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Development of ARPES analysis method using Bayesian Inference and application to cuprates

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High-Tc cuprate superconductors exhibit unique physical properties such as high superconducting transition temperatures, density wave formation, and bad metallic states. To understand their physical properties, it is necessary to quantitatively evaluate the many-body interactions that give rise to them. Since high-resolution angle-resolved photoemission spectroscopy (ARPES) spectra correspond to the imaginary part of the single-particle Green's function, quantitative analysis of the ARPES spectral shape allows us to experimentally extract the self-energy (Σ) that reflects information on many-body interactions. In conventional self-energy analysis methods, the self-energy is extracted by assuming some form of a one-electron band and checking whether the real part of the self-energy (ReΣ) and imaginary part of the self-energy (ImΣ) satisfy the Kramers-Kronig relation. However, this method cannot eliminate arbitrariness in determining the one-electron band, and the parameters cannot be optimized in a single step. It is required, therefore, to optimize all the parameters directly from an image plot of the ARPES spectrum without arbitrariness. In this study, we applied Bayesian inference [1] to analyze ARPES image plots of heavily overdoped $(Bi,Pb)_2Sr_2CuO_{6+\delta}$ ($T_C \sim 6$ K) to extract all parameters simultaneously.

We applied a new analysis method to the ARPES spectra shown in Fig. 1(a). Fig. 1(b) shows the simulated ARPES spectrum using optimized parameters. One can see experimental ARPES spectral features are well reproduced by the simulation. It is noted that the suppression of the ARPES spectral intensity below -0.4 eV which is known as waterfall structure is well reproduced by the self-energy due to the electron-electron interaction. It indicates that the waterfall structure mainly originated from many-body interactions but not from the matrix element effect. Solid blue lines in Fig. 1(c) show evaluated ReΣ and ImΣ, being compared with those obtained from the conventional method (red dots). The deviation is mainly from the transition matrix element effect which is included in the new method but not in the conventional method. This indicates how the transition matrix element affects the self-energy extraction.

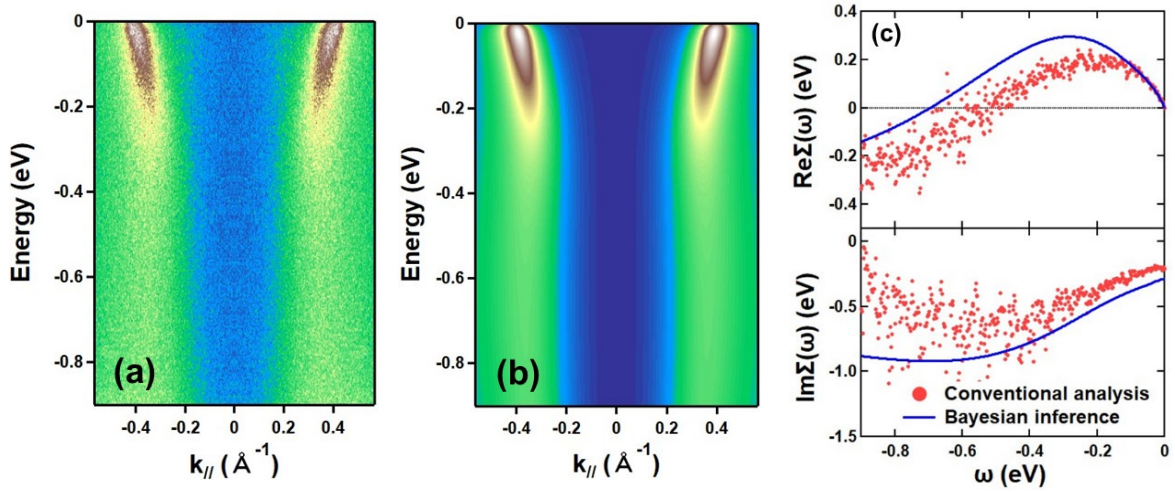

FIGURE 1. (a) Experimental data. (b) ARPES image plot simulated by the Bayesian inference method. (c)

Blue lines indicate evaluated total self-energy. Red dots show self-energy obtained from the conventional analysis method.

REFERENCES

1. S. Tokuda, S. Souma, K. Segawa, T. Takahashi, Y. Ando, T. Nakanishi & T. Sato, *Communications Physics,* **4**, 170 (2021).