Analysis of multiple bosonic couplings in the self-energy of the high-Tc cuprate superconductor $La_{2-x}Sr_xCuO_4$ using Bayesian inference

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To understand the mechanism of emergence of cuprate high-temperature superconductors, it is essential to clarify the interactions between electrons and bosons. In particular, the kink structure observed by angle-resolved photoemission spectroscopy (ARPES) has been regarded as a strong clue to electron–boson interactions [1–3]. However, there remains ongoing debate as to whether its origin is phonon in nature [2] or arises from magnetic interactions [3].

Lanzara *et al.* reported a universal kink structure appearing around 70 meV in Bi-based and La-based cuprate superconductors and suggested that it originates from electron–phonon coupling to the half-breathing phonon mode [2]. Furthermore, Zhou *et al.* performed high-resolution ARPES measurements on $La_{2-x}Sr_xCuO_4$ (LSCO) and investigated the kink structure in detail. By estimating the Eliashberg function $\alpha^2F(\omega)$ using the maximum entropy method (MEM), they demonstrated that electrons couple not to a single mode but to multiple phonon modes [4].

However, MEM has limitations in estimation accuracy, such as variations in the number and intensity of peaks in $\alpha^2F(\omega)$ depending on the choice of the prior function. In this study, we introduce Bayesian inference and determine the number of peaks by model selection based on the free energy. Figure 1 shows the real part of the self-energy, $\mathrm{Re}\Sigma$ of LSCO (x = 0.03) [5]. As a result, the model with the number of peaks (K = 3) yields both the minimum free energy and the maximum posterior probability, suggesting that three bosonic modes contribute to the kink structure. The three estimated peaks are located at approximately 31 meV, 51 meV, and 67 meV. By comparing these results with the phonon density of states obtained from first-principles calculations for La_2CuO_4 reported in previous studies [6], the physical origins of these bosonic modes can be interpreted as phonon. The peaks at about 51 meV and 67 meV are assigned to a bond-bending mode involving apical oxygen (LO_{2a} mode) and the oxygen bond-stretching phonon (LO_{1a} mode), respectively.

For the low-energy feature around 31 meV, two interpretations have been discussed in the literature. In Ref. [6], this peak is assigned to a low-energy mode (LE mode), whereas other first-principles studies report Cu–O bond-bending (buckling mode) in the energy range of 30–40 meV [7]. Therefore, the 31 meV peak may be attributed either to the LE mode proposed in Ref. [6] or to a buckling mode.

In this presentation, we report the results of a kink-structure analysis based on Bayesian inference and discuss the physical origins of these bosonic modes through comparison with previous studies.

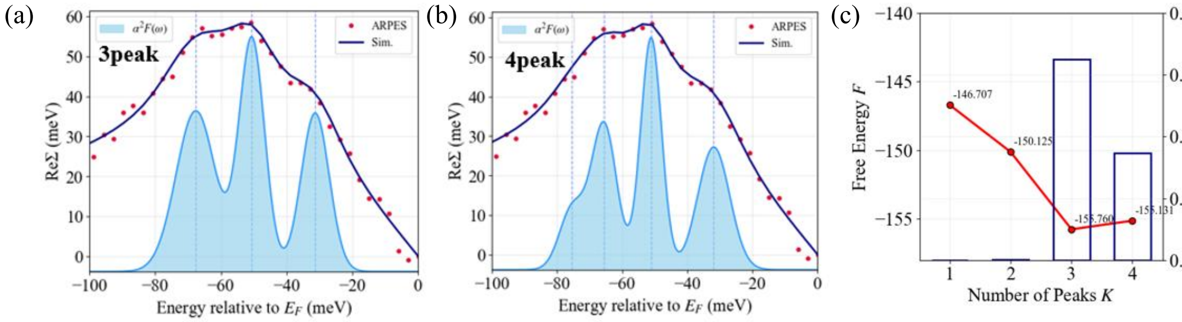

Figure 1.
(a), (b) Results of Bayesian fitting to the nodal-direction ReΣ(ω) of LSCO (x = 0.03) [5], assuming $\alpha^2F(\omega)$ with three peaks and four peaks, respectively.
(c) Results of model selection for the number of peaks (K) based on the Bayesian free energy (F) and the posterior probability (p).

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