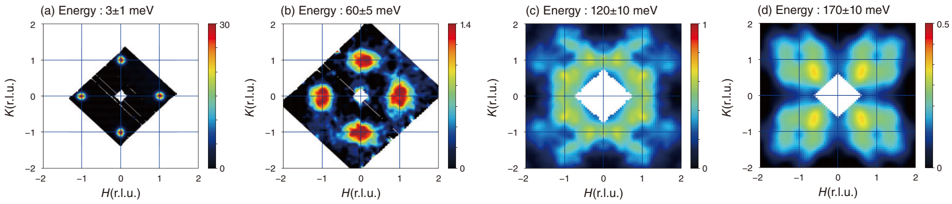
5–2 Linking Spin-Fluctuations to Electron Correlations

—A Combined Neutron and ARPES Study—



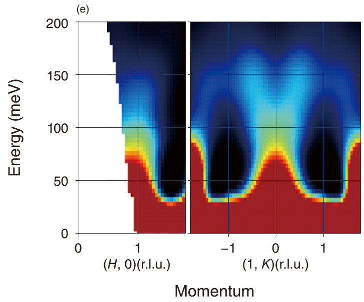


Fig.5-4 Spin excitations of the iron-based superconductor
Constant-energy maps in the (H, K) plane at energy transfers of (a) E = 3 ± 1 meV, (b) E = 60 ± 5 meV, (c) E = 120 ± 5 meV, and (d) E = 170 ± 10 meV; and (e) energy-band dispersion of spin excitations along the (1, K) high-symmetry direction.

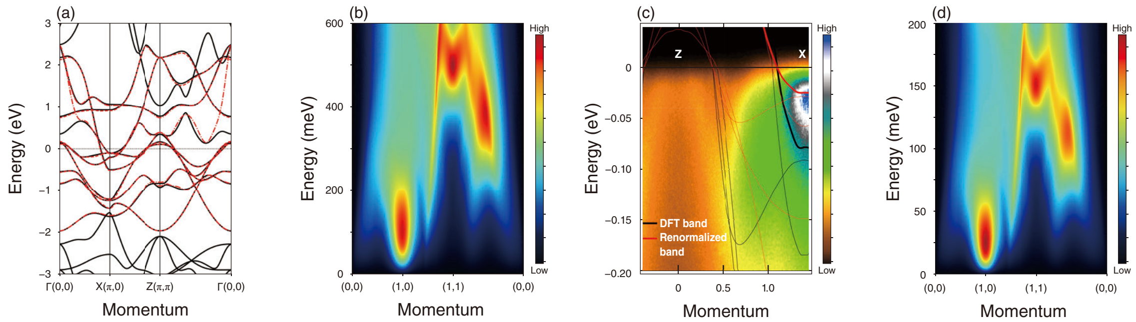


Fig.5-5 First-principles analysis of the spin excitation spectrum
(a) Electronic band structure of the iron-based superconductor obtained by first-principle calculations. (b) Spin excitation spectrum calculated using the model in Fig.5-5(a). (c) Comparison between ARPES and first-principles calculations. The black and red lines denote the original and renormalized bands, respectively. (d) Spin excitation spectrum calculated using the renormalized band structure.

The surprising discovery of high-T_c superconductivity in iron-based superconductors (FeSCs) has marked the beginning of a new era in superconductivity research. Earlier studies have suggested that FeSCs are weakly correlated materials, unlike cuprate superconductors, in which Mott physics is more fundamentally tied to superconductivity. However, increasing evidence suggests that electron correlations in FeSCs are much stronger than previously thought. The role of electron correlations is therefore the most interesting, yet not well understood, aspect of the physics in FeSCs.

Inelastic neutron scattering (INS) was used to study the effect of electron correlations on spin dynamics in FeSCs. INS measurements were performed using the BL01 4SEASONS installed at J-PARC. As seen in Fig.5-4, well-defined spin excitations were observed up to high-energy transfers of at least 200 meV.

To understand the obtained INS data, a first-principles analysis of the spin excitation spectrum was performed (Figs.5-5(a) and (b)). This analysis reproduced the spin-wave-like dispersive feature along the high-symmetry directions, but overestimated the energy scale of the excitations by a factor of three.

This overestimation of the spin excitation energy has important implications for the electronic state of FeSCs. In general, the electronic band structure determines the momentum- and energy-dependent structure of the spin excitation spectrum. The discrepancy between the experimental and theoretical spin excitations, therefore, suggests that the actual electronic structure of FeSCs deviates from that predicted from first-principles calculations.

To gain more insight into the electronic structure, angle-resolved photoemission spectroscopy (ARPES) was then performed on crystals from the same batch as was used for the INS measurements. From the ARPES data shown in Fig.5-5(c), one can notice that the experimental band structure displays a narrowing of the Fe-3*d* bands by a factor of three. This narrowing corresponds to an enhancement of the effective mass due to electron correlation effects.

Considering the strong sensitivity of the spin excitations to the underlying electronic structure, one can expect that the Fe-3*d* bandwidth narrowing due to electron correlations is directly reflected in the spin excitation energy scale. To confirm this, we re-evaluated the spin excitation spectrum by incorporating the effect of mass enhancement. As shown in Fig.5-5(d), the spin excitation bandwidth was reduced to approximately one third of its original width, yielding a broadly consistent description of the observed INS data.

The consistency between the results of the two momentum-resolved spectroscopic methods, INS and ARPES, demonstrates a quantitative link between the magnetic response and the underlying electronic structure of FeSCs, thus indicating that INS may be used as a momentum-resolved spectroscopy for determining the correlated electronic structure. The availability of more intense neutron sources in the next few years would further improve the potential of INS as a versatile and practical spectroscopic technique to investigate the electronic and magnetic structures on an equal footing.

Reference
Murai, N. et al., Effect of Electron Correlations on Spin Excitation Bandwidth in $Ba_{0.75}K_{0.25}Fe_2As_2$ as Seen via Time-of-Flight Inelastic Neutron Scattering, Physical Review B, vol.97, issue 24, 2018, p.241112-1–241112-6.