Effect of magnetic field on the spin resonance in FeTe$_{0.5}$Se$_{0.5}$ as seen via inelastic neutron scattering

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Inelastic neutron scattering and susceptibility measurements have been performed on the optimally-doped Fe-based superconductor FeTe$_{0.5}$Se$_{0.5}$, which has a critical temperature, $T_c$, of 14 K. The magnetic scattering at the stripe antiferromagnetic wave-vector $Q = (0.5, 0.5)$ exhibits a “resonance” at $\sim 6$ meV, where the scattering intensity increases abruptly when cooled below $T_c$. In a 7-T magnetic field parallel to the a-b plane, $T_c$ is slightly reduced to $\sim 12$ K, based on susceptibility measurements. The resonance in the neutron scattering measurements is also affected by the field. The resonance intensity under field cooling starts to arise at a lower temperature $\sim 12$ K, and the low temperature intensity is also reduced from the zero-field value. Our results provide clear evidence for the intimate relationship between superconductivity and the resonance measured in magnetic excitations of Fe-based superconductors.

The recent discovery of Fe-based superconductors has triggered tremendous interest in the field. One of the key questions to be answered is what is the pairing mechanism for the high critical temperature (high-$T_c$) superconductivity in these materials. It is now widely believed that pairing mediated by magnetic excitations is the most likely candidate for explaining the superconductivity. The “resonance” in magnetic excitations, where the spectral weight at the resonance energy shows a significant increase when the system enters the superconducting phase, has been observed in a number of these Fe-based superconductors, including BaFe$_2$As$_2$ (the 1:2:2 system) and the 1:1 system Fe$_{1+y}$Te$_{1-x}$Se$_x$. The resonance is always observed at the energy $h\Omega_0 \sim 5k_BT_c$, and near the antiferromagnetic (0, 0, 0.5) point (using notation with two Fe atoms per unit cell) although the propagating vectors for the spin-density-wave (SDW) in the parent compounds are different by 45° in these two systems. These results suggest that the resonance in the magnetic excitations should be similar across different Fe-based superconductor systems, and are closely related to the onset of superconductivity.

In these superconductors, angle resolved photoemission (ARPES) studies have provided evidence for electron and hole pockets that are nearly nested by the stripe antiferromagnetic wave-vector. A spin resonance detectable by neutron scattering is predicted to occur at a particular wave-vector only if that wave-vector connects portions of the Fermi surface that have opposite signs of the superconducting gap, so that observations of the resonance may provide important information relevant to the symmetry of the superconducting gap. Since superconductivity, and hence the coupling, is sensitive to magnetic field, one would naturally expect that an external magnetic field can also impact the resonance accordingly, as seen in YBa$_2$Cu$_3$O$_{6.6}$ (Ref. [20]) and in La$_{1.82}$Sr$_{0.18}$CuO$_4$ (Ref. [21]). Indeed, the magnetic field effect on the resonance in Fe-based superconductors has been observed in the 1:2:2 system BaFe$_{1.9}$Ni$_{0.1}$As$_2$ where the resonance energy and intensity have been partially reduced by an external field.

We have carried out an inelastic neutron scattering study on an optimally-doped 1:1 material—a single crystal of FeTe$_{0.5}$Se$_{0.5}$, with $T_c \approx 14$ K. We find that a resonance with energy $h\Omega_0 \approx 6$ meV = $5k_BT_c$, appears below $T_c$, consistent with previous findings. In a 7-T magnetic field parallel to the a-b plane, the superconductivity is partially suppressed, with reduced $T_c$ of 12 K. In the field, the resonance starts to appear at the reduced $T_c$, with lower intensity than that measured in zero field. This behavior demonstrates that the magnetic excitations have a close association with the superconductivity.

The single-crystal sample was grown by a unidirectional solidification method with nominal composition of FeTe$_{0.5}$Se$_{0.5}$. The bulk susceptibility was characterized using a superconducting quantum interference device (SQUID) magnetometer. In the susceptibility measurements, the sample was oriented so that a-b plane was parallel to the magnetic field. Neutron scattering experiments were carried out on the triple-axis spectrometer BT-7 located at the NIST Center for Neutron Research. A single crystal with mass of 8.9 g was used in the neutron experiment and firmly fixed to an aluminum plate. The lattice constants are $a = b = 3.80(8)$ Å, and $c = 6.14(7)$ Å using the notation where there are two Fe atoms in one unit cell. The data were collected in (HHL) scattering plane, defined by two vectors [110] and [001], and described in reciprocal lattice units (r.l.u.) of $(a^*, b^*, c^*) = (2\pi/a, 2\pi/b, 2\pi/c)$. A vertical magnetic field of 7 T was applied parallel to the a-b plane (along [110]) in the field-cooling (FC) measurements.

Energy scans have been performed at $Q = (0.5, 0.5, 0)$, as shown in Fig. 1(a). There is a large background at low energies coming from the superconducting magnet in which the sample resides, and this obscures the magnetic response in the raw data. However, if we compare the scans taken at 4 K and...
20 K, a significant amount of spectral weight shows up between 5 meV and 9 meV for the spectrum measured at low temperature (as indicated by the shading). If we subtract the 20 K data from the 4 K data as in Fig. 1(b), one can see a broad peak at 6 meV. This is consistent with that observed in 40% and 50% Se doped samples, in which resonance energies of 6.5 meV and 7 meV, respectively, were reported. Although a spin gap is not directly observed in the raw data, we do see from the background subtracted data in Fig. 1(b) that the difference of the intensity \(I_{4K} - I_{20K}\) becomes negative below 5 meV, which suggests that a gap opens below this energy at 4 K, consistent with the gap value obtained by Qiu et al.

To test the impact of a magnetic field, a 7-T field was applied at 20 K, and the sample was cooled in the field. In Fig. 2, we show background (20 K data, zero field) subtracted scans performed at different temperatures. At \(T = 12\) K, the difference between data taken with and without the field is very clear. With further cooling, the difference is still observable but becomes less pronounced. At \(T = 4\) K, the peak intensity for the 7-T scan is about 10% to 20% smaller than that of the zero-field data, while the 7-T spectrum seems to have more intensity filled in below the gap (5 meV).

We also performed some constant-energy (7-meV) scans along \((h, h, 0)\) through \(h = 0.5\). With a counting rate of 5 min/point, the change in signal at \(h \approx 0.5\) between 4 K and 20 K was consistent with the constant-Q scans; however, the signal-to-background level at this counting rate was not sufficient to provide a useful measure of the peak shape, nor to resolve changes due to field. Given finite beam time, it was not possible to measure both constant-Q and constant-energy scans with adequate statistics, so we decided to abandon the latter.

There is a sum rule for scattering from spin-spin correlations, and hence one might expect that the reduction of the resonance intensity by the field should result in an increase of spectral weight below the gap, as commonly seen in cuprates as well as in BaFe\(_{1.9}\)Ni\(_{0.1}\)As\(_2\) (Ref. 32). As discussed above, it is consistent with our results in principle, but the large background makes it impossible to follow the behavior to lower energies. In cuprates, Demler et al. analyzed a model of coexisting but competing phases of superconductivity and SDW order, and successfully predicted the field-induced static magnetic order observed experimentally. We have searched for SDW order around \((0.5, 0.5, 0)\), but no evidence of such field-induced order was found.

We have measured the bulk susceptibility in 0-T and 7-T field as well, and the results are shown in Fig. 3(a). In zero field, the system enters a superconducting state at 14 K, and becomes fully diamagnetic below 12 K. In the 7-T field, superconductivity is partially suppressed, and \(T_c\) has been reduced to 12 K. As a result of the suppressed superconductivity, the resonance intensity has also been reduced as shown in Fig. 2.

Fig. 3(b) gives another perspective of the impact of the field on the resonance. There we plot the intensity, integrated from 6 meV to 7 meV, as a function temperature obtained for the measurements with and without the field. The intensity \(I(T)\) was fit with the mean-field theory using \(T_{c,8}\) determined by the onset of the diamagnetism in Fig. 3(a), with
In summary, we observed a resonance at $\hbar \Omega_0 \approx 6 \text{ meV}$ in FeTe$_{0.5}$Se$_{0.5}$ ($T_c = 14 \text{ K}$). The temperature dependence of the intensity is consistent with the scaling $1 - (T/T_c)^{1/2}$. A 7 T magnetic field partially suppresses superconductivity, and lowers $T_c$ to about 12 K, determined from the bulk susceptibility. In the field, the resonance starts to appear at the lowered $T_c$, 12 K, with intensity reduced. These results are consistent with the picture that the resonance is related to quasiparticle scattering in the superconducting phase, and is reduced when superconductivity becomes weaker, either by heating or applying an external magnetic field.

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