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The effect of spin fluctuations on the *c*-axis thermoelectric power in underdoped cuprate

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Abstract

A theory of the thermoelectric power due to the interlayer hopping assisted by spin fluctuations has been developed. The prediction of the theory captures the main features of experiment. Thus, we argue that the *c*-axis thermoelectric power exhibiting metallic behaviour while the *c*-axis electronic conductivity appears to be nonmetallic in the underdoped cuprate may be properly understood within the theory.

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 over a wide range of temperatures above T_c, the infrared conductivity deviates from the Drude form, showing a relaxation rate proportional to the frequency, and the nuclear spin–lattice relaxation rate shows an anomalous temperature dependence different from that in normal metals [1, 2].

The above anomalous physical properties have been explained in terms of antiferromagnetic spin fluctuations in two-dimensional metals [3–11]. As for the *c*-axis thermoelectric power and the *c*-axis electronic conductivity, the measurements show that within the low-doping regime the *c*-axis thermoelectric power exhibits metallic behaviour while the *c*-axis electronic conductivity appears to be nonmetallic [12–14]. To date, there has been no consensus concerning this anomalous behaviour, though various proposals exist [15–17]. In the paper [18] I have developed a theory of the *c*-axis electronic conductivity due to the competition between interlayer direct hopping and the hopping assisted by the spin fluctuations. Since the anomalous behaviour of the *c*-axis electronic conductivity can be explained in terms of the effect of the antiferromagnetic spin fluctuations [18], we naturally expect the antiferromagnetic spin fluctuations to affect the *c*-axis thermoelectric power 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 thermoelectric power on the basis of the model of the interlayer hopping assisted by spin fluctuations. In section 3 we discuss our results. The paper concludes with a summary in section 4.

2. The theory

Following the idea of the paper [18], the Hamiltonian describing c-axis transport properties due to the interlayer hopping assisted by the spin fluctuations can be written as

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

where $H^{(1)}$ is the Hamiltonian for the one-layer carrier of the hopping junction. It contains all many-body interactions. Similarly, $H^{(2)}$ has all the physics for the two-layer 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 also they commute term by term. The interlayer hopping assisted by the spin fluctuations can be written as

$$H_T = \frac{J}{\sqrt{N}} \sum_{\boldsymbol{k}\boldsymbol{k}'\mu\mu'} (\boldsymbol{S}(\boldsymbol{k}' - \boldsymbol{k})\boldsymbol{\sigma}_{\mu\mu'} C^{(1)\dagger}_{\boldsymbol{k}\mu} C^{(2)}_{\boldsymbol{k}'\mu'} + \boldsymbol{S}(\boldsymbol{k} - \boldsymbol{k}')\boldsymbol{\sigma}_{\mu'\mu} C^{(2)\dagger}_{\boldsymbol{k}'\mu'} C^{(1)}_{\boldsymbol{k}\mu}). \tag{2}$$

Here J is the constant of the interlayer hopping assisted by the spin fluctuations, $\boldsymbol{\sigma}_{\mu\mu'}$ is the Pauli matrix element, $\boldsymbol{S}(\boldsymbol{q})$ is the spin fluctuation operator, $C^{(i)\dagger}_{\boldsymbol{k}\mu}$ $(C^{(i)}_{\boldsymbol{k}\mu})$ is the i-layer carrier creation (annihilation) operator. Physically, the interlayer hopping assisted by the spin fluctuations arises from the spin fluctuation scattering (represented by the $\boldsymbol{S}(\boldsymbol{q})$ which couples to the quasi-particles with strength J) which is analogous to the standard case of phonon-assisted hopping [19], except that the spin fluctuation operator replaces the phonon operator. Then the current operator of the interlayer hopping assisted by the spin fluctuations is given by

$$j_c = \frac{iedJ}{\sqrt{N}} \sum_{\boldsymbol{k}\boldsymbol{k}'\mu\mu'} (\boldsymbol{S}(\boldsymbol{k}' - \boldsymbol{k})\boldsymbol{\sigma}_{\mu\mu'} C^{(1)\dagger}_{\boldsymbol{k}\mu} C^{(2)}_{\boldsymbol{k}'\mu'} - \boldsymbol{S}(\boldsymbol{k} - \boldsymbol{k}')\boldsymbol{\sigma}_{\mu'\mu} C^{(2)\dagger}_{\boldsymbol{k}'\mu'} C^{(1)}_{\boldsymbol{k}\mu}). \tag{3}$$

After the standard procedure has been applied to calculate the ensemble average of j_c (cf. reference [20]), the ensemble average of j_c for the case in the presence of both a weak electric field (E) and a small temperature gradient (ΔT) in the c-axis direction is given by the following formula:

$$\begin{aligned}\langle j_c \rangle = \frac{6J^2e^2d^2}{VN} \int\int \frac{\mathrm{d}\omega_1}{2\pi} \frac{\mathrm{d}\omega_2}{2\pi} \sum_{\boldsymbol{k}\boldsymbol{q}} \operatorname{Im} \chi^{-+}(\boldsymbol{k}, \omega_1) A^{(1)}(\boldsymbol{q}, \omega_1 + \omega_2) A^{(2)}(\boldsymbol{k}+\boldsymbol{q}, \omega_2) \\ \times (n_F(\omega_1 + \omega_2) + n_B(\omega_1))\left(-\frac{\partial n_F(\omega_2)}{\partial \omega_2}\right)\left(E - \frac{\omega_2}{eT}\Delta T\right)\end{aligned} \tag{4}$$

where e is unit charge. d is the c-axis interlayer distance. $A^{(i)}(\boldsymbol{k}, \omega_i)$ is the spectral function for the electron in the i-layer, $n_F(\omega)$ is the Fermi function, $n_B(\omega)$ is the Bose function, $\operatorname{Im} \chi^{-+}(\boldsymbol{k}, \omega)$ is the spin fluctuation spectral function.

The thermoelectric power S_c is determined by the relation between the electrical current $\langle j_c \rangle$ and the temperature gradient ΔT:

$$\langle j_c \rangle = \sigma_c (E - S_c \, \Delta T). \tag{5}$$

From equations (4) and (5) with $\langle j_c \rangle = 0$, we can obtain

$$\sigma_c = e^2 \int \frac{\mathrm{d}\omega}{2\pi} \left(-\frac{\partial n_F(\omega)}{\partial \omega}\right)\sigma(\omega) \tag{6}$$

$$S_c = -\frac{|e|}{\sigma_c T} \int \frac{\mathrm{d}\omega}{2\pi} \left(-\frac{\partial n_F(\omega)}{\partial \omega}\right)\omega\sigma(\omega) \tag{7}$$

with the differential conductivity

$$\sigma(\omega) = \frac{6J^2 d}{\hbar a^2}\frac{1}{N^2}\int\frac{\mathrm{d}\omega'}{2\pi}\sum_{\boldsymbol{kq}} \mathrm{Im}\,\chi^{-+}(\boldsymbol{k},\omega')A(\boldsymbol{q},\omega'+\omega)A(\boldsymbol{k}+\boldsymbol{q},\omega) \times (n_F(\omega'+\omega)+n_B(\omega')). \tag{8}$$

Here a is the ab-plane lattice constant. $A(\boldsymbol{k},\omega)$ is the spectral function for the electron in the layer.

Then from equations (6), (7) and (8) we obtain the c-axis electronic conductivity σ_c and thermoelectric power S_c of the hopping assisted by the spin fluctuations.

3. Results

In this section we first introduce the spin fluctuation spectral function $\mathrm{Im}\,\chi^{-+}(\boldsymbol{k},\omega)$ and the spectral function of the electron in layer $A(\boldsymbol{k},\omega)$ that are used in equation (8) for calculating the c-axis electronic conductivity σ_c and thermoelectric power S_c of the hopping assisted by the spin fluctuations. Then we present the results obtained by using the formula that was outlined above and give a discussion.

In order to simplify the computations, we take the phenomenological form of the spin fluctuation spectral function [21–23]:

$$\chi^{-+}(\boldsymbol{k},\hbar\omega) = \sum_j \frac{\alpha(\xi/a)^2}{1+\xi^2(\boldsymbol{q}-\boldsymbol{Q}_j)^2 - \mathrm{i}\omega/\omega_{sf} - (\omega/\Delta_{sw})^2} \tag{9}$$

where ξ is the magnetic correlation length. ω_{sf} is an energy scale for the antiferromagnetic paramagnons that determine the antiferromagnetic spin dynamics. α is an overall temperature-independent constant and $\boldsymbol{Q}_j$ are the positions of the peaks in momentum space which are assumed to be incommensurate, i.e. $\boldsymbol{Q}_j = (1\pm\delta, 1)\pi/a$ and $\boldsymbol{Q}_j = (1, 1\pm\delta)\pi/a$. $\hbar\Delta_{sw}$ is a typical energy of propagating spin waves which comes into play at high frequencies. $\hbar\Delta_{sw} = \hbar c_{sw}(a/\xi)$. c_{sw} is the spin-wave velocity.

For the same reason, the spectral function of the electron in layer $A(\boldsymbol{k},\omega)$ is taken as

$$A(\boldsymbol{k},\omega) = \frac{\Gamma(T)}{(\omega-\varepsilon_{\boldsymbol{k}})^2+\Gamma^2(T)}. \tag{10}$$

Here $\Gamma(T) = \Gamma_0 + \Gamma_1 T$. $\varepsilon_{\boldsymbol{k}}$ is the single-particle energy spectrum in the layer, which has the following form:

$$\varepsilon_{\boldsymbol{k}} = -2t(\cos k_x a + \cos k_y a) - 4t'\cos k_x a\cos k_y a - \mu \tag{11}$$

where t is the nearest-neighbour, t' is the next-to-nearest-neighbour and μ is the chemical potential.

Taking equation (9), the phenomenological form of the spin fluctuation spectral function, and equation (10), the spectral function of the electron in the layer, we have performed a calculation for the c-axis electronic conductivity σ_c and thermoelectric power S_c of YBCO. In the computation, we choose $\hbar\omega_{sf} = 60 + 0.8T$ K, $\omega_0 = \omega_{sf}(\xi/a)^2$, $\hbar\omega_0 = 60$ meV, $\alpha = 9\times10^{-3}$ meV^{-1}, $\hbar c_{sw} = 180$ meV and $\delta = 0.21$ for the values of the parameters of the spin fluctuation spectral function [21–23]. The values of the parameters of the single-particle energy spectrum used are $t = 350$ meV, $t'/t = -0.3$ and $\mu/t = -1.05$ [24, 25]. Also $\Gamma_0/t = 0.235$ and $\Gamma_1/t = 4\times10^{-4}$ K^{-1} [26]. The result is plotted as the S_c versus T curve in figure 1. The solid curve shows the values from theory. The agreement between our theoretical calculation and experiment [12] is satisfactory. The $\rho_c(T)/\rho_c(T = 300$ K$)$ versus T curve is plotted in figure 2 ($\rho_c(T) = 1/\sigma_c(T)$). It shows that the c-axis electronic conductivity

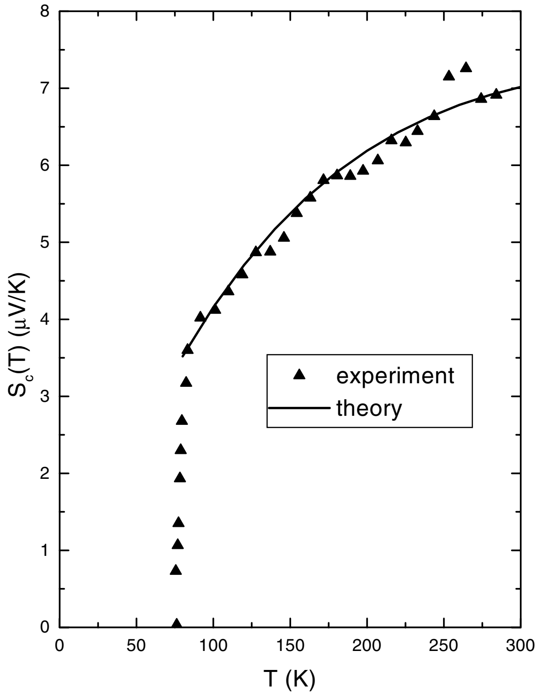

Figure 1. S_c versus T for YBCO in the underdoping regime. The parameters used are as follows: $\hbar\omega_{sf} = 60 + 0.8T$ K, $\omega_0 = \omega_{sf}(\xi/a)^2$, $\hbar\omega_0 = 60$ meV, $\alpha = 9 \times 10^{-3}$ meV^{-1}, $\hbar c_{sw} = 180$ meV, $\delta = 0.21$, $t = 350$ meV, $t'/t = -0.3$, $\mu/t = -1.05$, $\Gamma_0/t = 0.235$ and $\Gamma_1/t = 4 \times 10^{-4}$ K^{-1}.

appears to be non-metallic and the theoretical calculation captures the main features of the experiment. Therefore we conclude that the antiferromagnetic spin fluctuation affects c-axis transport properties and plays an important role in leading to the anomalous behaviour of c-axis transport properties in underdoped cuprate.

In order to further understand why the spin fluctuations favour at the same time metallic behaviour of the thermoelectric power and insulating behaviour of the resistivity, we investigate their analytical behaviours at low temperature (i.e. $|\mu| \gg T$). For $|\mu| \gg T$ we can use

$$\frac{\partial n_F(\omega)}{\partial \omega} \approx -\delta(\omega - \mu).$$

Then $\sigma_c(T) \sim T$ [18], while

$$S_c \sim T \frac{\partial \ln \sigma_c(\omega)}{\partial \omega}\bigg|_{\omega=\mu}.$$

It is noted that the linear T-dependence of the c-axis electronic conductivity $\sigma_c(T)$ originating from the hopping assisted by the spin fluctuations leads to insulating behaviour of the resistivity ($\rho_c(T) = 1/\sigma_c(T)$). This result is just the opposite to the usual case in the electron–spin fluctuation scattering mechanism [27, 28]. The physical origin of this effect is that for the hopping conduction process the electron–spin fluctuation scattering assists the c-axis transport of electrons, while for the usual case it plays the role of hindering the motion of electrons along the direction of the applied field. On the other hand, we note that the linear T-dependence of the thermoelectric power S_c originating from the hopping assisted by the spin fluctuations is similar in form to the diffusion thermoelectric power in metals [29].

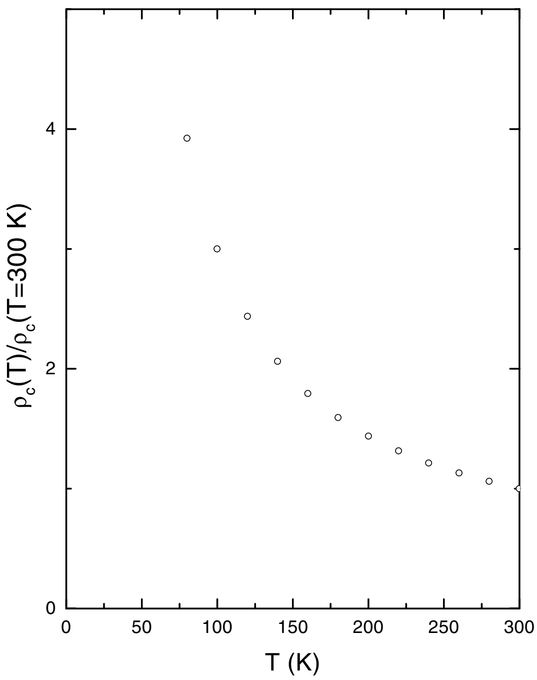

Figure 2. $\rho_c(T)/\rho_c(T = 300\ \text{K})$ ($\rho_c(T) = 1/\sigma_c(T)$) versus T for YBCO in the underdoping regime. The parameters used are the same as in figure 1.

4. Concluding remarks

In this paper we develop a theory of the thermoelectric power due to the interlayer hopping assisted by the spin fluctuations. The theoretical analysis results capture the main features of experiment. Thus, we argue that the anomalous behaviour of the *c*-axis electronic conductivity and the thermoelectric power in the underdoped cuprates may be properly understood by considering the mechanism of the interlayer hopping assisted by spin fluctuations.

Acknowledgments

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References

[1] Penning C H and Slichter C P 1990 *Physical Properties of High Temperature Superconductors* vol 2, ed D M Ginsberg (Singapore: World Scientific) pp 269–367
[2] Bell K S, Coffey P, Meltzer D E, Pines D and Schrieffer J R (ed) 1990 *Proc. Los Alamos Symp. on High Temperature Superconductivity* (Reading, MA: Addison-Wesley)
[3] Pines D 1991 *Physica* C **185–189** 120
[4] Moriya T, Takahashi Y and Ueda K 1991 *Physica* C **185–189** 114
[5] Tomeno I, Machi T, Tai K, Koshizuka N, Kambe S, Hayashi A, Ueda Y and Yasuoka H 1994 *Phys. Rev*. B **49** 15 327
[6] Arf B 1992 *Phys. Rev*. B **45** 2352
[7] Wu Hang-sheng and Lou Ping 1991 *Z. Phys.* B **85** 3

[8] Lou Ping 1994 *J. Phys.: Condens. Matter* **6** 3767
[9] Lou Ping 1995 *J. Phys.: Condens. Matter* **7** 5351
[10] Lou Ping 1997 *Physica* C **274** 248
[11] Lou Ping 1998 *Commun. Theor. Phys.* **30** 117
[12] Crommie M F, Zettl A, Barbee T W III and Cohen M L 1988 *Phys. Rev.* B **37** 9734
[13] Crommie M F, Briceno G and Zettl A 1989 *Physica* C **162–164** 1397
[14] Nakamura Y and Uchida S 1993 *Phys. Rev.* B **47** 369
[15] Kaiser A B and Mountjoy G 1991 *Phys. Rev.* B **43** 6266
[16] Xing D Y, Liu M and Ting C S 1988 *Phys. Rev.* B **43** 11 992
[17] Nagaosa N 1995 *Phys. Rev.* B **52** 10 561
[18] Lou Ping 1999 *J. Phys.: Condens. Matter* **11** 7569
[19] Buke C B 1969 *Tunneling in Solids* (New York: Academic) pp 238–43
[20] Mahan G D 1981 *Many Particle Physics* (New York: Plenum) section 3.8
[21] Stojkovic B P and Pines D 1997 *Phys. Rev.* B **55** 8576
[22] Morr D K and Pines D 1998 *Phys. Rev. Lett.* **81** 1086
[23] Morr D K and Pines D 2000 *Preprint* cond-mat/0004378
[24] Jaklic J and Prelovsek P 2000 *Adv. Phys.* **49** 1
[25] Tohyama T and Maekawa S 2000 *Supercond. Sci. Technol.* **13** R17
[26] Here $\Gamma(T) = \Gamma_0 + \Gamma_1 T$ represent the scattering rate, but Γ_0 does not represent the impurity scattering rate. Thus the parameter value of $\Gamma(T)$ is reasonable. For example, when $T = 300$ K, $\Gamma(300) = 124$ meV agrees with the values that other papers obtain. See
Puchkov A V, Basove D N and Timusk T 1996 *J. Phys.: Condens. Matter* **8** 10 049
or
Timusk T and Statt B 1999 *Rep. Prog. Phys.* **62** 61
[27] Ito T, Takenaka K and Uchida S 1993 *Phys. Rev. Lett.* **70** 3995
[28] Monien H, Pines D and Takigawa M 1991 *Phys. Rev.* B **43** 258
[29] Abrikosov A A 1988 *Fundamentals of the Theory of Metals* (Amsterdam: North-Holland) section 6.1