Experimental Determination of Competing Magnetic Interactions in FeSe

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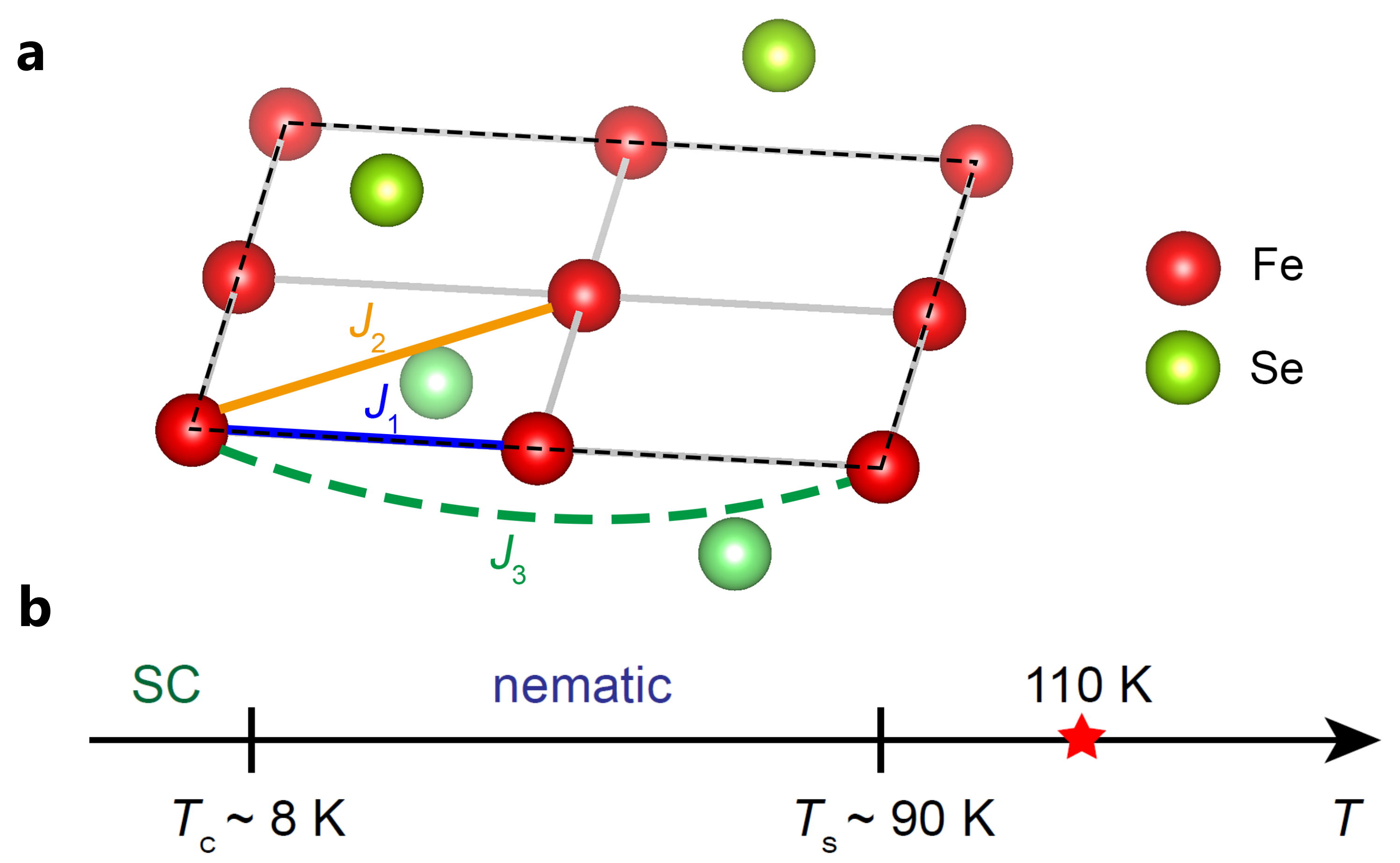
Abstract

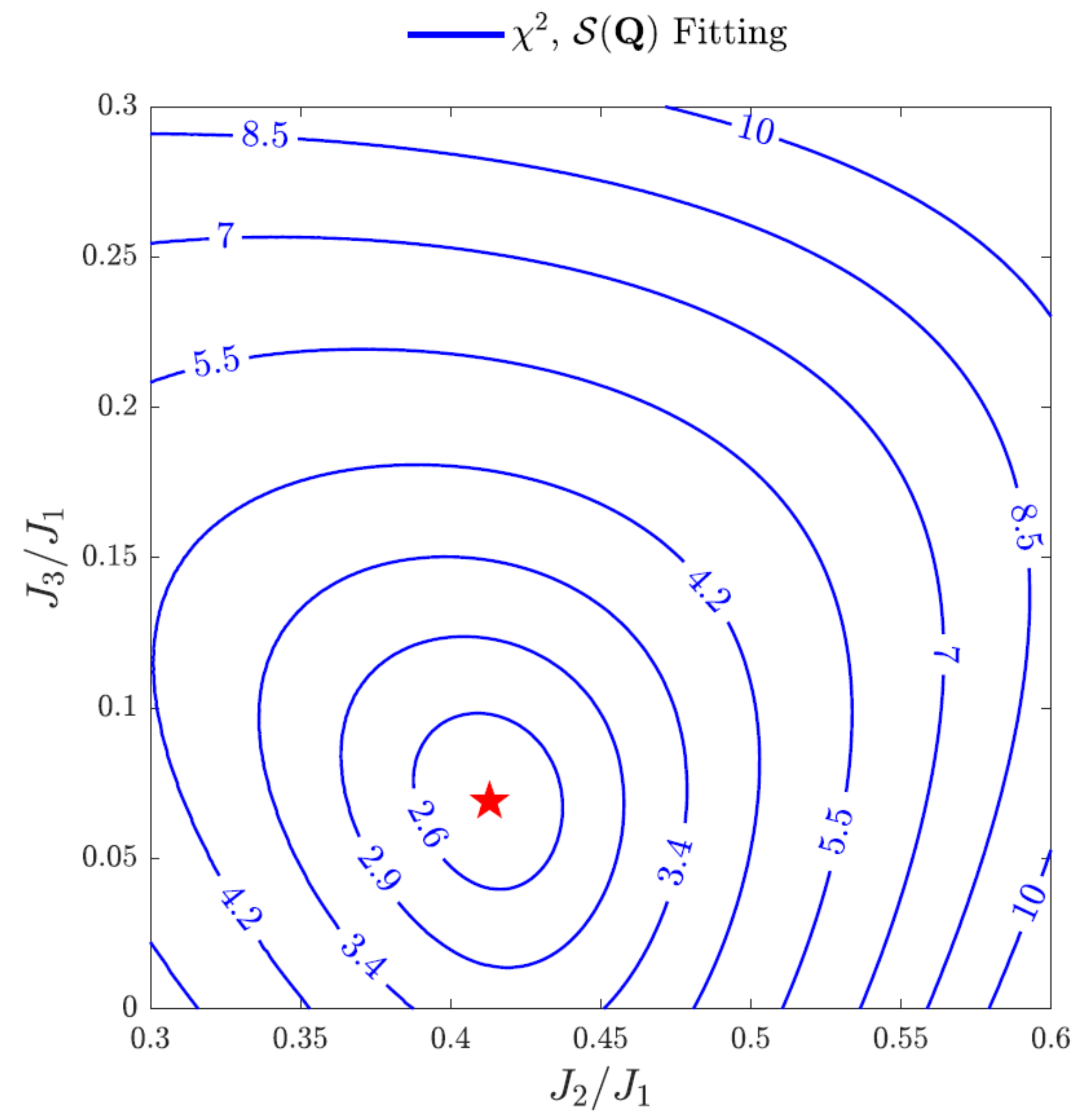
Magnetism plays a central role in the unconventional superconductivity of iron-based superconductors. Unlike typical iron-based systems with static antiferromagnetic order and spin wave excitations, FeSe exhibits extended nematic paramagnetic phase with large fluctuating moment and quite unusual spin excitation spectrum. Various theoretical models have been proposed to elucidate the nature of these exotic magnetic properties, which are generally attributed to the frustration arising from competing magnetic interactions. However, the magnetic ground state of FeSe is still under debate. Here we determine the exchange interactions in FeSe from inelastic neutron scattering data at 110 K using self-consistent Gaussian approximation (SCGA) method. Mapped to Heisenberg model with nearest-neighbor (J_1), next-nearest-neighbor (J_2) and third-nearest-neighbor (J_3) in-plane exchange couplings, $J_2/J_1 = 0.413 \pm 0.051$ and $J_3/J_1 = 0.069 \pm 0.060$ are extracted from the experiment in an unbiased way. Our results evidence the strongly frustrated exchange interactions in FeSe and shed light on the origin of nematic paramagnetic state.

Crystal structure and phase diagram of FeSe



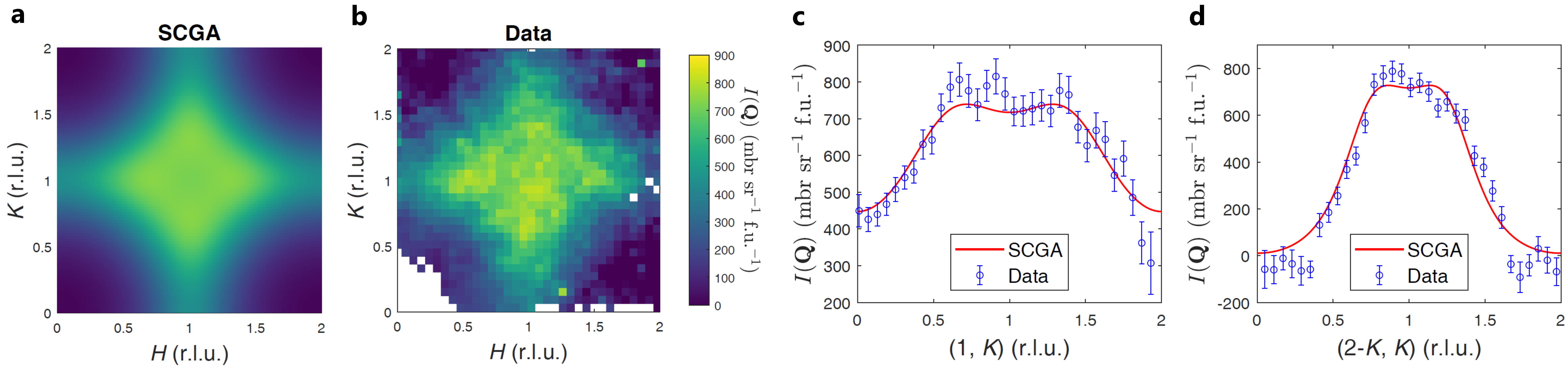
a, Crystal structure of FeSe. J_1, J_2, and J_3 denote the 1st, 2nd, and 3rd-nearest-neighbor in-plane exchange couplings, respectively. The black dashed lines represent the orthorhombic (4-Fe) unit cell, which is used throughout our presentation. **b**, Phase diagram of FeSe. The red star emphasizes the magnetic interactions are extracted from the inelastic neutron spectrum[1] measured at 110 K.

Determination of magnetic interactions in FeSe



Contour plot of the goodness of fit χ^2 between calculations and neutron scattering data. The equal-time magnetic structure factor $\mathcal{S}(\mathbf{Q})$ is calculated through self-consistent Gaussian approximation (SCGA) for the J_1-J_2-J_3 Heisenberg model at $k_BT/J_1 = 0.86$ which is optimized from global fit. The red star denotes the best fitted interaction parameters.

Momentum dependence of calculated equal-time structure factor and energy-integrated $I(\mathbf{Q})$ data



a, The equal-time structure factor calculated using SCGA for the optimized parameters $k_BT/J_1 = 0.86$, $J_2/J_1 = 0.413$ and $J_3/J_1 = 0.069$. **b**, Energy-integrated intensity $I(\mathbf{Q}) = \int_0^{E'} \left(1 + e^{-E/k_BT}\right) I(\mathbf{Q}, E)dE$ obtained from the measured magnetic intensity $I(\mathbf{Q}, E)$ of FeSe at T = 110 K, with the Fe^{2+} magnetic form factor corrected. $E' = 220$ meV is the upper limit of the spin excitation energy. **c-d**, Momentum dependence of $I(\mathbf{Q})$ along several paths in the reciprocal space, and comparison with SCGA calculations.

Conclusion

- $J_2/J_1 = 0.413 \pm 0.051$ and $J_3/J_1 = 0.069 \pm 0.060$ are extracted from the experiment (T = 110 K), which evidence the strongly frustrated exchange interactions in FeSe.
- The realistic interaction parameters of FeSe satisfy the prerequisite for the theoretically proposed S = 1 nematic quantum-disordered phase[2], and naturally explain the transfer of spectral weight from Néel to the stripe spin fluctuations as lowering the temperature across T_s (ref. 1, 3).

References

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