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Optical Conductivity in the Manganite $La_{1-x}Sr_xMnO_3$ (x=0.175)

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Abstract— ***We have calculated the optical conductivity $\sigma(\omega)$ in the manganite $La_{1-x}Sr_xMnO_3$ (x=0.175). We connected with Jahn-Teller polarons. We set the delta-functions appearing in $\sigma(\omega)$ as Gaussian. We have deduced the c-axis optical conductivity $\sigma_c(\omega)$ of an interband-type from fitting parameters. The interband-gap is positioned approximately at 2.3 eV and the orbital excitation is related to the peak at 0.5 eV in our theory. The global form of our theory corresponds to the experimental data. Our analysis can be also applied to $Pr_{0.5}Sr_{0.5}MnO_3$ nicely because of the form of $\sigma(\omega)$ similar to that for $La_{1-x}S_xMnO_3$.***

Keywords— ***Optical Conductivity, Manganite, Gaussian form, delta-functions, polaron***

I. Introduction

The colossal magnetoresistance (CMR) phenomena have renewed in recent years especially for the perovskite manganites, $R_{1-x}A_xMnO_3$ (RAMO: R=rare-earth; A=divalent cation) [1,2]. These manganites show a very rich phase diagram depending on the doping concentration, temperature, and pressure: antiferromagnetic (AFM) insulator, ferromagnetic (FM) metal, charge ordered (CO) insulator [3]. A variety of these phenomena suggest that several interactions originating from the spin, charge, lattice degrees of freedom are competing. For instance, the correlation between ferromagnetism and metallic conductivity for $0.2 < x < 0.5$ was explained qualitatively in terms of the double exchange model [1]. On the other hand, small lattice polaron effects due to a strong Jahn-Teller electron-phonon interaction are thought to be responsible for anomalous properties of manganites [4-8]. Optical conductivities of colossal magnetoresistance manganites have been investigated extensively, since they showed drastic spectral weight changes with temperature variation [9-15]. Especially, in ferromagnetic (FM) metallic states, their optical conductivity spectra $\sigma(\omega)$ showed a large incoherent peak near 0.5 eV. It has been argued that a few peaks of anomalous incoherent absorption should be related to Jahn-Teller polaron or orbital excitations [9-15]. Since ferromagnetism and ferroelectricity are very useful in spintronics, information storages, sensors, etc., multiferroics with spontaneous magnetization and polarization are promising candidates to design advanced devices with faster speeds, more functions, and energy saving [16].

II. Calculation of the Optical Conductivity

In this paper, we explain the optical data of $La_{1-x}Sr_xMnO_3$ (x=0.175, T_c=283 K) at T=250 K using the Jahn-Teller polaron model. Even though our Hamiltonian is as same as others [8], we calculate the optical conductivity more practically and concretely than Lee et al. [8]. The effective Hamiltonian incorporating the electron-phonon interaction is written as [8]

$$H = t < \cos\frac{\theta}{2} > \sum_{i,\delta} c_{i+\delta}^{+} c_i + \sum_{\vec{q}} \omega_q a_{\vec{q}}^{+} a_{\vec{q}}$$
$$+\sum_{i,\vec{q}} c_i^{+} c_i e^{i\vec{q}\cdot\vec{R}_i} M_q (a_{\vec{q}} + a_{-\vec{q}}^{+}), \quad (1)$$

where the hopping t connects neighboring sites, $< \cos\frac{\theta}{2} >$ double exchange parameter, $a_{\vec{q}}^{+}$ phonon creation operatror, M_q electron-phonon matrix. The optical conductivity $\sigma(\omega)$ can be determined by using the Kubo formula of the current-current correlation function [17],

$$\sigma(\omega) = \frac{1-e^{-\beta\omega}}{2\omega} \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} < J_\alpha^{+}(\tau) J_\alpha(0) >, \quad (2)$$

where the current operator $\vec{J}$ is $\vec{J} = it < \cos\frac{\theta}{2} > e \sum_{j,\delta} \vec{\delta} c_{j+\delta}^{+} c_j$, $\beta = k_B T$ and T is the temperature.

To evaluate $\sigma(\omega)$, let's consider the well-known polaron canonical transformation[8,17];

$$\tilde{H} = e^S H e^{-S}, \; S = -\sum_{j,\vec{q}} c_j^{+} c_j e^{i\vec{q}\cdot\vec{R}_j} \frac{M_q}{\omega_q} (a_{\vec{q}} - a_{-\vec{q}}^{+}).$$

The transformed Hamiltonian $\tilde{H}$ is given by

$$\tilde{H} = t < \cos\frac{\theta}{2} > \sum_{j,\delta} c^{+}_{j+\delta} c_j X^{+}_{j+\delta} X_j + \sum_{\vec{q}} \omega_q a^{+}_{\vec{q}} a_{\vec{q}}$$
$$-\Delta \sum_j c^{+}_j c_j \quad (3)$$

with $X_j = \exp[\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{R}_j} \frac{M_q}{\omega_q}(a_{\vec{q}} - a^{+}_{-\vec{q}})], \Delta = \sum_{\vec{q}} \frac{M_q^2}{\omega_q}, e^S c_j e^{-S} = c_j X_j$, $\tilde{H}$ corresponds to the shifted H by a polaron energy Δ. It becomes for sufficiently low temperatures

$$\sigma(\omega) \approx \frac{t^2(1-e^{-\beta\omega})}{2\omega} < \cos\frac{\theta}{2} >^2 e^2 \sum_{\delta,\delta'} \sum_{j,j'} (\vec{\delta}\cdot\vec{\delta}')$$
$$\times \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} < c^{+}_j(\tau) c_{j+\delta}(\tau) c^{+}_{j'+\delta} c_{j'} > \quad (4)$$
$$\times < X^{+}_j(\tau) X_{j+\delta}(\tau) X^{+}_{j'+\delta} X_{j'} > .$$

In the Heisenberg representation of quantum mechanics, the time development of operators is given by [17]

$$O(\tau) = e^{i\tilde{H}\tau} O e^{-i\tilde{H}\tau} \quad (5)$$

so that the operator obeys the equation

$$\frac{\partial}{\partial\tau} O(\tau) = i[\tilde{H}, O(\tau)]. \quad (6)$$

For the operator, this becomes

$$\frac{\partial}{\partial\tau} c_i(\tau) = i[\tilde{H}, c_i(\tau)] = -i\omega_i c_i(\tau) \quad (7)$$

which has the simple solution

$$c_i(\tau) = e^{-i\omega_i\tau} c_i$$
$$\omega_i = t < \cos\frac{\theta}{2} > e^{i\vec{q}\cdot\vec{R}_i} \sum_{j,\delta} X^{+}_{j+\delta} X_j - \Delta$$
$$a_q(\tau) = e^{-i\omega_q\tau} a_q \quad (8)$$
$$c_i = \sum_k e^{-i\vec{k}\cdot\vec{R}_i} c_k$$
$$\vec{q} = \vec{k}(c^{+}_{j+\delta}) - \vec{k}(c_j) = \vec{k}(X_j) - \vec{k}(X^{+}_{j+\delta}).$$

For $\tilde{H}$, it becomes

$$\frac{\partial}{\partial\tau} X_j(\tau) = i[\tilde{H}, X_j(\tau)] = -i\omega^j_{e-p} X_j(\tau)$$
$$\omega^j_{e-p} = \sum_q e^{i\vec{q}\cdot\vec{R}_j} M_q (e^{-i\omega_q\tau} a_q + e^{i\omega_{-q}\tau} a^{+}_{-q}) \quad (9)$$
$$X_j(\tau) = e^{-i\omega^j_{e-p}\tau} X_j,$$

where we assume $\omega_q = \omega_{-q}$ and ω^j_{e-p} is closely related to an optical phonon in connection with Jahn-Teller polarons.

The final optical conductivity becomes

$$\sigma(\omega) \approx \frac{t^2(1-e^{-\beta\omega})}{2\omega} < \cos\frac{\theta}{2} >^2 e^2 \sum_{\delta,\delta'}\sum_{j,j'} (\vec{\delta}\cdot\vec{\delta}')$$
$$\times < c_j^+ c_{j+\delta} c_{j'+\delta}^+ c_{j'} >< X_j^+ X_{j+\delta} X_{j'+\delta}^+ X_{j'} >$$
$$\times \frac{\delta(\omega - <\omega_{j+\delta} - \omega_j>)\delta(\omega - <\omega_{e-p}^{j+\delta} - \omega_{e-p}^{j}>)}{\delta(\omega)\omega} \quad (10)$$
$$\equiv \hat{\sigma}(\omega=0)(1-e^{-\beta\omega})\frac{\delta(\omega - <\omega_{j+\delta} - \omega_j>)\delta(\omega - <\omega_{e-p}^{j+\delta} - \omega_{e-p}^{j}>)}{\delta(\omega)\omega},$$

where $<\omega_{j+\delta} - \omega_j>$ is a mean value of orbital excitations, $<\omega_{e-p}^{j+\delta} - \omega_{e-p}^{j}>$ corresponds to a mean value of Jahn-Teller phonons.

The total optical conductivity is

$$\sigma_t(\omega) = \sigma(\omega) + s\sigma_c(\omega), \quad (11)$$

where σ_c is a c-axis optical conductivity of the interband-type and s is a scaling coefficient as same method as Alexandrov et al. [11,12]. We have a fit with experiments in sufficient correspondence for $La_{1-x}Sr_xMnO_3$ (x=0.175, T_c=283 K) at T=250 K as shown in Fig.1. We assume the δ -function is a Gaussian-type. As Alexandrov et al.[11,12] suggested the importance of rescaled c-axis optical conductivity, we deduce this and therefore optical conductivity at high energies has good correspondence with experimental data and we obtain two anomalies at 2.3 eV, 2×2.3 eV where 2.3 eV is the interband gap. As shown in Eq.(11), 0.5 eV peak in $\sigma(\omega)$ is confirmed by the orbital excitation for our formulation. The $\delta(\omega - <\omega_{j+\delta} - \omega_j>) \cong \frac{0.5\,eV}{(\omega - 0.5eV)^2 + (0.5eV)^2}$ is centered at $\omega = 0.5eV$ and have the half-width 0.5 eV. This orbital excitation corresponds to the experimental peak at 0.5 eV in Takenaka et al. [10]. The $\delta(\omega) \cong \frac{0.2\,eV}{(\omega)^2 + (0.2eV)^2}$ have the peak at $\omega = 0eV$ and corresponds to the measured peak in Takenaka et al. [10]. From our fitting result, we know that σ_c have a non-zero value from $\omega = 2.3eV$ corresponding to the interband gap. The anomaly of experimental data [10] at $\omega \cong 4.6eV$ results from the harmonics of the interband gap, here 2×2.3 eV. Since Jahn-Teller phonons are non-dispersive, it becomes $<\omega_{e-p}^{j+\delta} - \omega_{e-p}^{j}> \cong 0$. As shown in Fig.1, the global form of our theory corresponds to the experimental data so that the optical conductivity is dominated by small polarons. Although our Hamiltonian is same as others [8], our method of approximation to obtain the optical conductivity is different from them. Our more concrete and simple mathematical approach give something meaningful in comparison with original work [8]. The rough correspondence between our results and experimental data [10] at low energies mainly results from our treatments of delta-functions as simple Gaussian.

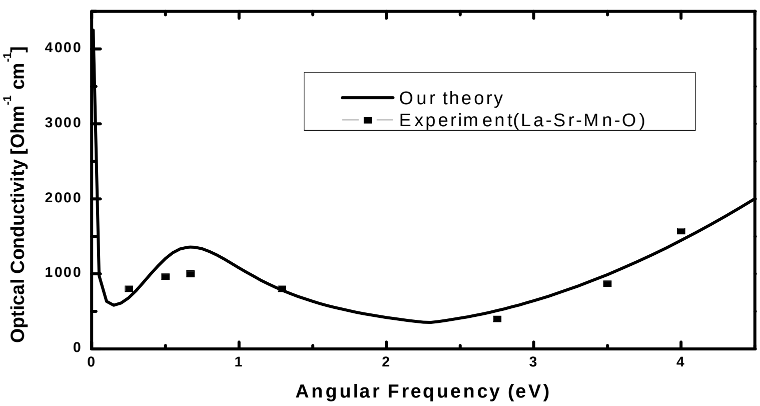

Fig. 1 We use the experimental data [10] for $La_{1-x}Sr_xMnO_3$ (x=0.175) at T=250 K.

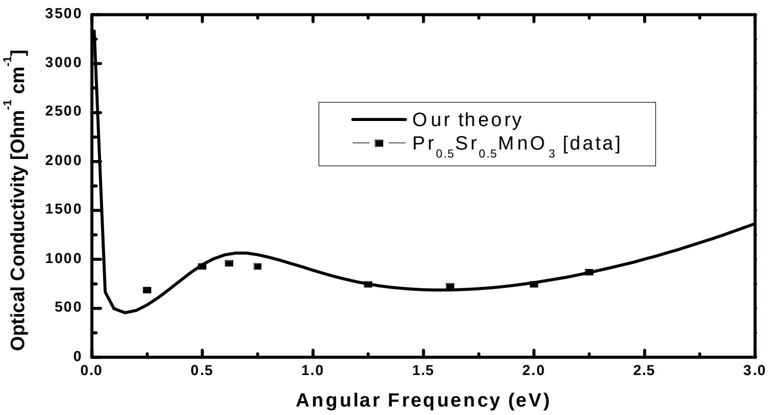

Fig. 2 We have fitted our theory with the experiment for $Pr_{0.5}Sr_{0.5}MnO_3$ [9] at T=230 K.

III. CONCLUSIONS

In conclusion, we have developed the theory of the optical conductivity in doped manganites with a strong electron-phonon interaction. We have found delta-functions of the Gaussian form to explain the experiments. Our analysis can be also applied to $Pr_{0.5}Sr_{0.5}MnO_3$ [9] nicely because of the form of $\sigma(\omega)$ similar to that for $La_{1-x}S_xMnO_3$ shown in Fig.2.

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