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THE STATE OF ITINERANT CHARGE CARRIERS
AND THERMOELECTRIC EFFECTS IN CORRELATED OXIDE METALS

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Abstract

We analyzed the physics of transport processes and, in particular, the thermoelectric power in the mercurocuprates and other cuprates to get a better insight into the state of the carriers in these compounds. The actual problems related to the complicated mechanisms of carriers scattering above Tc are discussed. The experimental studies of thermoelectric power showed that the state of carriers in cuprates can be influenced by many complicated scattering processes, however the underlying mechanism for the linear decreasing of the TEP with increasing the temperature for most hole-doped HTSC cuprates is still not yet known. The actual problems related to the complicated mechanisms of carriers scattering above Tc are discussed for a few models of charge transport. A comparison between the analytical and experimental results is also made.

It is concluded that the crucial factor for the understanding of the transport properties of correlated oxide metals is the nature of itinerant charge carriers, i.e. renormalized quasiparticles.

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1 Introduction

There is considerable current interest in the properties of transition metal and rare-earth metal oxides. Copper and manganese oxides with perovskite structure, both pure and doped, are characterized by the anomalous transport properties. The copper high temperature oxides have been extensively investigated since their discovery. Particular importance is the question of interrelation of normal state properties and superconductivity. However a satisfactory overall picture of the nature of this high-Tc behaviour is still in the process of evolution [?]. Unfortunately, we have, at the present time, no generally accepted and complete formal theory of HTSC [?]. The essence of the problem is in the inherent interaction (and coexistence) between charge and spin degrees of freedom which are coupled in a very nontrivial self-consistent way [?]. This explains why the problem of the nature of the itinerant charge carriers in cuprates and manganites has attracted considerable attention. The normal state electronic properties are determined by the state of itinerant charge carriers too and it is of particular importance to investigate transport characteristics of the correlated oxides.

It is well established that the CuO_2 layers are responsible for the superconductivity in cuprates and that the electrical properties are governed by a charge carrier density of these layers. The studies of the mercurocuprate family of high-temperature superconductors (HTSC) has been the object of special interest during the last years because of their pronounced layered structure and the highest transition temperatures [?],[?].

To more fully characterize the normal and superconducting state properties of correlated copper oxides extensive studies of the electrical resistivity, Hall effect and thermoelectric power (TEP) measurements were performed for the broad interval of temperatures during the last decade.

The TEP or Seebeck coefficient measures the voltage generated in a metal by a temperature gradient [?], [?] . Thermopower measurements provide an important complementary method to characterize the state of the itinerant charge carriers in metals and semiconductors. In simple metals TEP measurements permit to study small changes in the Fermi surface. But even for simple metals and, moreover, for transition and rare-earths metals and compounds the interpretation of TEP data is much more difficult than that of thermal and electrical conductivities. TEP is very sensitive to higher order scattering processes. On the other hand, experimentalists are well aware of a great sensitivity of TEP to impurities and to the inhomogeneity of the specimen.

Nevertheless, the measurements of the thermoelectric power and other thermoelectric effects are considered as a convenient diagnostic tool to determine the character of the charge carriers in the normal state of the superconductive copper oxides and in the overdoped composition [?]-[?]. The transport data and, in particular, the TEP measurements play an important role in the investigation of the state of the itinerant charge carriers in $La - Ca$ manganites, inspiring both theoretical models and the interpretation of experimental results.

In spite of the fact that the temperature behaviour of the TEP in metals and alloys is a subject area in which there has been considerable activity for many years [?],[?], there are still substantial differences in its interpretation. It is possible to say that TEP :" is easy to measure, difficult to interpret"! For example, it is commonly believed that there can be no thermoelectric effects in superconductors. This is based on the early experiments on the Seebeck effect and on the Thomson heat, which show that in the usual stationary-state arrangement these effects vanish in the superconducting state. However, V.L. Ginsburg [?] conjectured that in a superconducting state the thermoelectric effects do not disappear, although it is not generally easy to observe them.

In the present paper we will analyze the TEP results above Tc and will not be concerned with the complicated problem of TEP for superconducting state. Our aim is to find a reasonably and workable model for the rationalization of the observed TEP data for high Tc cuprates and especially for the mercurocuprates.

2   TEP Measurements in the Cuprates

There has been a great interest in the studies of transport properties in the normal state of the copper oxides. A great deal of research has been devoted to measure the TEP. The earlier measurements were done on the La-based copper oxides $La_{2-x}M_xCuO_4$. For sample $La_{1.85}Sr_{0.15}CuO_4$ the measurements of TEP were performed in Ref. [?]. In the normal state above Tc, the transport coefficients indicate positive charge carriers with a concentration $p = 6.10^{21}cm^{-3}$. The TEP behaviour above Tc is unconventional; it displays a broad hump centered at 150 K. Below 150 K the TEP slowly drops with temperature and then drops abruptly to zero around Tc. Below 34 K the TEP is zero within experimental uncertainty. Well above the transition region the TEP is far different from that expected for a simple metal. In particular, the TEP is very nonlinear with temperature and the large, broad hump centered at 150 K appears to be both too wide and at too high temperature to be ascribed to the usual phonon-drag effect. The linear decreasing of the TEP with increasing the temperature is seen, but as yet there is no clear explanation as to its cause. Such a behaviour must be attributed to the very special scattering processes, however the underlying mechanism for the linear decreasing of the TEP with increasing the temperature for most hole-doped HTSC cuprates is still unknown.

Complementary TEP measurements were reported [?] for some La_2CuO_{4-y} oxides with Ba and Sr doping. The main efforts were devoted to the investigation of the effects of doping. The temperature dependencies of TEP were measured and similar behaviour was observed. The extensive studies of the temperature variation of the TEP in single-layer copper oxide were made in Ref. [?]. It was concluded that the hump in the TEP versus T curve cannot be accounted for easily by either phonon-drag or mass-enhancement mechanism found in metals and alloys. It is interesting to note that in Ref. [?] the trend in TEP behaviour for small concentration was

Table 1: SUMMARY OF EXPERIMENT
(TEP(S) is measured in $\mu V/K$;
n is the number of layers in elementary cell)

Sample \ Data	T_c	n	Θ_D	S(290K)	S_{max}	$S(\geq T_c)$	Ref
$La_{1.85}Sr_{0.15}CuO_4$	38	1	413	+ 14.2	+ 20.5	+ 11	11
$La_{2-x}Sr_xCuO_4$	-	1	413	+20	+ 32	+15	7
$Tl_2Ba_2CuO_{6+y}$	4-84	1	-	-12 to -15	-	-	16
$Bi_{1.6}Pb_{0.5}Sr_{0.9-y}La_yCu_{1.05}O_z$	11-16	2	-	2-3	16-17	1.5	15
$YBa_2Cu_3O_{7-y}$	92	2	-	3	3.8	-	13,16
$Tl_2Ba_2CaCu_2O_8$	108	2	-	17	-	-	29
$YBa_2Cu_3O_7$	92	2	410	2.2	2.5	-	40
$YBa_2Cu_3O_{6.6}$	65.9	2	-	22	31.7	-	16
$(Y,Yb)_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$	85.5	2	-	1-2	2-3	-	14
$Bi_2Sr_2CaCu_2O_8$	95	2	250	1-2	6	-	16,29
$Bi_2Sr_2CaCu_2O_{7.965}$	120	2	-	-	14.5	-	10,29
$HgBa_2CaCu_2O_{6+y}$	127	2	-	3-5	12	8	26
$HgBa_2Ca_2Cu_3O_{8+y}$	135	3	-	5	20	18	26
$HgBa_2Ca_4Cu_5O_{12}$	110-113	5	-	25	-	-	28

ascribed to the presence of strong correlations. It was argued that the temperature dependencies of TEP cannot be viewed as those for the simple, uncorrelated wide-band materials. This was the important confirmation of the fact that the Hubbard model is relevant for describing of the basic physics of these materials. This was confirmed also in Ref. [?] for TEP measurements in the $YBa_2Cu_3O_{7-y}$. The study of TEP over a fairly wide range of doping was made for polycrystalline samples $(Y,Yb)_{1-x}Ca_xBa_2Cu_3O_{7-\delta}$ showing characteristic evolution (see Fig.1) of $S(T)$ as a function of the doping state of the CuO_2 planes [?]. The TEP has a very diverse and unusual temperature dependence and even absolute values that are partially summarized in Table 1. Variations of physical properties of $Bi_{1.6}Pb_{0.5}Sr_{0.9-y}La_yCu_{1.05}O_z$ with the La-concentration y across the superconducting-nonsuperconducting metal boundary were investigated in Ref. [?]. It was found that TEP has a systematic change with y and exhibits quite unusual behaviour even in the nonsuperconducting metallic phase. The temperature dependence of TEP was fitted by the expression

$$S = AT + \frac{BT^\alpha}{(T + \Theta)^\alpha} \qquad (1)$$

where A is rather insensitive to the carrier concentration or y and B gives the T-independent part of TEP at high temperatures ($T >> \Theta$) and depends on y roughly linearly in the metallic region of $y \leq 0.6$. It is tempting to consider the first term as the one of ordinary metal and the second one as the contribution from the existence of the unusual mechanism.

In an important paper [?] TEP measurements were systematized as a function of hole concentration p for a number of oxides. This was stimulated by the fact that many superconducting

cuprates show a parabolic variation of T_c with hole concentration p; there is a minimum and a maximum hole concentration for superconductivity. In oxygen stoichiometric $La_{2-x}Sr_xCuO_4$ this dependence is given by [?]

$$T_c/T_{c,max} = 1 - 82.6(p - 0.16)^2 \qquad (2)$$

The systematic trend in the concentration dependence of TEP was revealed. It was shown that a universal correspondence of the room-temperature TEP with p over the whole range of doping can be supposed. The results , which almost fit each other, have been obtained for various compounds spanning the entire doping range from the very underdoped to the strongly over-doped regime. It was a remarkable observation also that there are close similarities in the TEP of several compounds and a change in sign of the room-temperature TEP near the maximum T_c. The correlation of the room-temperature S(290) for $Y_{1-x}Ca_xBa_2Cu_3O_6$ was established in Ref. [?]. This gives further confirmation of the reliability of the universal correlation between the TEP and the hole concentration. The correlation may be conveniently parameterized by the relation

$$S(290) = 372\exp(-32.4p) \quad for \quad 0.00 \leq p \leq 0.05 \qquad (3)$$

$$S(290) = 992\exp(-38.1p) \quad for \quad 0.05 \leq p \leq 0.155 \qquad (4)$$

$$S(290) = 139p + 24.2 \quad for \quad p \geq 0.05 \qquad (5)$$

In fact, all transport properties of HTSC exhibit a systematic dependence upon hole concentration. The TEP behaviour is the most representative and notable, as it shows the additional measurements of TEP in cuprates [?]- [?]. The representative results, which are shown in Fig.2, were obtained in Ref. [?]. In this paper the TEP $S(T)$ was measured for $YBa_2Cu_3O_{7-\delta}$ and $YBa_2Cu_4O_8$ as a function of Zn substitution and hole concentration p. A strong enhancement in $S(T)$ is correlated with the smooth opening of an energy gap in the normal-state spectrum. It was concluded that the TEP is determined by the strength of electron-electron interactions, which vary strongly with doping rather than by details of any scattering process.

3   Crystal Structure and Properties of the Mercurocuprates

The homologous series $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ is of special interest because it culminates the fascinating features of HTSC and are still most high-Tc representatives of cuprates (see Fig.3). Recently, there has been great progress in synthesis of high quality samples [?]- [?] and detailed structural studies.

The highest superconducting transition temperature at ambient pressure was observed for the third ($n = 3$) of Hg-based copper-mixed oxide series $HgBa_2Ca_2Cu_3O_{8+\delta}$(Hg-1223) with Tc (onset) at 135 K after which a saturation seemed to be reached . This feature of the highest Tc for $n = 3$ is analogous to that which occurred in the $Tl-$ and $Bi-$based series. There are

important differences between the mercurocuprates and the thallium analogue. One of the main differences is the one connected with the partially occupied oxygen sites in the region between CuO_2 planes, occupancy for which in mercurocuprates is very small. Thus the doping state of mercurocuprates can be controlled by changing the excess oxygen content.

As already mentioned, the different members of the mercurocuprate family are found to exhibit different optimal superconducting transition temperatures which increase up to the third member, after T_c decreases. An important and general structural feature of the mercurocuprates is that the apical $Cu - O$ distances are larger than the corresponding distances in the other cuprates and the Cu and O atoms forming the CuO_2-layers are coplanar. These structural features could be responsible for the highest transition temperature.

The charge carriers in active CuO_2 planes are the fundamental degrees of freedom which are primarily responsible for the essential physics. The problem how doping will modify the charge and spin distribution of the system is not well understood for HTSC [?]. Contrary to the insulating behaviour the doped systems are still not completely understood and create a number of controversy. This confirms the statement that the question about the true nature of carriers in the copper oxides is the topic which is one of the central in the field and is still open. It was emphasized that the distribution of charge among the CuO_2 layers should be understood in order to describe adequately the variation of T_c with the number of CuO_2 layer per unit cell in layered cuprates with three or more CuO_2 planes.

The carrier concentration p is a crucial factor determining the critical temperature $T_c(p)$ [?]. It was supposed that in HTSC a charge redistribution may occur between the reservoir block and active block under various conditions like applied high pressure or with the changing of composition, such as oxygen stoichiometry. In the multilayer structures there is a possibility of charge redistributing between the layers within a unit cell thus leading to models of "inequivalent" CuO_2 layers [?]. The inequivalent layer models reveal essential local physics arising from the sensitivity to the transition of one of the subsystems to the superconducting state so that p should rearrange when the system becomes superconducting. In the case considered here, i.e. the mercurocuprate family with $n \geq 3$, the different number of holes in inner and outer CuO_2 planes will reflect the possible charge redistribution transfer with the "reservoir" block.

The superconducting transition temperature dependence from the number n of CuO_2 planes in copper oxides was described recently in papers [?], [?] in the framework of workable phenomenological model and compared with experimental data.

4   TEP in the Mercurocuprates

The measurements of the TEP in the mercurocuprates were performed in papers [?] - [?]. In paper [?] the TEP of $Hg - 1223$ samples were measured. In the normal state, the TEP of the annealed samples shows a similar shape as a function of temperature: it decreases as temperature

increases, with the rate of decrease slowing down at higher temperatures. The TEP remains positive up to room temperature. In terms of universal correlation [?], [?] the observed data suggest that the studied samples were underdoped.

In paper [?] the temperature dependence of the TEP for $Hg - 1222$ and $Hg - 1223$ samples was measured. The peculiar temperature dependence is similar to that reported for other high-T_c superconducting cuprates. The TEP monotonically decreases with increasing the degree of oxidation and shows negative values in overdoped region. The results of TEP measurements indicate that $Hg - 1222$ follows the universal relation between $S(290)$ and T_{cmax}/T_c or the hole concentration of Ref. [?]. That is to say, $S(290)$ decreases monotonically with increasing the hole concentration and exhibits a slightly positive value of approximately $3 - 5\mu V/K$ for optimally doped samples. For the $Hg - 1223$ samples the temperature dependence of TEP is similar to that observed in $Hg - 1222$ as well as other high-Tc cuprates. An interesting observation was made as regards to the room-temperature TEP $S(290K)$. It decreases systematically with increasing the Cu valency, suggesting that it also follows the universal relation of Ref. [?].

The recent measurements of thermal conductivity versus temperature [?] over a broad range of doping in $YBCO$ and $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ (n = 1,2,3) suggest that small domains of localized holes develop for hole concentration near $p = 1/8$. The data imply a mechanism for localization that is intrinsic to the CuO_2 planes and is enhanced via pinning associated with oxygen-vacancy clusters. The peculiar charge- and spin-ordered phases, like stripe order may exist at CuO_2 planar hole concentrations near $p = 1/8$ for which the modulation wavelength is commensurate with the lattice. The neutron scattering experiments suggest (however not ultimately) that stripe modulation (when an appropriate pinning potential is present) are disordered and/or fluctuating in $LSCO$ and $YBCO$. There are some additional evidences for the existence of localized holes in the CuO_2 planes. It is important to understand more clearly whether localized holes are a general feature of cuprates and contribute to short-ranged charge-spin segregation and the normal-state pseudogap. In paper [?] it was concluded that a fraction of the doped holes in the CuO_2 planes become localized near the particular doping level. The authors conjectured the formation of nanoscale, hole-localized domains that are pinned near oxygen-vacancy clusters. This suggests a possible connection with the physics of stripe formation and raises questions about the generality of this phenomenon and the role of oxygen vacancies. The measurements of TEP in this paper were made for the mercurocuprates with $p = 0.104 - 0.205$ and the data are qualitatively similar to that of other results.

5   TEP and Models of Transport

It is widely recognized that the unusual normal-state properties of the high-Tc cuprates are strongly related to the unusual electronic ground state which may give rise to formation of the high-Tc superconducting state. To get a better insight into the transport properties of cuprates

we analyzed the thermoelectric power. The diffusion TEP is related to dc electrical conductivity σ in the semiclassical Mott's model [?] by

$$S_0 = -\frac{\pi k_B^2 T}{3|e|}\frac{\sigma'(E_F)}{\sigma(E_F)} \tag{6}$$

where the derivative is made with respect to energy and is evaluated at the Fermi energy E_F. The conductivity can be related to Fermi-surface parameters as

$$\sigma = \frac{e^2}{12\pi^3\hbar}\tau(E_F)vS_F \tag{7}$$

where S_F is the Fermi-surface area. The sign of the thermopower will indicate the sign of the majority carrier because of the S_F term. Recently such kind of theory has been used recently for a describing the experiments on thermoelectric effects in La-based cuprates [?].

This approach is based on the Sommerfeld expansion, as most theoretical works, in spite of the fact that in some systems of correlated electrons the application of this expansion may lead to considerable errors. It is a low temperature expansion and is suitable when temperature tends to zero. The additional assumptions are that the physical properties which are responsible for the DOS and relaxation time are analytic near and on the Fermi surface, which is valid for a Fermi liquid model.

To write down the Sommerfeld expansion explicitly, let us consider a function $A(\omega)$ which at the Fermi energy E_F can be expanded

$$\int_{-\infty}^{\infty}(-\frac{df}{d\omega})A(\omega)d\omega = A(E_F) + \frac{\pi^2}{6}(k_BT)^2(\frac{d^2A}{d^2\omega})_{\omega=E_F} + ... \tag{8}$$

Here $f(\omega)$ is the Fermi function. The next step is to determine the transport relaxation time $\tau(\omega,T)$. The transport properties of the isotropic metals are determined by

$$L_n = \int_{-\infty}^{\infty}(-\frac{df}{d\omega})\omega^n\tau(\omega,T)d\omega \tag{9}$$

Here the energy dependence of DOS and electron velocity was neglected. This is not reliable for the TEP, since the thermopower is particularly sensitive to the changes of the density of states at the Fermi level. The expression for the resistivity has the form with these notations

$$\rho = \frac{m}{pe^2}L_0^{-1} \tag{10}$$

where p is the conduction electron density. For the diffusion TEP we obtain

$$S_d = \frac{L_1}{eTL_0} \tag{11}$$

The above formulae were derived within a free-electron-approximation and for Boltzmann transport model. For this model the diffusion TEP is expected to be linear in temperature according to the expression

$$S = \frac{\pi^2}{2}\frac{k_B}{e}\frac{T}{T_F} = 142(\frac{T}{T_F})\frac{\mu V}{K} \tag{12}$$

A deviation from linearity indicates that special electronic scattering processes are occurring. In addition to the diffusion TEP in metals there may exist a phonon-drag TEP contribution which can give a large enhancement to the total TEP. An estimation for phonon-drag contribution shows that this will be the case at roughly 0.2 - 0.1 the Debye temperature Θ_D. This phonon-drag enhancement (if it exists) will usually manifest itself in TEP as a large peak at low temperatures. Hence, the TEP within the simplified free-electron model for a simple metal should be linear in temperature at high temperatures and may exhibit a phonon-drag peak near $T \approx 0.1\Theta_D$.

In the theory of thermoelectric effects an important role play the Gorter-Nordheim relation. This relation connects the total TEP S_d due to two different types of scattering mechanisms $\alpha = 1, 2$ with the partial TEPs. The G-N relation can be written as

$$S_d = \rho^{-1} \sum_\alpha S_{d\alpha} \rho_\alpha \tag{13}$$

This rule is based on the assumption that the two transition probabilities for the scattering of the conduction electrons by two channels are independent. Formally this is expressed by

$$\tau^{-1}(\omega) = \tau_1^{-1}(\omega) + \tau_2^{-1}(\omega); \quad \rho = \rho_1 + \rho_2 \tag{14}$$

There are special situations, especially in strongly correlated systems, when the Gorter-Nordheim relation does not fulfil.

In paper [?] a more general expression for the TEP has been derived. It has the following form

$$S = -\frac{k_B}{e} \int (\frac{\omega - E_F}{k_B T}) \frac{\sigma(\omega)}{\sigma} d\omega; \quad \sigma = \int \sigma(\omega) d\omega \tag{15}$$

However, the derived expression has general validity when correlation effects are neglected.

To discuss the TEP more carefully, it is necessary to know the chemical potential as a function of T. The microscopic derivation must include the correct heat and charge fluxes

$$S = \frac{1}{eT} [\frac{L_1}{L_0} - \mu] \tag{16}$$

$$L_0 = \frac{1}{V} \int_0^\infty dt' \int_0^\beta d\lambda < v_x(-i\hbar\lambda) v_x(t') > \tag{17}$$

$$L_1 = \frac{1}{V} \int_0^\infty dt' \int_0^\beta d\lambda < Q_x(-i\hbar\lambda) v_x(t') > \tag{18}$$

The partial analysis of TEP for the $t - J$ model near the half-filling was made in Ref. [?]. For the $t - t' - J$ model the variational numerical calculations of the TEP dependence on the concentration of carriers were performed by Trugman [?]. In both papers [?], [?] the decreasing of TEP with increasing of temperature above the broad hump was not explained.

A simple phenomenological model for the interpretation of the TEP measurements on $YBa_2Cu_3O_{7-y}$ was proposed in Ref. [?]. The results were interpreted assuming that the carriers conduct in a narrow band, where the carrier concentration in the band and the dominant scattering mechanism are determined by the concentration of oxygen vacancies. Recently, Ashkenazi [?], [?] proposed a scenario for an explanation of transport properties of correlated oxides.

The systematic behaviour of the resistivity, Hall constant and TEP was derived within a picture of a striped structure with three types of carriers. To get the typical behaviour observed in the cuprates the TEP has been parameterized as Eq.(1) (see Ref. [?]). The effect of the doping of a cuprate within this picture is both in changing the density of the charged stripes within a CuO_2 plane, and in changing the concentration of carriers ("stripons") n^p within a charged stripes. The corresponding contribution in TEP was given by

$$S^p = \frac{k_B}{e} \ln[\frac{1-n^p}{n^p}]$$ (19)

The possible role of a static charge ordering into hole-rich stripes on the temperature behaviour of TEP was discussed qualitatively in Ref. [?] in the context of normal state properties of the $La_{2-x}Ba_xCuO_4$ under different hydrostatic pressures. The same was done very recently in paper [?] for the mercurocuprates with $n = 3, 5$.

An alternative interesting approach for the accounting of the transport data of cuprates is related to the phenomenology of two-lifetime physics in the cuprates, which was discussed in Refs. [?], [?]. This phenomenology is based on the Anderson's conjecture that there are two transport relaxation times in the cuprate metals which independently govern the decay of electrical and Hall currents. The experiment shows that in $La_{2-x}Sr_xCuO_4, x = 0.17$

$$\rho_{xx} \sim \Gamma_{tr} \sim T; \quad \frac{\rho_{xy}}{R_H} \sim \frac{\Gamma_H}{\omega_c}$$ (20)

And for the inverse Hall relaxation time

$$\Gamma_H \sim aT^2 + b$$ (21)

The conjecture was that

$$\theta_H^{-1} \sim aT^2 + b \Longrightarrow \Gamma \sim aT^2 + b$$ (22)

and

$$\sigma_{xx} \sim \frac{1}{\Gamma_{tr}}$$ (23)

$$\sigma_{xy} \sim (\frac{1}{\Gamma_{tr}})(\frac{\omega_c}{\Gamma_H})$$ (24)

The remarkable experimental confirmation was the observation that

$$\sigma_{xy} \sim \tau_{tr}\tau_H$$ (25)

This observation suggests that the two different relaxation rates at each point on Fermi surface may exist. In other words, the experimental observations are taken to indicate the existence of two separate and essentially decoupled scattering times governing longitudinal transport and Hall transport. These two intrinsic lifetimes are assumed to coexist at all points on the Fermi surface.

Table 2: TWO LIFETIMES PHENOMENOLOGY

Standard metal	$\sigma_{xx} \sim \tau$	$\sigma_{xy} \sim \omega_c \tau^2$	$\tan\theta_H \sim \omega_c \tau$	$\tilde{S} \sim T$
Cuprates	$\sigma_{xx} \sim \tau_{tr}$	$\sigma_{xy} \sim \omega_c \tau_{tr}\tau_H$	$\tan\theta_H \sim \omega_c \tau_H$	$\tilde{S} \sim \tilde{S}_0 - bT; S/T = a + bR_H(T)$

Two lifetime physics in the cuprates consider it as the single band materials, so there at least the Hall effect should be understandable. This phenomenology for the cuprates is summarized in Table 2. Here τ_{tr} and τ_H are the transport and Hall relaxation times respectively, $\omega_c = eB/m$ is the cyclotron frequency and θ_H is the Hall angle:

$$\rho_{xx} = \frac{m^*}{pe^2}\frac{1}{\tau_{tr}}; \quad \tan\theta_H = \rho_{xy}/\rho_{xx} = \omega_c\tau_H \tag{26}$$

It is well known that under the condition of the equality of the effective masses and relaxation times for transversal and longitudinal motion the Hall constant is given by

$$R_H = \frac{1}{pe} \tag{27}$$

In the cuprates the τ_{tr} has a temperature dependence which varies with doping, but $\tau_H \sim bT^{-2}$, and b is only a weakly doping dependent, even in underdoped materials when the pseudogap has opened. Since the Hall angle $\theta_H = \tan^{-1}(\sigma_{xy}/\sigma_{xx})$ involves $1/\tau_H$ only, it implies that

$$\cot\theta_H = 1/\omega_c \sim aT^2 \tag{28}$$

This equation shows that the Hall angle, rather than R_H, is the most incisive probe of the anomalous effect because it does not involve τ_{tr}. In this spirit the theory introduces two independent lifetimes at every $\vec{k}$ point

$$l_1 = \vec{v}_{F1}\tau_1; \quad l_2 = \vec{v}_{F1}\tau_2$$

Microscopic derivation within this picture is still controversial; it is not clear how to make response functions couple selectively to each lifetime to obtain suitable results. The full construction of the two lifetimes phenomenology is not the scope of the present paper. We shall confine ourselves to the estimations of the TEP within this approach.
The consideration of the thermoelectric conductivity [?]

$$\beta_{xx} = -(\frac{\pi^2 k_B}{3e})(\frac{k_B T}{E_F})\frac{pe^2}{m}\tau_{TE} \tag{29}$$

in combination with the electrical conductivity, $\sigma_{xx} = (pe^2/m)\tau_{tr}$ leads to the following expression for the dimensionless thermopower

$$\tilde{S} = \frac{eS}{k_B} = (\frac{\tau_{TE}}{\tau_{tr}})(\frac{\pi^2}{3})(\frac{k_B T}{E_F}) \tag{30}$$

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From the analysis of the optimally doped compounds [?], the authors conclude that the TEP contains an unusual constant part, $\tilde{S} \approx \tilde{S}_0 - bT$ where $\tilde{S}_0 \sim 0.1$, which indicates that

$$\tau_{TE}^{-1} = T^2 / W_{th} \tag{31}$$

is a factor $T / \eta W_{th}$ smaller than the transport relaxation rate. Here

$$W_{th} = (3\tilde{S}_0 / \pi^2 \eta) E_F \sim 0.1 E_F \tag{32}$$

Here the conclusion of paper [?] was taking into account that in YBCO, the transport scattering rate $1/\tau_{tr}$ that appears in resistivity is linear in T above the transition temperature T_c, viz. $\hbar/\tau_{tr} = \eta k_B T$, with $\eta \approx 2$.

From this consideration a conclusion has been made [?] that the comparable size and temperature dependence of τ_{TE}^{-1} and τ_H^{-1} suggest that the same type of quasiparticle carries both the Hall current and the thermocurrent.

This conjecture was formalized as the scaling of thermopower with the Hall constant $R_H(T)$ in the following form

$$\frac{S}{T} = \frac{e\tilde{l}_0}{2E_F}[\omega_\rho^{-2} + \omega_c^{-1} R_H(T)] \tag{33}$$

Here $\tilde{l}_0 = \pi^2 k_B^2 / 3e^2$ is the Lorentz number. So for a given doping

$$\frac{S}{T} = a + bR_H(T) \tag{34}$$

It was argued that an analysis of the TEP data which was based on this scaling gives an indication that the two lifetimes may be responsible for anomalous thermopower in $Tl - 2212$ and $YBCO$ thin films and the magnetotransport in $Tl_2Ba_2CuO_{6+\delta}$ [?]. It was speculated that carriers scatter from objects [?] with $(\frac{Q}{P}) = \frac{e}{k_F}$ but phases are independent around Fermi surface (metallic environment). Scattering is sensitive to conjugation symmetry. The consistent microscopic picture and corresponding theory are still open questions for this phenomenological approach. It should be emphasized that there is the more conventional class of transport models which exploits the fourfold anisotropy of the cuprate Fermi surfaces and postulates the existence of an anisotropic scattering rate whose magnitude and temperature dependence is different on different parts of Fermi surface.

6   Electron-Phonon Interaction Effects and TEP

The temperature dependence of metallic diffusion TEP arising from electron-phonon enhancement was studied for LSCO high-Tc superconductors in Ref. [?]. The role of electron-phonon interaction in producing the peculiar normal and superconducting properties of cuprates is not fully transparent. As we argued before, the TEP is the least understood of the transport properties. The thermoelectricity coefficients of a metal are enhanced at low temperatures by large many-body effects which must be taken into account in any quantitative calculation of TEP.

The thermoelectric coefficients consist of two components, the electron diffusion and phonon-drag. Many-body effects appear only in the electron-diffusion component. This component is determined by energy derivatives of quasi-particle properties. It is convenient to distinguish the two categories of many-body effects, one of which has to do only with intrinsic properties of the quasi-particles, such as mass and velocity, and the other which is associated with quasi-particle scattering.

The first category consists of two effects. One is the enhancement of the bare mass of the carrier by a factor $(1 + \lambda)$, which appears in the thermoelectric coefficients as an enhancement in the density of states at the Fermi energy by this same factor. Small, but strongly energy dependent corrections to the quasi-particle velocity, over and above the $(1 + \lambda)$ correction, are the second effect, which can also produce a significant contribution to some thermoelectric coefficients.

The second category contains several effects, amongst them a many-body corrections to the scattering of electrons by phonons and subtle many-body corrections to the scattering of electrons by impurities.

By measuring selected thermoelectric effects in metals, it has been shown that all of the thermoelectric coefficients are enhanced by the factor $(1 + \lambda)$. The many-body effects of quasiparticle scattering are competing with the alternative interpretations of the same observable data, primarily interpretations based upon anisotropic electron-impurity scattering.

For the cuprates, it was argued [?] that diffusion TEP is enhanced at low temperatures by the $(1 + \lambda)$ factor, where λ is the electron-phonon interaction parameter. The calculation of the temperature dependence of metallic diffusion TEP, including additional effects arising from velocity and relaxation-time renormalization and from the higher-order diagrams, gives [?]

$$S_d = S_0[1 + a\lambda\lambda_s(T)] \tag{35}$$

where S_0 is the bare diffusion TEP, a is the constant, and λ_s is the normalized temperature-dependent enhancement of TEP. When one scattering mechanism dominates, and if the density of states does not vary too sharply near the Fermi level, the bare TEP S_0 will be approximately linear in temperature for nonmagnetic metals. The other important requirement for the observation of the electron-phonon enhancement effect in TEP is the absence of the phonon-drag term, which in normal crystals is the dominant contribution to TEP at intermediate temperatures. For the most hole doped cuprates the TEP does not show any sign of phonon drag. However, some authors have tried to describe the unusual temperature dependence of TEP at high temperatures $T \geq 0.1 - 0.2\Theta_D$ as the contribution from the phonon drag effects via the function

$$S(T) = S_d + S_g \sim AT + B/T \tag{36}$$

In paper [?] it was speculated that the broad hump is a manifestation of special phonon-drag scattering which is related to the unusual lattice softening effects. The authors supposed that it

was possible that soft modes could couple to the charge carriers under a temperature gradient through phonon-drag scattering.

7 Conclusions

In summary, in this paper we have analyzed the temperature dependence of the TEP in hole-doped cuprates. The mechanism which causes the observed unusual behaviour is not clear at the present time. We noted that not all of earlier theories support the observable temperature dependence. There are several possibilities to account for the unusual temperature behaviour which was observed. We presented a few models of transport with which there is hope to rationalize some portion of experimental data for the cuprates. Clearly more work is needed to verify these models and approaches to the consistent and fully microscopic theory of transport processes and TEP in correlated oxide metals.
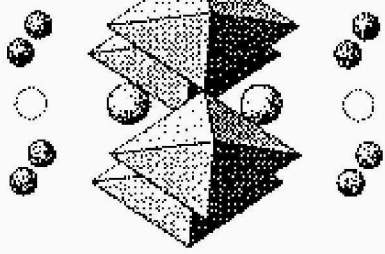
8 Acknowledgements

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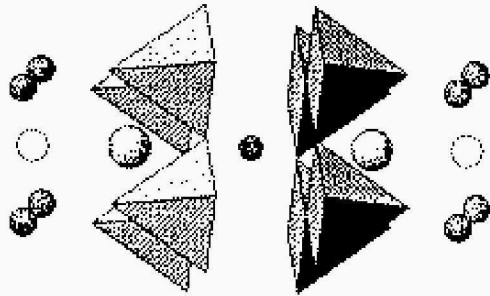
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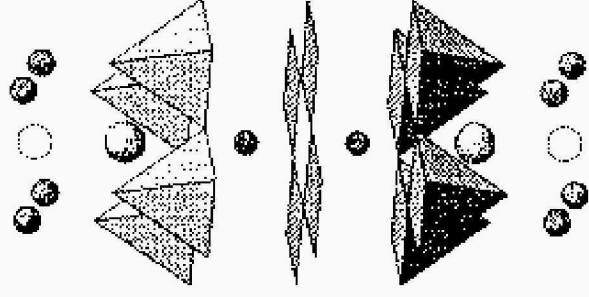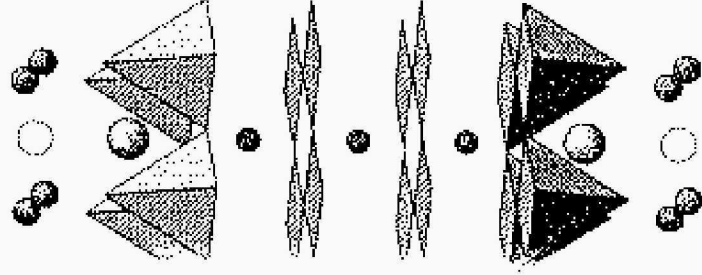[40] A. B. Kaiser and G. Mountjoy, Phys. Rev. B43 (1991) 6266.

n = 1   n = 2   n = 3   n = 4

CuO₂ polyhedra

Hg
Ba
Ca
Interstitial O (δ) – partially occupied