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Nuclear magnetic resonance effect and adaptation

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ABSTRACT: *A prototypical electron-doped iron-based superconductor LaFeAsO1−xHx goes through an antiferromagnetic (AF) stage for $x \geq 0.49$. We have performed atomic attractive reverberation (NMR) estimations on LaFeAsO0.4H0.6 at 3.7 GPa to research the attractive prop-erties in the region of a pressing factor incited quantum basic point (QCP). The linewidth of 1H-NMR spectra expands at low temperatures under 30 K, proposing that the turn minutes stay requested at 3.7 GPa. The conjunction of gapped and gapless turn ex-references was affirmed in the arranged state from the unwinding time T1 of 75As. The pressing factor initiated QCP is assessed to be 4.1 GPa from the pressing factor reliance of the gapped excitation.*

I. INTRODUCTION

A prototypical electron-doped iron-basedpnictide $\mathrm{LaFeAsO1}_{-x}\mathrm{H}_x$(0 x 0.6) exhibits unique electronicpropertiesinaheavilycarrier-dopedregime: a superconducting (SC) phase with double-domes structure expands in a wide regime (0.05 < x <0.49)[1]andanantiferromagnetic(AF)phasemanifests itself by further H doping (0.49 x) [2–4]. Band calculations show that both Fermi surfaces and nesting vectors change by H doping: the two hole pockets present at Γ point in the lightly H- dopedregimealmostdisappearintheheavilyH-dopedregime[5,6].ThechangeinthenestingvectorsduetoHdopingwouldcauseachangeinwave-vector(q)dependentspinsusceptibilityχ(q,ω)and would allow for the appearance of two AF phases in the lightly and heavily H-dopedregimes.

The AF phase in the heavily H-doped regime is stronglysuppresseduponapplyingpressure[7].We have performed nuclear magnetic resonance (NMR) measurements on LaFeAsO0.4H0.6 at 3.7 GPa, and we have found that the spin excitation gapappearing at the AF phase vanishes at around 4.1 GPa. We haveinvestigatedthemagneticpropertiesin thevicinityofapressure-inducedquantumcritical point (QCP)(c4.1GPa).

II. EXPERIMENTAL APPARATUSES AND CONDITIONS

A pressure of 3.7 GPa was applied using a NiCrAl- hybrid clamp-type pressure cell as shown in Fig. 1 [8]. We have used a mixture of Fluorinert FC-70 and FC-77 as the pressure-transmitting medium. Acoilwoundedaroundthepowdersamplesandan opticalfiberwiththeRubypowdersgluedontop

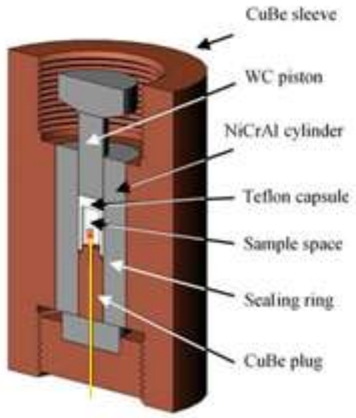

Figure1:ANiCrAlhybridclamptypepressurecell[8].AcoilwoundedaroundthepowdersamplesandanopticalfiberwiththeRubypowderswereinsertedintothe sample space.

wereinsertedintothesamplespaceofthepressure cell [8]. The size of the coil was 2.4 mm in di- ameter and 3.5 mm in length, and the number of windingswas18turns.Thepressurewasmonitored through Ruby fluorescence measurements. TheR1 and R2 lines at ambient pressure, 3.0 and 3.7 GPa are shown in Fig. 2. The wavelength of the R1 or R2 peak shifts linearly with respect topressure. TheshiftofthewavelengthΔλsatisfiestherelation P(GPa)=Δλ(nm)/0.365.

NMR measurements for the powder samples were acquired using a conventional coherent-pulsed NMRspectrometer.Therelaxationrate(1/T1)was measured using a conventional saturation-recovery methodforthesampleswhoseFeAsplanesarepar- allel to the appliedfield.

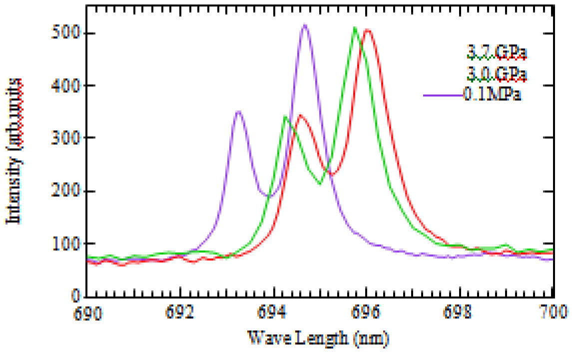

Figure2: Rubyfluorescencespectra.Thesmallerand largerpeakscorrespondtotheR2andR1transitions, respectively.

III. EXPERIMENTAL RESULTS

i. ^{1}H-NMRspectra

^{75}As(I=3/2)-NMRspectrabroadenduetothenu-

clearquadrupoleinteraction,whichmakesdifficult to investigate the antiferromagnetic (AF) state. However, 1H(I = 1/2) is free from the nuclear quadrupole interaction. Therefore, the 1H signal is narrow at a paramagnetic state, and the broad- eningintheAFphasedirectlyreflectsthemag-

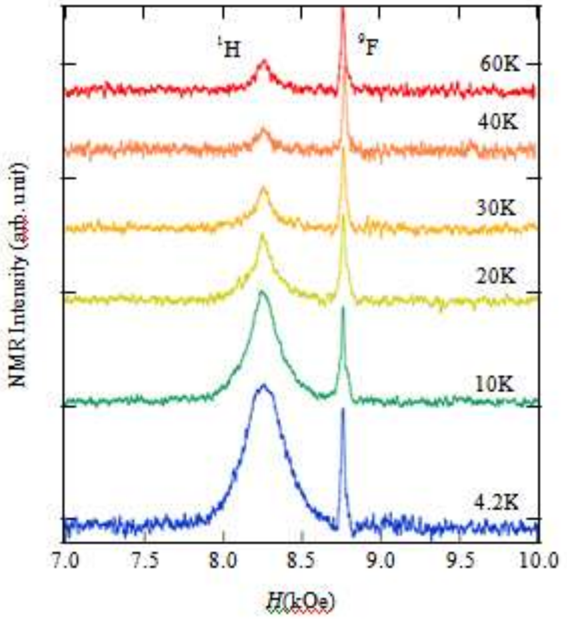

Figure 3: ^{1}H-NMR spectra for LaFeAsO0.4H0.6 mea- suredat3.7GPaand35.1MHz.The^{9}Fsignalorig- inatesfromthepressure-transmittingmedium,amix- ture of Fluorinert FC-70 andFC-77.

Figure4:Theincreasein^{1}Hlinewidthduetotheor- dered spin moments. T_N represents theantiferromag- netic (AF) transitiontemperature.

nitude of the spin moments. Figure 3 shows 1H- NMR spectra measured at 3.7 GPa and 35.1 MHz. Thesharpsignalof9Foriginatesfromthepressure- transmitting medium mentioned above. Thetem-
perature dependence of the linewidth is shown in Fig. 4 together with the data at ambient pressure [2, 4]. The onset of the broadening in Fig. 4 cor- responds to the AF transition temperature (T_N). Themaximumspinmomentisestimatedtobe1.80
μ_B[4]. As seen in Fig. 4, $T_N$is about 100 K at ambientpressureanddecreasesto30Kat3.7GPa. The pressure-induced QCP is expected at a much higher pressureregime.

ii. 1/T1T for75As

△

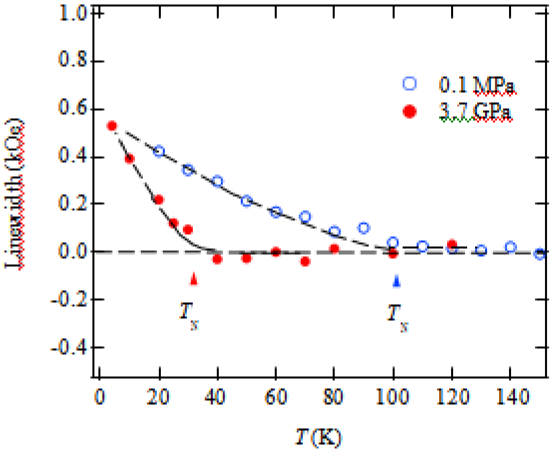

Figure4:Theincreasein1Hlinewidthduetotheor- dered spin moments. TN represents theantiferromag- netic (AF) transitiontemperature.

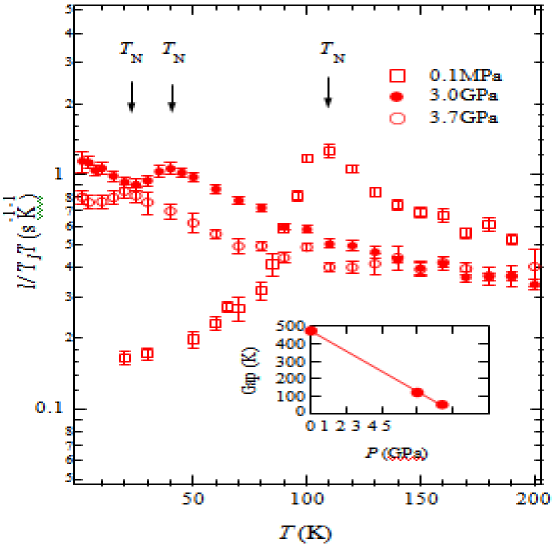

Figure5:Relaxationrateof^{75}Asdividedbytempera- ture,1/T1TforLaFeAsO$_{0.4}$H$_{0.6}$.$T_N$representstheAF transitiontemperature.Theinsetshowsthepressure dependenceofthespinexcitationgapΔ(SeeEq.(1)).

shows 1/T1T for 75As, and the peaks correspondto T_N. The values of $T_N$determined from 1/T1T are consistent with those obtained from the linewidth of 1H. At low temperatures just below T_N,1/T1T
is expressed as follows:
The relaxation rate divided by temperature 1/T1T providesameasureoflow-energyspinfluctuations.
1

——

T1T $\propto$

e^{-} T

(1)

Ingeneral,neglectingthewave-number(q)depen- dence of the hyperfine coupling constant, 1/T1T is proportionaltotheimaginarypartofthesuscepti-

bility: 1/T1T $\propto \Sigma_q \mathrm{Im}\chi(q,\ \omega)/\omega$ where ω represents a NMR frequency. 75As is preferred to 1H for T1 measurements, because FeAs layers are hardlyaf-

fected by the random distrubution of hydrogen in $\mathrm{LaO1}_{-x}\mathrm{H}_x$layers. Furthermore, owing to the nuclearquadrupoleinteraction,onecanpickupthe

^{75}As signals coming from the powders whoseFeAs planes are parallel to the applied field. Figure5

where Δ represent the spin excitation gap. The

pressure dependence of Δ is shown in the inset to Fig. 5. Assuming that Δ shows the linear depen- dence, the pressure-induced QCP is estimated to be 4.1 GPa.

IV. DISCUSSION

The activated spin excitation as shown in Eq. (1) originates from a spin density wave (SDW). However,1/T1TalsoshowsCurie-WeissbehaviorbelowT$_N$. The behavior is not observed at ambient pres- sure and it is characteristic of the critical behav- iornearthepressure-inducedQCP.Thecoexistence of the gapped and gapless excitations are specific to this system. In this system, major Fermi sur- facesareelectronpocketswithasquare-likeshape intwodimensionalkspace.Somepartsoftheelec- tron pockets would contribute to the nesting and the SDW formation. The critical behavior would originate from the other parts of the Fermi surfaces.Thenestingconditionbecomesworseandthe bandwidth becomes broader with increasing pressure.Owingtotheseeffects,theactivatedbehavior shown in Eq. (1) would disappear at the pressure- inducedQCP.

V. CONCLUSIONS

We performed NMR measurements on LaFeAsO0.4H0.6 at 3.7 GPa to investigate the magneticpropertiesinthevicinityofthepressure- induced QCP. We have found that the SDW ordered state still remains at 3.7 GPa. The pressure-induced QCP is estimated to be 4.1 GPa from the pressure dependence of the spin excitation gap. The gapless excitation observed as the Curie-Weiss behavior of 1/T1T coexists with the gapped excitation, implying that each excitation originates from different parts within the Fermisurfaces.

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