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Effect of spin fluctuations on the *c*-axis electronic conduction in $YBaCu_2O_{7-\delta}$

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Abstract. A theory of the *c*-axis electronic conduction due to the competition between interlayer direct hopping and the hopping assisted by the spin fluctuations has been developed and on this basis the experimental results of $YBa_2Cu_3O_{7-\delta}$ have been interpreted. Our theoretical analysis fits the experimental results excellently and provides good evidence that the spin fluctuations affect the *c*-axis electronic conduction and lead to the anomalous behaviour.

1. Introduction

It is well known that the most striking features of high-T_c oxides are their anomalous physical properties above their transition temperature T_c. For example, the electrical resistivity is linear in temperature in a wide range of temperatures above T_c, the infrared conductivity deviates from the Drude form, showing a relaxation rate proportional to the frequency, the nuclear spin–lattice relaxation rate shows an anomalous temperature dependence different from that in normal metals etc [1, 2].

The above anomalous physical properties have been explained in terms of antiferromagnetic spin fluctuations in two-dimensional metals [3–11]. For the *c*-axis electronic conduction of $YBa_2Cu_3O_{7-\delta}$ measurements show semiconducting-like behaviour in the underdoped regime and metallic behaviour in the overdoped regime above the superconducting transition temperature [12–14]. To date, there is no consensus concerning the *c*-axis electronic conduction, though various proposals exist [15–18]. Since the nearly linear temperature dependence of in-plane electrical resistivity can be explained in terms of the antiferromagnetic spin fluctuations [19], we expect naturally that the antiferromagnetic spin fluctuations affect the *c*-axis electronic conduction and lead to the anomalous behaviour.

The rest of the paper is organized as follows. In section 2 we develop a theory of the *c*-axis electronic conduction, on the basis of the model of the competition between interlayer direct hopping and the hopping assisted by spin fluctuations. In section 3 we discuss our results and compare them with experimental data. The paper concludes with a summary in section 4.

2. The theory

The Hamiltonian describing *c*-axis electronic conduction due to the competition between interlayer direct hopping and the hopping assisted by the spin fluctuations can be written as follows:

$$H = H^{(1)} + H^{(2)} + H_T \tag{2.1}$$

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where $H^{(1)}$ is the Hamiltonian for the layer-1 carrier of the hopping junction. It contains all many-body interactions. Similarly, $H^{(2)}$ has all the physics for the layer-2 carrier of the hopping junction. These two are considered to be strictly independent. Not only do these two operators commute, $[H^{(1)}, H^{(2)}] = 0$, but they commute term by term. The hopping is caused by the term H_T in (2.1):

$$H_T = J \sum_{\vec{k}\vec{k}'\mu\mu'} \left\{ \vec{S}(\vec{k}' - \vec{k})\vec{\sigma}_{\mu\mu'})C^{(1)+}_{\vec{k}\mu} C^{(2)+}_{\vec{k}'\mu'} + (\vec{S}(\vec{k} - \vec{k}')\vec{\sigma}_{\mu'\mu})C^{(2)+}_{\vec{k}'\mu'} C^{(1)}_{\vec{k}\mu} \right\} + \sum_{\vec{k}\vec{k}'\mu\mu'} \left\{ D^{\mu\mu'}_{\vec{k}\vec{k}'} C^{(1)+}_{\vec{k}\mu} C^{(2)}_{\vec{k}'\mu'} + D^{\mu'\mu}_{\vec{k}'\vec{k}} C^{(2)+}_{\vec{k}'\mu'} C^{(1)}_{\vec{k}\mu} \right\} \tag{2.1a}$$

where J is the constant of the interlayer hopping assisted by the spin fluctuations, $D^{\mu\mu'}_{\vec{k}\vec{k}'}$ is the interlayer direct hopping matrix element, $\vec{\sigma}_{\mu\mu'}$ is the Pauli matrix element, $\vec{S}(\vec{q})$ is the spin fluctuation operator and $C^{(i)+}_{\vec{k}\mu}$ $\left(C^{(i)}_{\vec{k}\mu}\right)$ is the i-layer carrier creation (annihilation) operator. Physically, the interlayer direct hopping arises from Giaver tunnelling and the interlayer hopping assisted by the spin fluctuation arises from the spin fluctuations scattering (represented by the $\vec{S}(\vec{q})$ which couples to the quasiparticles with strength J) which is analogous to the standard case of phonon-assisted hopping [30] except for the spin fluctuation operator replacing the phonon operator. The type of Feynman diagram that arises in the following calculation of the hopping current is shown in the appendix. The paper [17] also proposed a similar model but without a quantitative result.

After the standard procedure applied to the single-particle hopping current equation (cf [20]), the hopping current is given by the following formula:

$$I = I_d + I_{sf} \tag{2.2}$$

$$I_d = 2e \sum_{\vec{k}\vec{k}\mu\mu'} \left| D^{\mu\mu'}_{\vec{k}\vec{k}'} \right|^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} A^{(1)}_{\mu}(\vec{k}, \omega) A^{(2)}_{\mu'}(\vec{k}', \omega + eV)[n_F(\omega) - n_F(\omega + eV)] \tag{2.2a}$$

$$I_{sf} = 6J^2 e \iint \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{d}\omega'}{2\pi} \sum_{\vec{k}\vec{q}} \mathrm{Im}\, \chi^{-+}(\vec{k} - \vec{q}, eV + \omega - \omega') A^{(1)}_{\mu}(\vec{q}, \omega) A^{(2)}_{\mu'}(\vec{k}, \omega')(n_F(\omega) + n_B(eV + \omega - \omega'))(n_F(\omega' - eV) - n_F(\omega')) \tag{2.2b}$$

where I_d is the interlayer direct hopping currents, I_{sf} is the currents of the hopping assisted by the spin fluctuations. $A^{(i)}_{\mu}(\vec{k}, \omega)$ are the spectral functions for the electrons in layer i, $n_F(\omega)$ is the Fermi function, $n_B(\omega)$ is the Bose function, V is the voltage and $\mathrm{Im}\, \chi^{-+}(\vec{k}, \omega)$ is the spin fluctuation spectral function.

Because we primarily study the interlayer hopping of the quasiparticle, we simply choose the following the free-quasiparticle approximation for $A^{(i)}_{\mu}(\vec{k}, \omega)$ (as in [20] 796)

$$A^{(i)}_{\mu}(\vec{k}, \omega) = 2\pi\delta\left(\omega - \varepsilon^{(i)}_{\vec{k}\mu}\right). \tag{2.3}$$

Then from the equations (2.2a), (2.2b) and (2.3) we obtain

$$I_d = 4\pi e \sum_{\vec{k}\vec{k}'\mu\mu'} \left| D^{\mu\mu'}_{\vec{k}\vec{k}'} \right|^2 \delta\left(\varepsilon^{(2)}_{\vec{k}'\mu'} - \varepsilon^{(1)}_{\vec{k}\mu} - eV\right) \left[n_F\left(\varepsilon^{(1)}_{\vec{k}\mu}\right) - n_F\left(\varepsilon^{(2)}_{\vec{k}'\mu'}\right) \right] \tag{2.4a}$$

$$I_{sf} = 6J^2 e \sum_{\vec{k}\vec{q}} \mathrm{Im}\, \chi^{-+}\left(\vec{k}, \varepsilon^{(1)}_{\vec{q}\mu} - \varepsilon^{(2)}_{\vec{k}+\vec{q}\mu'}\right) \left(n_F\left(\varepsilon^{(1)}_{\vec{q}\mu}\right) + n_B\left(\varepsilon^{(1)}_{\vec{q}\mu} - \varepsilon^{(2)}_{\vec{k}+\vec{q}\mu'}\right) \right) \times \left(n_F\left(\varepsilon^{(2)}_{\vec{k}+\vec{q}\mu'} - eV\right) - n_F\left(\varepsilon^{(2)}_{\vec{k}+\vec{q}\mu'}\right) \right). \tag{2.4b}$$

Table 1. The fit parameters η, σ_d and λ for samples in figures 1–4.

Samples	η (mΩ cm mol emu^{-1} K^{-1})	σ_d (mΩ^{-1} cm^{-1})	λ (mol emu^{-1} K^{-1}mΩ cm^{-1})	λ/σ_d (mol emu^{-1} K^{-1})
0.03	44.84	0.338 3	5.911	17.473
0.12	77	0.034	3.4	100
0.22	127.88	0.002 467	1.124	455.68
0.32	135	0.000 25	0.315	6300

For equation (2.4*a*) we assume that the density of states on both layers is roughly constant:

$$\sum_{\vec{k}} \to \int \frac{\mathrm{d}^3\vec{k}}{(2\pi)^3} \to N^{(1)} \int \mathrm{d}\varepsilon^{(1)}_{\vec{k}\mu}$$

$$\sum_{\vec{k}'} \to \int \frac{\mathrm{d}^3\vec{k}'}{(2\pi)^3} \to N^{(2)} \int \mathrm{d}\varepsilon^{(2)}_{\vec{k}'\mu'} \tag{2.5}$$

and $\left|D^{\mu\mu'}_{\vec{k}\vec{k}'}\right| \approx |D|^2$. Then equation (2.4*a*) becomes

$$I_d = 4e^2 N^{(1)} N^{(2)} \pi |D|^2 V. \tag{2.6}$$

For equation (2.4*b*) the first step is to do the $\vec{q}$-summation:

$$\sum_{\vec{q}} \to \int \frac{\mathrm{d}^3\vec{q}}{(2\pi)^3} \to \frac{1}{(2\pi)^2} \int \mathrm{d}\varepsilon^{(1)}_{\vec{q}\mu} \int \frac{m}{\vec{k}}\, \mathrm{d}\varepsilon^{(2)}_{\vec{k}+\vec{q}\mu'}. \tag{2.7}$$

Then

$$I_{sf} = \frac{3J^2e^2mV}{2\pi^2} \sum_{\vec{k}} \int \mathrm{d}\varepsilon^{(1)}_{\vec{q}\mu}\, \mathrm{Im}\,\chi^{-+}\left(\vec{k}, \varepsilon^{(1)}_{\vec{q}\mu}\right) \left(n_F\left(\varepsilon^{(1)}_{\vec{q}\mu}\right) + n_B\left(\varepsilon^{(1)}_{\vec{q}\mu}\right)\right). \tag{2.8}$$

For the $\vec{k}$-summation we have

$$\sum_{\vec{k}} \frac{1}{|\vec{k}|} \to \frac{1}{(2\pi)^2} \int_0^{k_c} \mathrm{d}^2\vec{k}. \tag{2.9}$$

Then equation (2.8) becomes

$$I_{sf} = \frac{3J^2e^2mV}{2\pi^2} \frac{1}{(2\pi)^2} \int_0^{k_c} \mathrm{d}^2\vec{k} \int_0^{\infty} \mathrm{d}\omega\, \mathrm{Im}\chi^{-+}(\vec{k}, \omega) \left(\coth\left(\frac{\beta\omega}{2}\right) - \tanh\left(\frac{\beta\omega}{2}\right)\right) \tag{2.10}$$

where we have used $\varepsilon^{(1)}_{\vec{q}\mu} \to \omega$.

From equations (2.6) and (2.10) we obtain the *c*-axis electronic conduction due to the competition between interlayer direct hopping and the hopping assisted by the spin fluctuations as follows:

$$\sigma_c = \sigma_d + \sigma_{sf} \tag{2.11}$$

with

$$\sigma_d = 4e^2 N^{(1)} N^{(2)} \pi |D|^2 \tag{2.11a}$$

$$\sigma_{sf} = \frac{3J^2e^2m}{2\pi^2} \frac{1}{(2\pi)^2} \int_0^{k_c} \mathrm{d}^2\vec{k} \int_0^{\infty} \mathrm{d}\omega\, \mathrm{Im}\,\chi^{-+}(\vec{k}, \omega) \left(\coth\left(\frac{\beta\omega}{2}\right) - \tanh\left(\frac{\beta\omega}{2}\right)\right). \tag{2.11b}$$

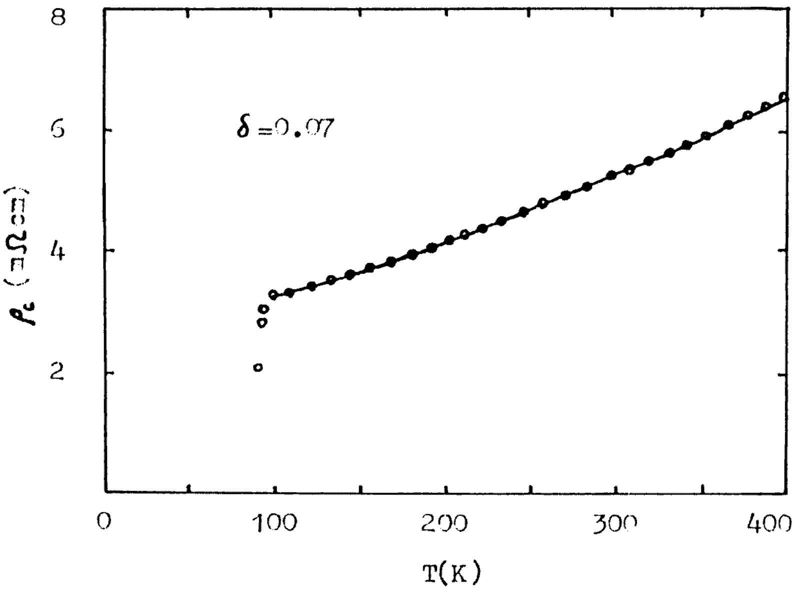


Figure 1. ρ_c versus T (solid line) from equation (3.1), experimental data (open circles) from [27] for $\delta = 0.07$.

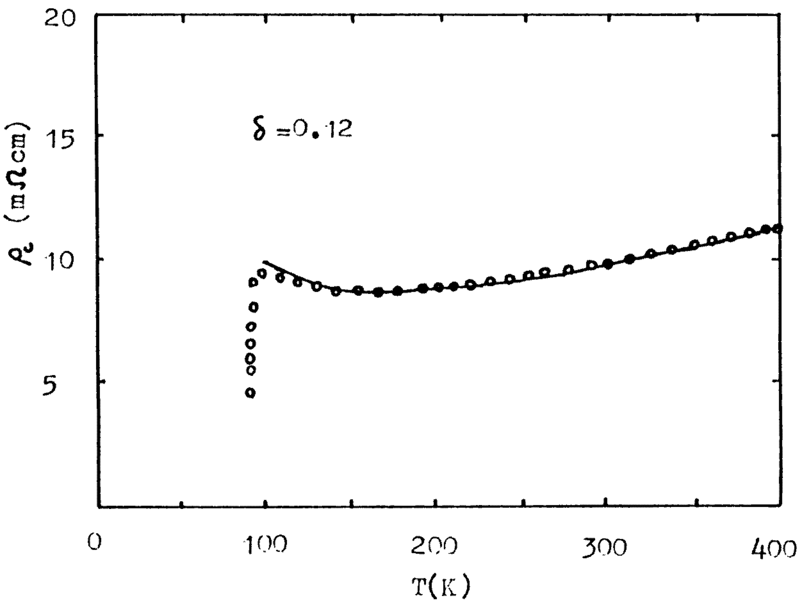


Figure 2. ρ_c versus T (solid line) from equation (3.1), experimental data (open circles) from [27] for $\delta = 0.12$.

For the spin fluctuation spectral function, we take the model of Millis, Monien and Pines (MMP) [21]:

$$\operatorname{Im} \chi^{-+}(\vec{k}, \omega) = \frac{\chi_Q(T)\omega/\omega_{sf}}{[1 + \xi^2(\vec{k} - \vec{Q})^2]^2 + \omega^2/\omega_{sf}^2} \tag{2.12}$$

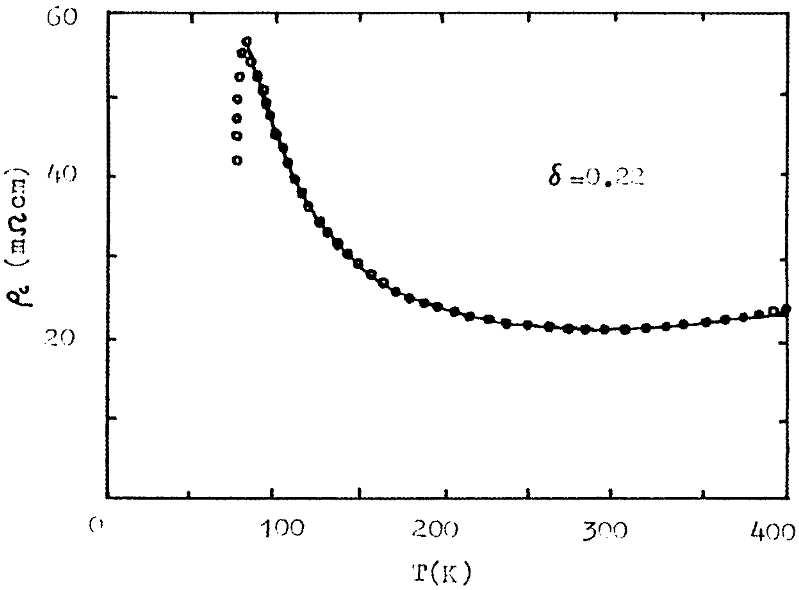


Figure 3. ρ_c versus T (solid line) from equation (3.1), experimental data (open circles) from [27] for $\delta = 0.22$.

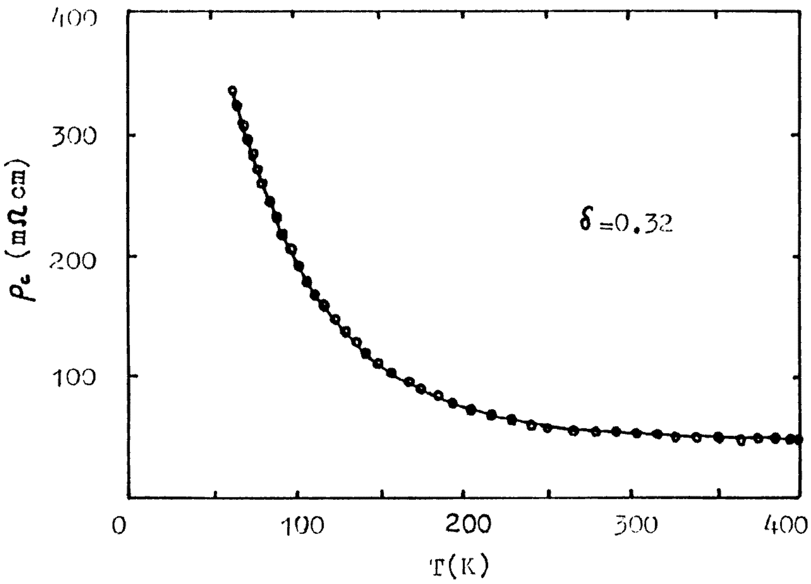


Figure 4. ρ_c versus T (solid line) from equation (3.1), experimental data (open circles) from [27] for $\delta = 0.32$.

where $\chi_Q(T)$ is the static spin susceptibility at the antiferromagnetic wave vector $\vec{Q}$ and ξ is the temperature-dependent antiferromagnetic length. In the normal state, $\chi_Q(T) = \chi_0(T)(\xi/a)^2\sqrt{\beta'}$, where $\chi_0(T)$ is the experimentally measured uniform spin susceptibility which is in general temperature dependent. $\hbar\omega_{sf}$ is a typical energy scale for the

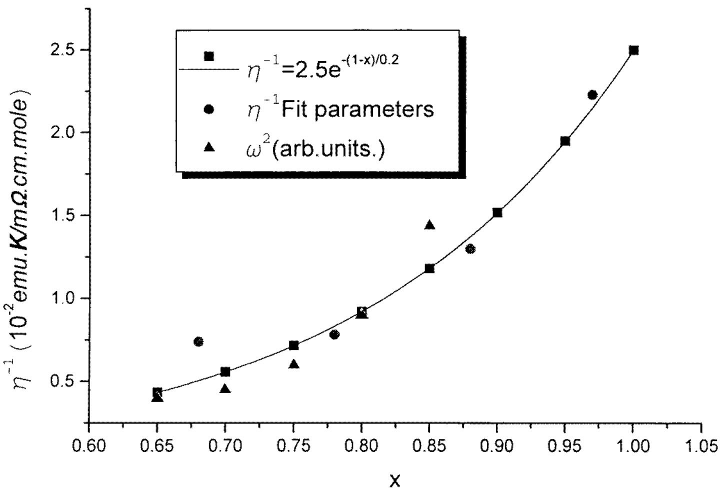


Figure 5. η^{-1} and ω_p^2 versus doping x. Fit parameters (circles), formula (squares and solid line) and experimental data (triangles) from [28].

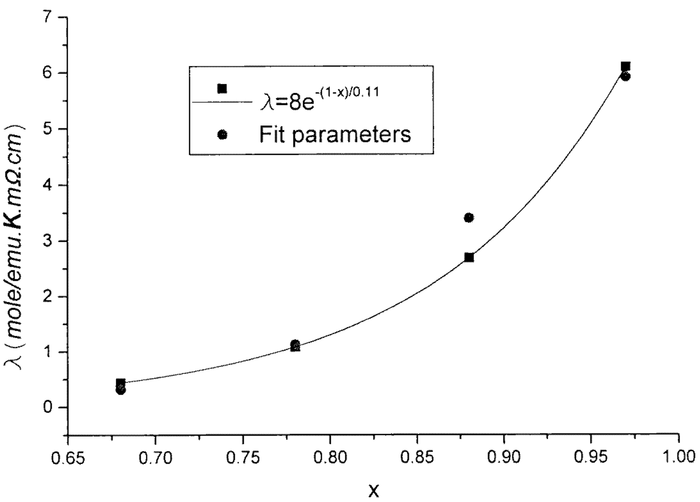


Figure 6. λ versus doping x. Fit parameters (circles), formula (squares and solid line).

antiferromagnetic paramagnons that describe the antiferromagnetic spin dynamics, which is given by $\omega_{sf} = \Gamma/\sqrt{\beta'}\pi(\xi/a)^2$, where Γ plays the role of a magnetic Fermi energy and β' is a constant.

Using equation (2.12), expression (2.11*b*) may be evaluated (cf [22]) to give the following result:

$$\sigma_{sf} = A\chi_0(T)T \tag{2.13}$$

with

$$A = \frac{3e^2J^2mk_B\sqrt{\beta'}d}{8\pi^3}\int_0^\infty \mathrm{d}x\{\tan^{-1}(x/z) - \tan^{-1}(x/z(1+r))\}[\coth(x/2) - \tanh(x/2)]$$

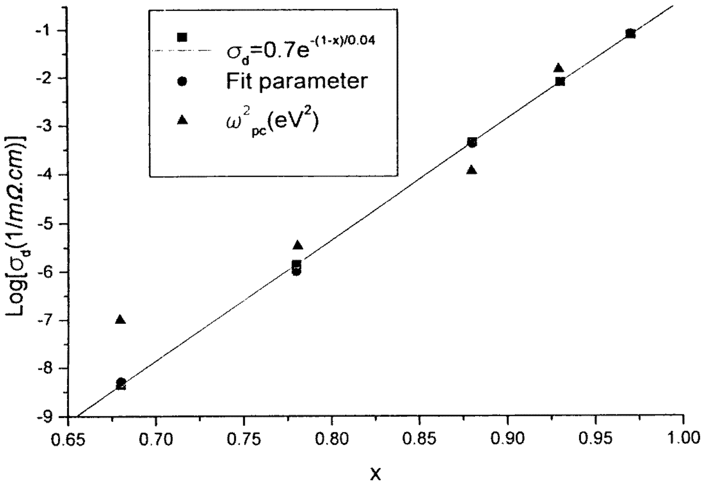


Figure 7. σ_d and ω_{pc}^2 versus doping x. Fit parameters (circles), formula (squares and solid line) and experimental data (triangles) from [29].

where $z = \omega_{sf}/k_B T$ and $r = 4\Gamma/\sqrt{\beta'}\omega_{sf}$. For $YBa_2Cu_3O_{7-\delta}$, A is constant independent of temperature. In equation (2.13), T is the absolute temperature. $\chi_0(T)$ is the uniform spin susceptibility. It reflects the c-axis electronic conduction due to hopping assisted by the spin fluctuations. Because the in-plane electrical resistivity $\rho_{ab} \propto \chi_0(T)T$ [19, 23, 24] which is based on the fact that the in-plane electrical resistivity ρ_{ab} arises from electrons being scattered by spin fluctuation, we obtain that the c-axis electronic conduction due to hopping assisted by the spin fluctuations is proportional to the in-plane electrical resistivity, i.e.

$$\sigma_{sf} \propto \rho_{ab} \tag{2.14}$$

$\sigma_{sf} \propto \rho_{ab} \propto \chi_0(T)T$ indicates that the c-axis electronic conduction σ_{sf} and the in-plane electrical resistivity ρ_{ab} have a common origin, i.e. the effect of spin fluctuation.

Using equations (2.11), (2.11*a*) and (2.13) and considering the c-axis electrical resistivity of the CuO_2 layer which is proportional to ρ_{ab} also, we have the following result:

$$\rho_c = \eta\chi_0(T)T + \frac{1}{\sigma_d + \lambda\chi_0(T)T} \tag{2.15}$$

where η, σ_d and λ are constants independent of temperature. ρ_c is the c-axis electrical resistivity of $YBa_2Cu_3O_{7-\delta}$. In the following section, we will discuss our results and compare them with experimental data.

3. Comparison with experiment

From the result of the previous section the c-axis electrical resistivity of $YBa_2Cu_3O_{7-\delta}$ can be expressed by the following formula:

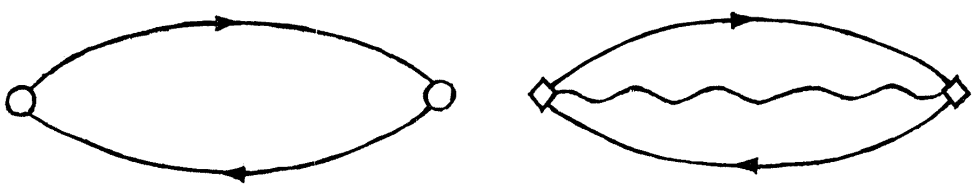
$$\rho_c = \eta\chi_0(T)T + \frac{1}{\sigma_d + \lambda\chi_0(T)T} \tag{3.1}$$

where $\chi_0(T)$ represents the uniform spin susceptibility. T is the absolute temperature. η, σ_d and λ are constants independent of temperature. The second term represents the c-axis electronic conduction due to the competition between interlayer direct hopping and the hopping assisted by the spin fluctuations.

First we note that η, σ_d and λ and are not affected by Zn doping and $\chi_0(T)$ of $YBa_2Cu_3O_{7-\delta}$ is not affected by Zn doping either [12]. Thus both the magnitude and T dependence of ρ_d do not change with Zn doping, which is in agreement with the experiment [12, 25]. Second for $\chi_0(T)$ of $YBa_2Cu_3O_{7-\delta}$ we use the experimental values [26]. Then the least-squares fits of the theoretical expression equation (3.1) to the experiment [27] are shown in figures 1–4. The solid curve is obtained from equation (3.1).The fit parameters η, σ_d and λ for samples in figures 1–4 are given in table 1. We find that the parameter λ/σ_d increases from overdoping to underdoping states. Since λ/σ_d represents the competition between interlayer direct hopping and the hopping assisted by the spin fluctuations, we can conclude that in the underdoped regime the interlayer hopping assisted by the spin fluctuations is dominant. On the other hand we can find that each parameter shows a doping dependence as in figures 5–7. In figure 5 we plot the values of η^{-1} and ω_p^2 (the Drude spectral weight) as a function of doping x. These values of ω_p^2 are taken from paper [28], which estimated the Drude spectral weight from the magnetic penetration depth or optical conductivity spectrum. Both η^{-1} and ω_p^2 show the same doping dependence and indicate that the fit parameter η^{-1} is reasonable. In figure 6 we plot the values of λ and find that $\lambda \cong \eta^{-2}$, which indicates that σ_{sf} and ρ_{ab} have the same origin. In figure 7 are plotted the values of σ_d and ω_{pc}^2 and (the Drude spectral weight of the c-axis) as a function of doping x. These values of ω_{pc}^2 are taken from paper [29], which estimated the Drude spectral weight from the optical conductivity spectrum. Both and σ_d and ω_{pc}^2 show the same doping dependence and indicate that the fit parameter σ_d is reasonable. The fitting is satisfactory and seems to support our model of the c-axis electronic conduction due to the competition between interlayer direct hopping and the hopping assisted by spin fluctuations.

4. Summary

In this paper we develop a theory of the c-axis electronic conduction, on the basis of the model of the competition between interlayer direct hopping and the hopping assisted by spin fluctuations, and obtain a theoretical expression of the c-axis electronic resistivity of $YBa_2Cu_3O_{7-\delta}$. Our theoretical analysis fits the experimental results excellently and provides good evidence that the mechanism of the c-axis electronic conduction of $YBa_2Cu_3O_{7-\delta}$ is the competition between interlayer direct hopping and the hopping assisted by the spin fluctuations.



(a) (b)

Figure A1. (a) Diagram of the current–current correlation function associated with the quasiparticle direct interlayer hopping current. The open circle vertices denote $D_{kk'}^{\mu\mu'}$ in the text. (b) Diagram of the current–current correlation function associated with the quasiparticle interlayer hopping (assisted by spin fluctuations). The square vertices denote J in the text.

Appendix. The Feynman diagrams that arise in calculation of the hopping current

The type of Feynman diagram that arises in the calculation of the hopping current is shown in figure A1. The solid lines represent the exact one electron propagators for layer 1 and layer 2. The wavy line represents the spin fluctuation propagator.

Acknowledgments

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