Carrier localization, Anderson transitions and stripe formation in hole-doped cuprates

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Abstract. Three distinctly different scenarios are proposed for the carrier localization in three-dimentional (3D) lightly doped cuprates in which the self-trapping and pairing of hole carriers (i) near the small-radius dopants and (ii) in a defect-free deformable lattice lead to the formation of the extrinsic and intrinsic (bi)polaronic states in the charge-transfer gap of the cuprates, and (iii) the self-trapping of hole carriers away from the large-radius dopants results in the formation of the in-gap hydrogenic impurity states. We have shown that the extrinsic and intrinsic 3D large bipolarons exist in La-based lightly doped cuprates at $\eta = \varepsilon_\infty/\varepsilon_0 < 0.127$ and $\eta < 0.138$, respectively, where $\varepsilon_\infty(\varepsilon_0)$ is the optic (static) dielectric constant. We use the uncertainty relation to obtain the specific conditions for the Anderson and new MITs in cuprates. The applicability limits of these MITs in La-based cuprates are clarified. Our results are in good agreement with the existing experiments on La-based cuprates.

1. Introduction

Understanding the mechanisms of carrier localization, metal-insulator transitions (MITs), stripe formation and suppression of high-T_c superconductivity in hole-doped cuprates remains one of the central issues in condensed matter physics. In hole-doped cuprates, the phenomena of carrier localization and MITs seem to be much more complicated by carrier-dopant (defect)-lattice or carrier-lattice interaction effects, which usually were ignored in the existing theoretical models. In reality, there are important unexplained differences between the MITs observed in lightly doped [1, 2, 3], underdoped [4, 5, 6] and optimally doped [7] cuprates. Another unresolved issue in the physics of high-T_c cuprates is the role of the electronic inhomogeneity and charge ordering in the phase separation in the form of alternating dynamic and static stripes [8, 9, 10, 11, 12], which is intimately related to carrier localization, MITs and superconductivity in these materials. Our main purpose is to understand the possible microscopic mechanisms leading to the carrier localization, MITs, stripe formation and suppression of superconductivity and to propose a unified theoretical description of these interrelated phenomena in the cuprates.

2. Possible Scenarios for Carrier Localization in Lightly Doped Cuprates

Hole doping of the cuprates produces first quasi-free holes having the mass m_b in the oxygen valence band. In polar cuprates, these hole carriers interacting both lattice vibrations and with lattice defects (e.g. dopants or impurities) are self-trapped either near the defects (defect-assisted extrinsic self-trapping) or in a defect-free deformable lattice (phonon-assisted intrinsic self-trapping). Therefore, the ground states of such hole carriers are their self-trapped (i.e.

localized extrinsic and intrinsic polaronic) states lying in the CT gap of the cuprates [13]. A large ionicity of the cuprates $\eta = \varepsilon_\infty/\varepsilon_0 << 1$ (where ε_∞ and ε_0 are the high-frequency and static dielectric constants, respectively) enhances the polar electron-phonon interaction and the tendency to polaron formation. Actually, the relevant charge carriers in hole-doped cuprates are large polarons [13, 14, 15, 16] and the strong electron-phonon interactions are responsible for enhancement of the polaron mass $m_p = (2.0 - 3.0)m_b$ [17] (where $m_b \simeq m_e$ is the free electron mass). The formation of nearly small Frölich polaron [18] might be also relevant. According to Ref.[13], the ground state energies or binding energies E_{ep} of extrinsic polarons would increase rapidly with decreasing ε_∞ from 5 to 3 or with increasing η from 0 to 0.12 and are equal to $E_{ep} \simeq (0.11 - 0.18)$ eV (for $\varepsilon_\infty = 3.5 - 4.5$ and $\eta = 0.12$) and $E_{ep} \simeq (0.086 - 0.14)$ eV (for $\varepsilon_\infty = 4$ and $\eta = 0 - 0.12$). Whereas the binding energies E_p of intrinsic polarons would decrease noticeably with increasing η from 0 to 0.12 (i.e. $E_p \simeq (0.085 - 0.065)$ eV for $\varepsilon_\infty = 4$ and $\eta = 0 - 0.12$), but E_p increases from 0.054 eV to 0.09 eV with decreasing ε_∞ from 4.5 to 3.5 at $\eta = 0.10$. We believe that the carrier-defect-phonon and carrier-phonon interactions together with the charge inhomogeneities play an important role in hole-doped cuprates and are responsible for the carrier localization and segregation. In these materials, the inhomogeneous spatial distribution of polaronic carriers leads to their segregation into carrier-rich and carrier-poor regions. Perhaps the carrier-defect-phonon and carrier-phonon interactions give rise to charge aggregation in carrier-rich metallic regions together with charge depletion in spatially separated carrier-poor regions with no mobile carriers. In general, the local charge inhomogeneity and the competition between the kinetic energy and the aligning interactions produce nanoscale self-organized structures called stripes. Further, the anisotropy of the dielectric constants (ε_∞ and ε_0) and smallness of η in the cuprates favor such a carrier segregation.

3. Possible mechanisms of metal - insulator transitions and stripe formation in cuprates

The binding energy of the intrinsic large bipolaron is defined as

$$\Delta_b = E_{bB} - 2\varepsilon_F, \tag{1}$$

At a certain doping level $n = n_c$ or $x = x_c = n_c/n_a$, $\Delta_b = 0$ and the large bipolaron will dissociate into two large polarons. Therefore, the critical carrier concentration n_c determined as

$$n_c = (m_p E_{bB})^{3/2}/3\pi^2\hbar^3 \tag{2}$$

For the LSCO system we can evaluate n_c using the parameter values $m_p = 2.1m_e$, $\varepsilon_\infty = 3.5 - 4.5$, $\eta = 0.04 - 0.08$, $E_{bB} \approx 0.01 - 0.10$ eV. We attempt to find the conditions under which such a insulator-to-metal transition occurs in doped materials.

The conditions for carrier localization or delocalization can be obtained by using the uncertainty principle: $\Delta p \Delta x \geq \hbar/2$. This uncertainty relation can be written as

$$\Delta x \cdot \Delta E \simeq \frac{\hbar^2(\Delta k)^2}{2m^*} \frac{1}{2\Delta k}, \tag{3}$$

Taking into account that in the impurity band the uncertainties in the energy of carriers is of order $W_I/2$ and the uncertainty in their wave vector is about $1/a_I$, the relation (3) can be rewritten in the form (cf.[19])

$$\Delta x \cdot \Delta E \cong W_I a_I/4 \tag{4}$$

Since, a random potential V_0 leads to the uncertainties in the energy $\Delta E \sim V_0/2$ and coordinate $\Delta x \sim a_H$ of carriers, the condition for Anderson localization can be written as

$$V_0/W_I > 0.5a_I/a_H, \tag{5}$$

We believe that the strong carrier-defect-phonon and carrier-phonon interactions can initiate MITs in cuprates. The condition for carrier localization or a new type of MIT can be written as

$$E_{pI}/W_I > 0.25a_I/R_I, \qquad (6)$$

from which it follows that the MIT is governed by the ratios E_{pI}/W_I and a_I/R_I.

We examine below the possibility of the Anderson and new MITs and stripe formation in La-based cuprates.

3.1. The Anderson-type metal-insulator transitions
In inhomogeneous hole-doped cuprates the randomness in dopant distribution affects on the depths of the potential wells of impurities. In disorder system the volume Ω_0 may contain two or more impurities at the random spatial distribution of dopants and the energy of a carrier in the field of l impurities is equal to lE_I [20]. One can expect that the depth of the potential well for the carrier varies from 0 to lE_I and $V_0/2 \simeq lE_I/2$. The case $l = 2$ is assumed to be more probable. Therefore, we can take $V_0 = 2E_I^H$ and write the condition (5) in the form

$$z \exp\left[-R/a_H\right] = a_H/a_I \qquad (7)$$

Taking into account that dopants form different superlattices with the site disorder, we obtain the following criteria for the Anderson-type MITs:

$$(z/n^{1/3}a_H)\exp[-1/n^{1/3}a_H] = 1 \quad \text{for} \quad z = 6, \qquad (8)$$

$$(\sqrt[3]{2} \cdot z/n^{1/3}a_H)\exp[-\sqrt{3}/\sqrt[3]{4} \cdot n^{1/3}a_H] = 1 \quad \text{for} \quad z = 8, \qquad (9)$$

$$(\sqrt[3]{4} \cdot z/n^{1/3}a_H)\exp[-2^{1/6}/n^{1/3}a_H] = 1 \quad \text{for} \quad z = 12. \qquad (10)$$

From equations (8),(9) and (10), we find $n^{1/3}a_H \simeq 0.3530$, $n^{1/3}a_H \simeq 0.3148$ and $n^{1/3}a_H \simeq 0.2618$, respectively. If we assume $a_H = 7 - 8\mathring{A}$ [1], we find $x_c \simeq 0.0116 - 0.0173$ (for $z = 8$), and $x_c \simeq 0.0163 - 0.0243$ (for $z = 6$) at which the coexistence of the metallic and insulating stripes and the transition from the metallic to the insulating behavior were observed in lightly doped cuprates (see [21, 22]). For example, experimental results show that the degeneration of hole carriers occurs at the appearance of the first metallic stripes for $x \approx 0.02$ [2].

3.2. The new metal-insulator transitions and stripe formation
The width of the energy band of extrinsic large polarons or impurities with tightly bound large polarons can be defined as (see [23])

$$W_I = 2z\alpha^3 v_0 D_0 \exp\left[-\alpha R\right] \qquad (11)$$

If v_0 would be of the order of R_I^3, the quantity $\alpha^3 v_0$ may be replaced by unity. The D_0 is of the order of E_{pI}. Thus, we obtain the following criteria for the new MITs from the relation (6):

$$(0.5z/n^{1/3}R_I)\exp[-1/n^{1/3}R_I] = 1 \quad \text{for} \quad z = 6,$$

$$(0.5\sqrt[3]{2} \cdot z/n^{1/3}R_I)\exp[-\sqrt{3}/\sqrt[3]{4} \cdot n^{1/3}R_I] = 1 \quad \text{for} \quad z = 8,$$

$$(0.5\sqrt[3]{4} \cdot z/n^{1/3}R_I)\exp[-2^{1/6}/n^{1/3}R_I] = 1 \quad \text{for} \quad z = 12,$$

from which it follows that $n^{1/3}R_I \simeq 0.651$ (for $z = 6$), $n^{1/3}R_I \simeq 0.453$ (for $z = 8$), $n^{1/3}R_I \simeq 0.3354$ (for $z = 12$). We are now able to evaluate n_c in La-based cuprates using the above values of $n_c^{1/3}R_I$. For $\varepsilon_\infty = 4.5$, and $\eta = 0.04 - 0.12$ the value of R_I is found

to vary between 8.44 and 9.91 $\overset{\circ}{A}$. In these cases, the MITs and stripe formation occur at $x_c \simeq 0.0539 - 0.0872$ (for $z = 6$) and $x_c = 0.0182 - 0.0294$ (for $z = 8$) in La- based cuprates with small-radius dopants. When $\varepsilon_\infty = 3.5$, $\eta = 0.04 - 0.12$ and $R_I \simeq 6.41 - 7.56$, the MITs and stripe formation occur in these systems at $x_c \simeq 0.1213 - 0.1990$ (for $z = 6$) and $x_c \simeq 0.0409 - 0.0671$ (for $z = 8$). For $\varepsilon_\infty < 3.5$ and $z = 6$, the metal-insulator boundary of La-based cuprates containing small-radius dopants lies in the deeply overdoped region ($x_c > 0.2$)

4. Conclusions

In this work we have studied the possible mechanisms of carrier localization, charge ordering, MITs and stripe formation and propose a unified theoretical description of these interrelated phenomena in inhomogeneous hole-doped cuprates. The phenomena of self-trapping and pairing of hole carriers in the vicinity of the dopants (impurities) and in a defect-free deformable lattice at their interaction with impurities, acoustic and optical lattice vibrations in 3D cuprate compounds have been investigated quantitatively using the continuum model of ionic crystal and adiabatic approximation. These distinctly different scenarios for carrier localization lead to the formation of the extrinsic large (bi)polaronic states, the hydrogenic impurity states (i.e. impurities with loosely bound free carriers or large polarons) and the intrinsic large (bi)polaronic states in the CT gap of the cuprates. The binding energies and sizes of the extrinsic and intrinsic large polarons and bipolarons are calculated variationally, taking into account the short- and long-range parts of the carrier-defect-phonon and carrier-phonon interactions. Using the uncertainty relation, we are able to obtain the specific conditions for the MITs caused by disorder, carrier-dopant-phonon and carrier-phonon interactions. Validity of the Anderson and new MITs for the La-based cuprates is clarified. Our results have shown that the Anderson MITs may occur in lightly doped cuprates containing large-radius dopants, while the new MITs take place in deeply underdoped ($x \approx 0.02 - 0.05$), slightly underdoped ($x \lesssim 0.13$), optimally doped ($x \gtrsim 0.15$) and deeply overdoped ($x > 0.2$) cuprates containing both the small-radius dopants and the large-radius dopants. Our results consistent with the experimental data on carrier localization, MITs and stripe formation in La-based cuprates.

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