Charge fluctuation in the CuO double chains of $PrBa_2Cu_4O_8$

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Abstract

The optical conductivity of the CuO double chains of $PrBa_2Cu_4O_8$ is calculated by the mean-field approximation for the coupled two-chain Hubbard model around quarter filling. We show that the ~40 meV peak structure, spectral shape, and small Drude weight observed in experiment are reproduced well when the stripe-type charge ordering is present. We thereby argue that the observed anomalous optical response may be due to the presence of stripe-type fluctuations of charge carriers in the CuO double chains.

Key words: charge fluctuation; charge ordering; CuO double chain; optical conductivity; $PrBa_2Cu_4O_8$

1. Introduction

The CuO double chains in $PrBa_2Cu_4O_8$ (see Fig. 1 (a)) provide a good opportunity for studying anomalous charge dynamics in one-dimensional (1D) strongly correlated electron systems [1–3] because the holes in the CuO_2 planes of this system are localized and thus the planes show insulating conductivity (except at low temperatures $\lesssim$140 K). Actually, anomalous charge dynamics of the CuO double chains has recently been reported [5,4]: A nuclear-quadrupole-resonance (NQR) experiment demonstrated the presence of anomalous spin-lattice ($1/T_1$) and spin-spin ($1/T_2$) relaxations [5] and an optical conductivity experiment clearly showed the presence of anomalous charge excitations at $\omega \gtrsim 40$ meV [4].

In this paper, we focus on the optical conductivity spectra $\sigma(\omega)$ observed by Takenaka *et al.* [4] and consider the origin of the appearance of the characteristic peak structure at $\omega \simeq 40$ meV as well as the presence of extremely small Drude weight.

We use the mean-field approximation to the extended Hubbard model defined on a lattice of coupled two chains (see Fig. 1 (b)) and calculate the ground-state phase diagram. We find that there appear two types of charge-ordered (CO) phases, depending on the parameter values, which are the CO phase with in-line–type ordering and CO phase with stripe-type ordering. We then calculate the optical conductivity spectrum $\sigma(\omega)$ for each of these two phases in the same approximation. In the following, we will present the calculated results and discuss their implications.

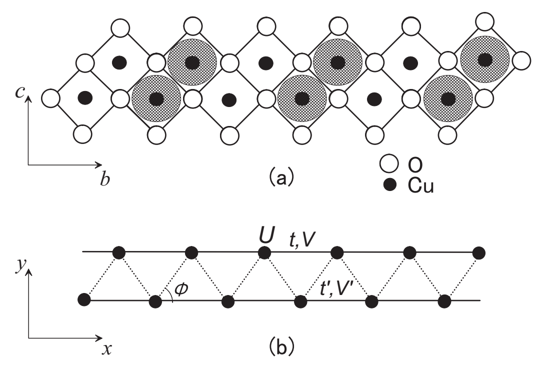

Fig. 1. Schematic representations of (a) the CuO double chain and (b) corresponding two-chain Hubbard model. The stripe-type CO discussed in the main text is schematically shown as shaded circles in (a).

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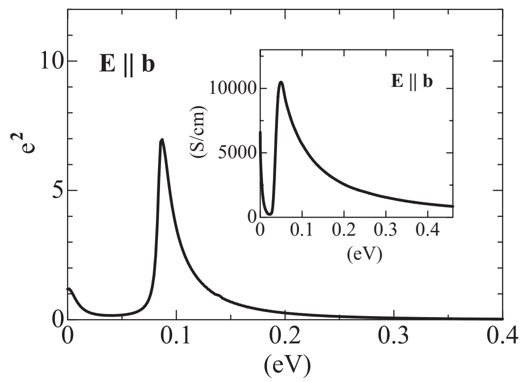

Fig. 2. Calculated optical conductivity spectrum compared with the experimental data of Takenaka *et al.* [4] (inset).

2. Calculated results and discussion

Let us first summarize the experimental features of the optical conductivity of $PrBa_2Cu_4O_8$ observed at room temperature [4]; (i) a broad peak structure with large spectral weight (98% of the total weight) located at $\omega \gtrsim 40$ meV and (ii) very small Drude weight (2% of the total weight). Another experimental feature of the charge dynamics found by the NQR experiment [5] is that the CuO double chains have a very slow fluctuation of the electric-field gradient caused by the spatial fluctuation of electronic charge carriers; the system may thus be in the vicinity of the long-range CO state.

Now, in Fig. 2, we compare our results with experiment. We find a good agreement; (i) The spectrum calculated for the stripe-type CO phase is in reasonable agreement with experiment. The spectra calculated for the in-line–type CO phase completely fail to agree with experiment. (ii) The observed very small Drude weight is well reproduced. (iii) The asymmetric spectral shape of the main peak structure, i.e., sharp in the lower energy side and broad in the higher energy side, is reproduced by our calculation. The width of the peak is however rather narrow compared with experiment. This may be due to the effect of electron correlations neglected in the mean-field approximation, i.e., the scattering of the quasiparticles may well broaden the spectra. (iv) As for the amplitude of the ordered charges, we find the calculated values of the order parameters to be $\delta = 0.013$ (per site) and $2S^z = 0.21$ (per site) for the parameter values used in Fig. 2. This value of δ is consistent with the experimental estimation where it has been pointed out that less than 0.02 holes per Cu are frozen [5].

Thus, we have demonstrated that the mean-field calculation of the optical conductivity for the two-chain Hubbard model reproduces well the experimental features of the charge excitations of the CuO double chains of $PrBa_2Cu_4O_8$, provided that the stripe-type CO phase is present. However, we should note that there is no experimental indication of the long-range CO in $PrBa_2Cu_4O_8$ but rather there is only the slow fluctuation of electronic charge degrees of freedom [4,5]. The time-scale argument may resolve this apparent contradiction; the fast time scale of the optical measurement should enable one to detect slowly fluctuating order parameters as virtually a long-range order. We therefore argue that the stripe-type charge fluctuations with very slow time scale of the order of $0.1-10$ MHz [5] should persist in the system and should be the origin of the $\sim$40 meV peak structure in the optical conductivity spectrum of the CuO double chains of $PrBa_2Cu_4O_8$.

In summary, we have calculated the optical conductivity of the two-chain Hubbard model by the mean-field approximation to consider the observed anomalous features of the charge dynamics of the CuO double chains of $PrBa_2Cu_4O_8$. We have argued that the stripe-type fluctuation of charge carriers with a very slow time-scale should be the origin of anomalous features of the observed optical conductivity spectra.

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