Reply to Valla’s Comment on “Multiple Bosonic Mode Coupling in Electron Self-Energy of (La$_{2-x}$Sr$_x$)CuO$_4$”

In his comment[1], Valla simulated the effect of energy resolution on the fine structure in the electron self-energy. By employing one energy resolution of $\Delta_{\text{exp}}=20$ meV in his simulation, he concluded that the fine structure in Re$\Sigma$ cannot be observed and the fine structure we identified[2] are most likely noise related.

First, let us look at data measured with an energy resolution better than 20meV[3]. Fig. 1 shows the measured real part of electron self-energy Re$\Sigma$ taken at an energy resolution of $\sim 15$meV for LSCO $x=0.03$ (Fig. 1a)[4] and at 12 meV for LSCO $x\sim 0.06$ (Fig. 1b). Clear fine structure, manifested as a curvature change, can be identified at 40$\sim 45$ meV and $\sim 60$meV. The measured Re$\Sigma$ is fitted by the same procedure as in[2]. The second derivative of the fitted Re$\Sigma$ reveals two additional weaker features at $\sim 25$meV and $\sim 80$meV.

The new data with better energy resolution are consistent with other data presented in[2]. The two features at 40$\sim 45$ and $\sim 60$meV are rather robust, showing up as main features in all the measurements. The higher energy feature at 70$\sim 80$ mev shows up more clearly in LSCO samples with higher doping, same as before[2]. The variation of the low energy feature at $\sim 25$ meV is relatively larger among different measurements, but the feature exists. Given consistent observations from different samples, different dopings, and under different experimental conditions, our findings are not explainable by random noise. As shown in[2] as well as in Fig. 1, experimental uncertainty including noise may affect the results, such as the small peak shift between 40 and 45 meV. However, bearing in mind the extreme challenging nature of this experiment, we consider the consistency satisfactory in this very first effort to get the fine structure in cuprates.

We now turn to the issue raised by Valla[1] about the effect of energy resolution on the fine structure. First we note that this simulation is model dependent because a specific electron-phonon coupling form was used[1]. We also note that this simulation is parameter sensitive, including the mode energy, mode strength, impurity scattering and how the resolution is included. We don’t think that one should take the simulation too literally as in[1]. For the sake of discussion, let us put these aside for the moment. We show in Fig.2 simulated Re$\Sigma$ under different energy resolutions in the same procedure as in[1] (Fig. 2a), and the corresponding second derivative (Fig. 2b). Four modes at 25, 40, 60, and 80meV are assumed in the $\alpha^2 F(\omega)$ to calculate the single particle spectral function. The mode positions are determined from Fig. 1b which were measured using a better energy resolution, and an impurity term $\sim 100$meV from MDC width at $E_F$ is added in the imaginary part of the self-energy.

As seen from Fig. 2, at a high energy resolution, the fine structure shows up as small peaks on the top of a broad self-energy feature. As the resolution deteriorates, the fine structure manifests themselves as a curvature change in Re$\Sigma$ which can be better identified as peaks in its corresponding second derivative. It is clear from Fig. 2b that at an energy resolution of 20 meV or even slightly worse, it is possible to identify the fine structure, albeit with a larger error bar. We stress that while it appears hard to discern features in the Re$\Sigma$ at an energy resolution of 20 meV, as claimed by Valla[1], the second derivative that we used, reveals them. The main reason here is that the fine structure is embedded in the curvature of the self-energy. Part of the issue is the separation between 45 and 61 meV mode, which is under an energy resolution of 20 meV[1]. The reason they are observable can be three-fold. As in Fig.2, one can still discern peaks in the second derivative even when the separation is slightly smaller than the resolution. The second is that the energy resolution quoted in our paper (18$\sim 20$meV)[2] was an overestimate as the beamline is conservatively calibrated. The third is a few meV shift of the 40 meV mode to 45 meV as a small experimental uncertainty is not unexpected.

A separate issue Valla raised is the distortion of Re$\Sigma$ at lower energy near the Fermi level $E_F$[1]. At a low energy resolution, the simulated Re$\Sigma$ exhibits a backbend near $E_F$ and gives rise to a finite value at $E_F$. For ex-
ample, at an energy resolution of 20meV, the ReΣ tends to level off in the energy range between 0 and ~20meV. This simulated result deviates markedly from our experimental results where the measured ReΣ extends to Fermi level almost linearly (Fig. 1). This discrepancy between data and simulation is well beyond the noise. This issue depends on many details of the simulation and its comparison with data that are beyond this short communication. However, the clear discrepancy between data and simulation drives home an important point. The real way for the author of [1] to substantiate his claim is not through a model specific, parameter and procedure sensitive simulation, but rather through experimental data with superior energy resolution and signal to noise ratio.

In summary, experiments with improved energy resolution more clearly reveals the fine structure of mode coupling which is consistent with other measurements. Even within the context of Valla’s simulation, at an energy resolution of 20meV, it is possible to observe fine structure as they are embedded in the curvature and will be revealed in the second derivative. We believe that the ensemble of data and the analysis make a strong case for multiple mode coupling in LSCO, with the most important modes near 40 and 60 meV.

FIG. 2: (a). Simulated real part of electron self-energy ReΣ at different energy resolutions. (b). Second derivative of the simulated ReΣ at different energy resolutions.

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[1] T. Valla, cond-mat/0501138
[2] X. J. Zhou et al., cond-mat/0405130
[3] This experiment is challenging because of the necessity to use a relatively high photon energy (\textasciitilde 55eV) for LSCO system. In this case, it is hard to compromise between two conflicting requirements: high energy resolution and high photon flux for a good statistics of data.
[4] This is the same data set as in Fig. 2(a2) in [2]. The data were measured at an energy resolution of \textasciitilde 15meV with 1 meV energy interval. To improve the statistics, every three adjacent data point are combined to obtain one data point in Fig. 1a.