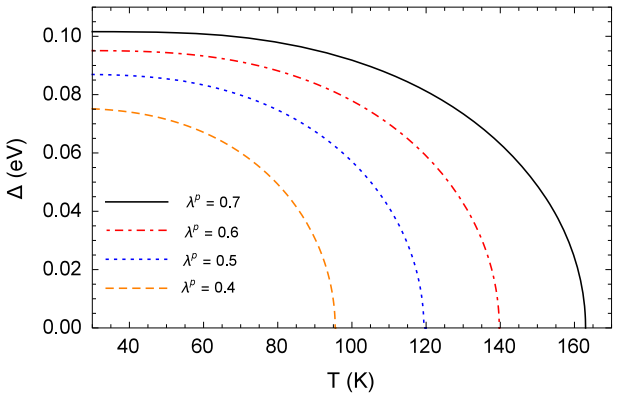

Figure 1. Temperature dependence of the SC gap Δ for different BCS-like coupling constants λ^p.

Then we obtain the following equations for $\Delta^*(p)$ and $T^*(p)$:

$$\Delta^*(p) = \frac{\varepsilon_A}{\sinh\left[\frac{\hbar^2(3\pi^2 n_a p)^{2/3}}{2m_p \tilde{V}^p}\right]}, \tag{8}$$

and

$$k_B T^*(p) \simeq 1.134\varepsilon_A \exp\left[-\frac{\hbar^2(3\pi^2 n_a p)^{2/3}}{2m_p \tilde{V}^p}\right], \tag{9}$$

where m_p is the mass of large polarons. It follows that both $\Delta^*(p)$ and $T^*(p)$ increase with decreasing doping, $p = n_p/n_a$ (where $n_a = 1/V_a$ is the density of the host lattice atoms, V_a is the volume per CuO_2 unit in the cuprates). Such doping dependences of the PG, $\Delta^*(p)$, and PG temperature $T^*(p)$ were observed experimentally in HTSCs [8,47,50–56].

The data in figure 2 demonstrate that there are two coexisting energy scales in the high-T_c cuprate superconductors: one associated with the SC T_c and the other, as inferred primarily from the antinodal region properties, with the PG T^*. As shown in figure 2, the predicted behaviour of T^* as a function of doping p is fairly consistent with the experimental results reported for Bi2212. We see that the PG cross-over temperature is above T_c of Bi2212, as observed in various experiments [8,51–56]. We determined doping from T_c via an empirical curve, $T_c = T_{c,max}[1 - 82.6(p - 0.16)^2]$, taking 96 K as the optimum T_c for Bi2212 [58].

The fact that the pseudogap measured in angle-resolved photoemission spectroscopy (ARPES) and scanning tunnelling spectroscopy (STS) experiments is only half the size of the gap in superconductor/insulator/superconductor (SIS), scanning tunnelling microscopy (STM), Raman and heat conductivity measurements, points to a pairing gap. So, although the origin of the pseudogap at finite doping remains uncertain, we are

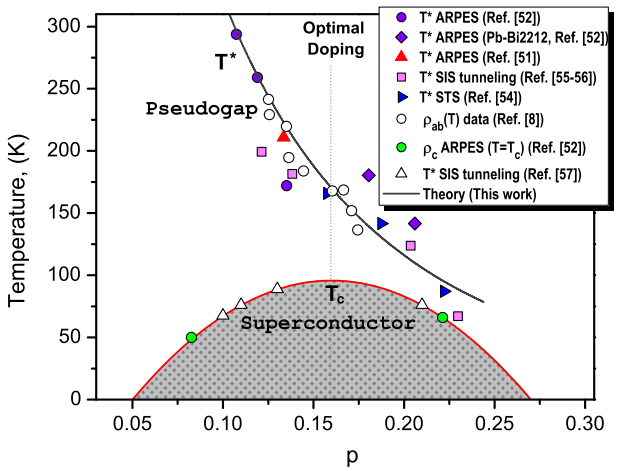

Figure 2. Proposed phase diagram $T^*(p)$ for $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) when $T_{c,max} \simeq 96$ K. The datapoints T^* were obtained as a function of hole doping p from the data of the ARPES measurements (refs [51,52]), STS [54] and SIS tunnelling experiments [55–57], and by analysing $\rho_{ab}(T)$ data (ref. [8]). The solid line is the fit to the experimental data (all symbols) using $T^*(p)$ (eq. (9)) with parameters $m_p = 2.1m_e$, $\varepsilon_A = 0.14$ eV, $\tilde{V}^p = 0.1$ eV and $n_a = 1 \times 10^{22}$ cm^{-3}.

of the opinion that it most likely reflects a pairing energy of some sort. To this end, the trend in figure 2 brings additional support to the picture discussed by many researchers that the reduction in the density of states at T^* is associated with the formation of electron pairs, well above the onset of phase coherence taking place at T_c (see, e.g. [59,60]). The pseudogap energy would then be the energy needed to break up a preformed pair. To conclusively address this point, it would be important to study very carefully the temperature dependence of the antinodal region (increases with underdoping) response below T_c; any further change with the onset of superconductivity, i.e. an increase in pseudogap energy, would confirm the two-particle pairing picture, while a lack thereof would suggest a one-particle band structure effect as a more likely interpretation of the pseudogap.

3. Relaxation time for lattice scattering

We now consider the scattering of charge carriers by the acoustic and optical lattice vibrations, in order to find the variation of relaxation times with the energy of the carrier and with the temperature of the crystal. We discuss the behaviour of energy- and temperature-dependent relaxation times determining the rate at which polaronic carriers and incoherent Cooper pairs are caused to change their $\vec{k}$-vectors and also their mobility in electric fields. Knowledge of the relaxation times for lattice

scattering will allow us to calculate the mobility of charge carriers of HTSCs.

From the Boltzmann transport equation and the principle of detailed balance, the relaxation time $\tau(\mathbf{k})$ of a carrier for any type of scattering is generally given by [61]

$$\frac{1}{\tau(\mathbf{k})} = \frac{V}{(2\pi)^3}\int \mathrm{d}^3\mathbf{k}' W(\mathbf{k},\mathbf{k}')(1-\cos\theta), \tag{10}$$

where $V = N\Omega$ is the crystal volume, $W(\mathbf{k},\mathbf{k}')$ is the scattering probability for charge carriers from $|\mathbf{k}\rangle$ to $|\mathbf{k}'\rangle$ states, θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$, N is the number of unit cells and Ω is the volume of a unit cell.

When we consider the lattice scattering, the transition rate of a carrier from the initial state $|\mathbf{k}\rangle$ to final state $|\mathbf{k}'\rangle$ is given by

$$W(\mathbf{k},\mathbf{k}') = \frac{2\pi}{\hbar}|\langle\mathbf{k}',\mathbf{q}'|H_{eL}|\mathbf{k},\mathbf{q}\rangle|^2 \times \delta[\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})\mp\hbar\omega_{\mathbf{q}}], \tag{11}$$

where H_{eL} is the electron-lattice (or phonon) interaction Hamiltonian and $|\mathbf{k},\mathbf{q}\rangle$ is given by the product of the electron wave function and the wave function of the scattering centre, which is a phonon $|\mathbf{q}\rangle$ with wave vector $\mathbf{q}$, $\varepsilon(\mathbf{k})$ and $\varepsilon(\mathbf{k}')$ are the energies of the initial and final states, $\hbar\omega_{\mathbf{q}}$ is the phonon energy.

3.1 *The relaxation time for carrier-acoustic phonon scattering*

The carrier-acoustic phonon interaction Hamiltonian is given by

$$H_{eL} = E_d\sum_{\mathbf{q}}\sqrt{\frac{\hbar}{2MN\omega_{\mathbf{q}}}}i\mathbf{q}\left(a_{\mathbf{q}}\mathrm{e}^{i\mathbf{qr}} - a^{+}_{-\mathbf{q}}\mathrm{e}^{-i\mathbf{qr}}\right), \tag{12}$$

where E_d is the deformation potential, M is the mass of atoms of the unit cell, $a^{+}_{\mathbf{q}}$ ($a_{\mathbf{q}}$) is the creation (annihilation) operator of a phonon, $\mathbf{r}$ is the position vector of the carrier.

In order to calculate the matrix element for this interaction Hamiltonian, we replace $|\mathbf{q}\rangle$ by $|n_{\mathbf{q}}\rangle$ (where $n_{\mathbf{q}}$ is the phonon number) and use the Bloch function

$$|\mathbf{k}\rangle = (N\Omega)^{-1/2}U_{\mathbf{k}}(\mathbf{r})\mathrm{e}^{i\mathbf{kr}}. \tag{13}$$

Then the wave functions of the initial and final states are given by

$$|\mathbf{k},\mathbf{q}\rangle = |n_{\mathbf{q}}\rangle\psi_{\mathbf{k}}(\mathbf{r}) \tag{14}$$

and

$$|\mathbf{k}',\mathbf{q}'\rangle = |n_{\mathbf{q}}+1\rangle\psi_{\mathbf{k}'}(\mathbf{r}), \tag{15}$$

respectively.

Further, the scattering probability $W(\mathbf{k},\mathbf{k}')$ is calculated by using the cyclic boundary conditions for the Bloch function

$$\sum_l \mathrm{e}^{i(\mathbf{k}-\mathbf{k}'-\mathbf{q})\mathbf{r}_l} = N,$$
$$\frac{1}{\Omega}\int u^*_{\mathbf{k}'}(\mathbf{r})u_{\mathbf{k}}(\mathbf{r})\mathrm{d}^3\mathbf{r} = 1 \tag{16}$$

and by taking into account the scattering processes corresponding to the phonon emission and absorption, and also the integral in eq. (10) with respect to $\mathbf{k}'$ is replaced by the integral over $\mathbf{q}$.

For acoustic phonons, the relation $\omega_{\mathbf{q}} = v_s q$ (where v_s is the sound velocity) holds, and the allowed values of $\mathbf{q}$ are determined on the basis of the relevant conservation laws ($\mathbf{k}' = \mathbf{k}\pm\mathbf{q}$ and $\varepsilon(\mathbf{k}') = \varepsilon(\mathbf{k})\pm\hbar\omega_{\mathbf{q}}$) as

$$q = 2k\left(\mp\cos\beta \pm \frac{m_p v_s}{\hbar k}\right), \tag{17}$$

where β is the angle between $\mathbf{k}$ and $\mathbf{q}$. When the condition $m_p v_s/\hbar k \ll 1$ is fulfilled (e.g., if $\hbar k \simeq m_p v_s = \sqrt{3m_p k_\mathrm{B}T}$, $m_p = 2m_e$, $v_s = 4\cdot 10^5$ cm/s and $T = 100$ K, the condition $m_p v_s/\hbar k < 0.084$ is fulfilled), the carrier-acoustic phonon scattering may be treated as elastic scattering. Under this condition, the allowed values of q range from 0 to $2k$. Above T^*, the expression for $\tau_{ac}(\mathbf{k})$ is then written as

$$\frac{1}{\tau_{ac}(\mathbf{k})} = \frac{V}{2\pi\hbar}\int_0^{2k} q^2\mathrm{d}q|V(\mathbf{q})|^2 \times \int_{\beta_{\min}}^{\beta_{\max}}\sin\beta\mathrm{d}\beta[(n_{\mathbf{q}}+1)\delta(\varepsilon(\mathbf{k}-\mathbf{q})-\varepsilon(\mathbf{k})) + n_{\mathbf{q}}\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k}))](1-\cos\theta), \tag{18}$$

where $V(\mathbf{q}) = E_d(\hbar/2MN\omega_{\mathbf{q}})^{1/2}i\mathbf{q}$ and the δ-function is written in the form

$$\delta\left[\frac{\hbar^2(\mathbf{k}\pm\mathbf{q})^2}{2m_p} - \frac{\hbar^2k^2}{2m_p}\right] = \frac{m_p}{\hbar^2kq}\delta\left[\frac{q}{2k}\pm\cos\beta\right]. \tag{19}$$

As far as we consider the elastic scattering, the vectors $\mathbf{k}$ and $\mathbf{k}'$ lie on the same energy surface (i.e. on the same sphere), and thus in this case the following relation holds:

$$1-\cos\theta = -\frac{q}{k}\cos\beta, \quad 0\le\theta\le\pi, \quad \frac{\pi}{2}\le\beta\le\pi. \tag{20}$$

Inserting relations (19) and (20) into eq. (18), using the approximation $n_{\mathbf{q}}+1 \approx n_{\mathbf{q}} \approx k_\mathrm{B}T/\hbar\omega_{\mathbf{q}} \gg 1$, and performing integration over q and β, we obtain

$$\tau_{ac}(\varepsilon) = \frac{\pi\hbar^4\rho_M v_s^2}{\sqrt{2}E_d^2 m_p^{3/2}k_\mathrm{B}T\sqrt{\varepsilon}}, \tag{21}$$

where ρ_M is the material density and $\varepsilon = \hbar^2k^2/2m_p$ is the energy of polarons.

3.2 *The relaxation time for carrier-optical phonon scattering*

In order to determine the relaxation time of large polarons at their scattering by longitudinal optical phonons in an ionic model, we consider the polarization of a crystal due to an ionic movement or longitudinal optical lattice vibrations given by [61,62]

$$P(\mathbf{r}) = e^* u(\mathbf{r})/\Omega \quad \text{or} \quad P(\mathbf{r}) = (N/V)e^* u(\mathbf{r}), \tag{22}$$

where e^* is the effective charge of ions, $u(\mathbf{r})$ is their relative displacement, $\Omega = 2a^3$, a is the distance between the nearest-neighbour ions.

The effective charge of ions is given by [62]

$$e^* = \sqrt{M\Omega\omega_0^2/16\pi^2\tilde{\varepsilon}}, \tag{23}$$

where $M = M_1M_2/(M_1 + M_2)$ is the reduced mass of ions (anions and cations) in the CuO_2 plane of the cuprates, ω_0 is the optical phonon frequency, $\tilde{\varepsilon} = (1 - \eta)/\varepsilon_\infty$ is the effective dielectric constant, ε_∞ and ε_0 are the high frequency and static dielectric constants, respectively.

When the condition $k_BT \ll \hbar\omega_0$ is satisfied, the relaxation time of large polarons scattered by optical phonons having the specific frequency $\omega_0 = \omega_{01}$ may be determined from the relation [61]

$$\frac{1}{\tau_{\text{op}}} = \frac{Vm_p^*(2\pi)^3e^{*2}e^2}{8\pi^2\hbar^2k^3NMa^6\omega_{01}} \exp\left[-\frac{\hbar\omega_{01}}{k_BT}\right] \times \left(2k\sqrt{k^2+k_0^2} - k_0^2 \ln\frac{\sqrt{k^2+k_0^2}+k}{\sqrt{k^2+k_0^2}-k}\right), \tag{24}$$

where k_0 is the wave vector corresponding to the polaron energy $\hbar\omega_{01}$:

$$\frac{\hbar^2k_0^2}{2m_p} = \hbar\omega_{01}. \tag{25}$$

For small k, the Taylor expansion of the expression in the square bracket with respect to $(k/k_0) \ll 1$ gives k^3/k_0. Next, we use the relation $\Omega = V/N = 2a^3$ and eq. (23). Then the relaxation time for polaron–optical phonon scattering is independent of the polaron energy and expressed as

$$\tau_{\text{op}} = \frac{4\sqrt{2}\pi\tilde{\varepsilon}(\hbar\omega_{01})^{3/2}}{\omega_{01}^2e^2\sqrt{m_p}} \exp\left[\frac{\hbar\omega_{01}}{k_BT}\right]. \tag{26}$$

4. The charge carrier mobility above and below T^*

The total scattering probability of polaronic carriers at their scattering by acoustic and optical phonons is defined as the sum of two possible scattering probabilities. In particular, the total relaxation time of polaronic carriers above T^* is given by

$$\frac{1}{\tau_p(\varepsilon)} = \frac{1}{\tau_{\text{ac}}(\varepsilon)} + \frac{1}{\tau_{\text{op}}} \tag{27}$$

and mobility

$$\mu_p(\varepsilon) = \frac{e\tau_p(\varepsilon)}{m_p}, \tag{28}$$

where

$$\tau_{\text{ac}}(\varepsilon) = \frac{A_p}{t\sqrt{\varepsilon}}, \qquad A_p = \frac{\pi\hbar^4\rho_M v_s^2}{E_d^2\sqrt{2}m_p^{3/2}k_BT^*},$$
$$t = \frac{T}{T^*}, \quad \tau_{\text{op}} = B_p \exp\left[\frac{\hbar\omega_{01}}{k_BT^*t}\right],$$
$$B_p = \frac{4\sqrt{2}\pi\tilde{\varepsilon}(\hbar\omega_{01})^{3/2}}{\omega_{01}^2e^2\sqrt{m_p}}.$$

Below T^*, the polaronic carriers in the energy layer of width ε_c around the Fermi surface take part in the BCS-like pairing and form Cooper pairs in the CuO_2 planes. If we use the property of δ-function $\delta[E(k') - E(k)] = (\mathrm{d}\varepsilon/\mathrm{d}E)\delta[\varepsilon(k') - \varepsilon(k)]$ in the expression for $\tau_p(k)$ below T^*, the relaxation time of large polarons at their BCS-like pairing is given by

$$\tau_{\text{BCS}}(\varepsilon) = \frac{E(\mathbf{k})}{|\xi(\mathbf{k})|}\tau_p(\varepsilon), \tag{29}$$

where $E(k) = \sqrt{\xi^2(k) + \Delta^{*2}}$ is the excitation spectrum of quasiparticles in the BCS-like PG state, $\xi(k) = \varepsilon(k) - \chi$, χ is the chemical potential of a polaronic Fermi gas. Therefore, we can consider polaronic Cooper pairs below T^* as an ideal Bose gas with chemical potential $\chi_B = 0$. The total relaxation time of polaronic Cooper pairs, which are scattered as the composite bosons at the acoustic and optical phonons below T^*, is determined from the relation

$$\tau_B(\varepsilon) = \frac{\tau_{\text{ac}}^c(\varepsilon)\tau_{\text{op}}^c(\varepsilon)}{(\tau_{\text{ac}}^c(\varepsilon) + \tau_{\text{op}}^c(\varepsilon))}, \tag{30}$$

where

$$\tau_{\text{ac}}^c(\varepsilon) = \frac{\pi\hbar^4\rho_M v_s^2}{E_d^2\sqrt{2}m_B^{3/2}k_BT^*t\sqrt{\varepsilon}},$$
$$\tau_{\text{op}}^c(\varepsilon) = \frac{4\sqrt{2}\pi\tilde{\varepsilon}(\hbar\omega_{02})^{3/2}}{\omega_{02}^2(2e)^2\sqrt{m_B}} \exp\left[\frac{\hbar\omega_{02}}{k_BT^*t}\right]$$

and $m_B = 2m_p$ is the mass of polaronic Cooper pairs.

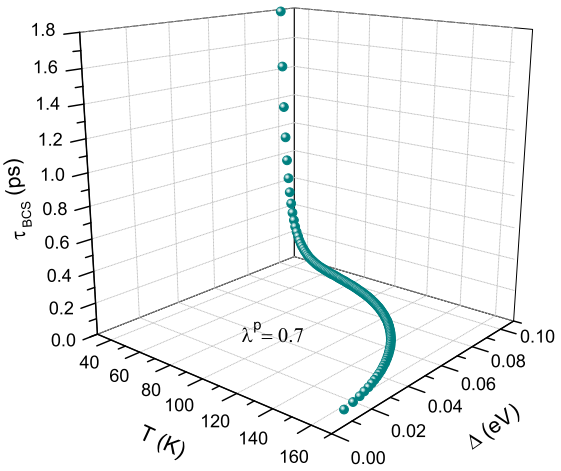

Figure 3. Relaxation time of polarons at their BCS-like pairing τ_{BCS} as a function of the temperature and SC gap Δ in the CuO_2 planes.

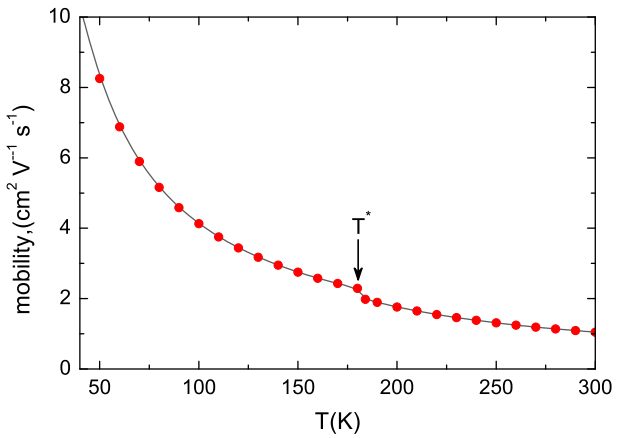

Figure 4. Temperature dependence of the charge carrier mobility above and below PG temperature in cuprate superconductors.

In figure 3, it is shown that the relaxation time of polarons at their BCS-like pairing τ_{BCS} is a function of the temperature and Δ within the CuO_2 planes. The SC gap Δ, which decreases with increasing temperature and related relaxation time τ_{BCS} also decreases with decreasing Δ.

Then, the expression for the mobility of bosonic Cooper pairs in the anisotropic cuprate superconductor at their scattering by acoustic and optical phonons can be written as

$$\mu_B(\varepsilon) = \frac{e\tau_B(\varepsilon)}{m_B}. \tag{31}$$

Figure 4 shows clearly that the charge carrier mobility (mobility of large polarons and bosonic Cooper pairs) vs. temperature in high-T_c cuprates exhibit a sharp drop at T^*.

5. Conclusion

In this work, we have studied polaron effects and the charge carrier mobility in HTSCs. We have calculated the mobility of polaronic carriers and bosonic Cooper pairs above and below the PG temperature T^*. Assuming the scattering of polaronic carriers and bosonic Cooper pairs at acoustic and optical phonons, we obtained appropriate expressions for the relaxation times of these carriers in high-T_c cuprates. In particular, we have derived different expressions for charge carrier mobility of cuprate superconductors above and below T^* by using the relaxation time approximation above T^* and considering BCS-like PG in the quasiparticle energy spectrum below T^*. It is shown that the scattering of polaronic carriers at acoustic and optical phonons is responsible for the charge carrier mobility above T^*. In particular, we have also found that the transition to the BCS-like PG regime and the mobility of bosonic Cooper pairs in the normal state of cuprates are responsible for the nonmonotonic temperature dependence of μ and upward deviation from the T-linear behaviour below T^*. Importantly, anomalous temperature behaviour of the charge carrier mobility in the PG state of cuprates is explained by the developed theory of charge transport naturally if one assumes that the polaronic carriers and bosonic Cooper pairs are scattered at different optical phonons having distinctive frequencies ω_{01} and ω_{02}.

We have also shown that the energy scales of the binding energies of large polarons and polaronic Cooper pairs are identified by PG cross-over temperature on the cuprate phase diagram.

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