Neutron Scattering and Scaling Behavior in URu_2Zn_{20}

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Abstract

Cubic compounds URu_2Zn_{20} and ***$YbFe_2Zn_{20}$*** are good candidates for studying the Anderson impurity model in periodic f compounds and: f-atom content is less than 5% of the total number of atoms, and the shortest f-atom/f-atom spacing is ~ 6Å.

We measured ***time-of-flight (PHAROS*** at ***LANSCE, LRMECS*** at ***IPNS)*** spectra for URu_2Zn_{20} and ***triple-axis (HB3, HFIR-ORNL)*** for $YbFe_2Zn_{20}$.

We observed a broad peak in dynamic susceptibility χ''(ΔE) centered at 16.5 meV for URu_2Zn_{20} and 7 meV $YbFe_2Zn_{20}$. Together with specific heat and susceptibility the, it is obviously that γ and χ scale inversely with the characteristic energy for spin fluctuations, $T_{sf} = E_{max} / k_B$. ***Kondo impurity model*** describes the behavior of the 4*f* compound $YbFe_2Zn_{20}$ very well but works badly for the URu_2Zn_{20}, suggesting that the scaling behavior of the actinide compounds arises from spin fluctuations of *itinerant* 5*f* electrons.

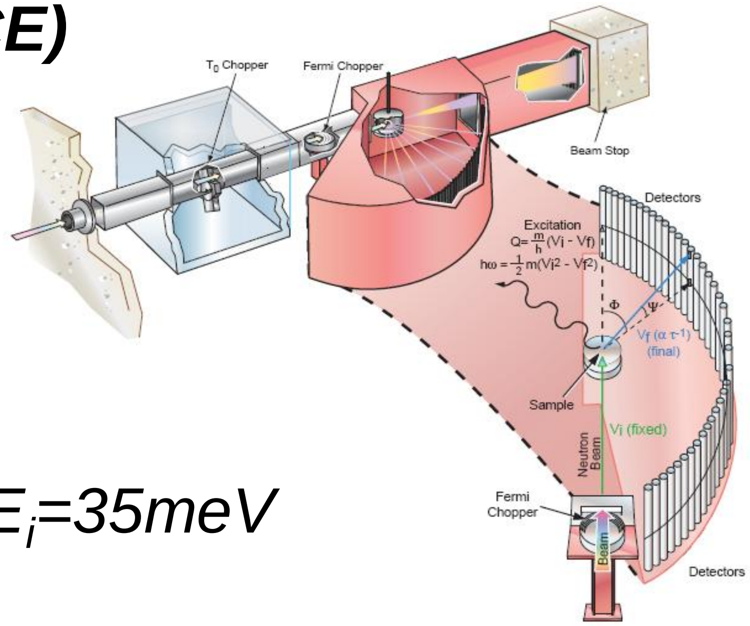
Motivation

For 4*f* electron rare earth Heavy Fermion compounds where the 4f orbitals are highly localized and hybridize only weakly with the conduction electrons.
the ***Anderson Impurity Model*** appears to give an excellent description of much of the experimental behavior.

Uranium compounds, the 5f orbitals are spatially extended and form dispersive bands through strong hybridization with the neighboring *s*, *p*, and *d* orbitals.
Hence, we might expect differences in the details of the behavior between the uranium and the rare-earth based heavy fermion materials, despite the common occurence of scaling behavior.

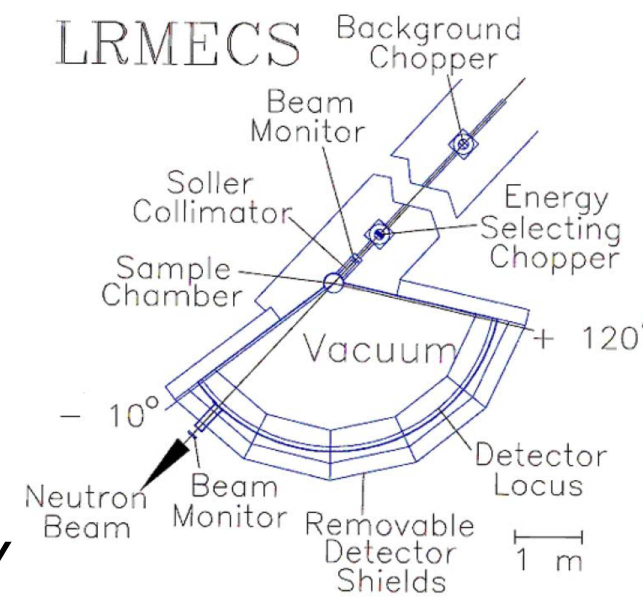
Experimental Details

Pharos Time-of–flight Spectrometer ***(LANSCE)***



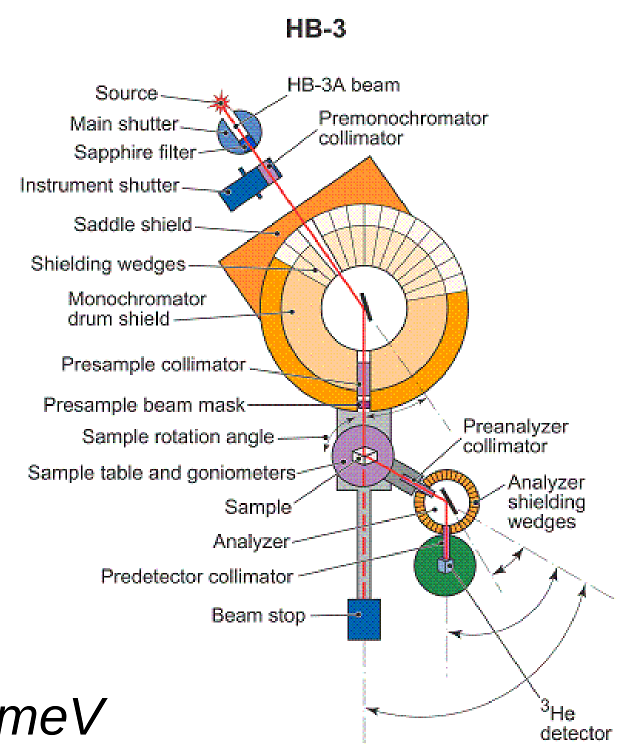
T=7K, E_i=35meV

LRMECS Time-of–flight Spectrometer ***(IPNS)***



T=10K, E_i=60meV

Triple-Axis Spectrometer HB-3 ***(HFIR-ORNL)***



T=2K, E_f=14.7 meV

Anderson Impurity Model:

- *The calculations show the presence of the low energy Kondo resonance and the spin excitation spectra at a scale of $k_B T_0$ governs the universal behavior of $C_m(T)$, $\chi(T)$ and neutron scattering cross section $\chi''(\Delta E)$. These properties are highly dependent on the orbital degeneracy N_J (= 2J + 1 for rare earths).*

- *Rajan's Coqblin-Schrieffer model for zero-temperature and zero-field limits[1]:*

$$\gamma_0 = \pi JR / 3T_K$$

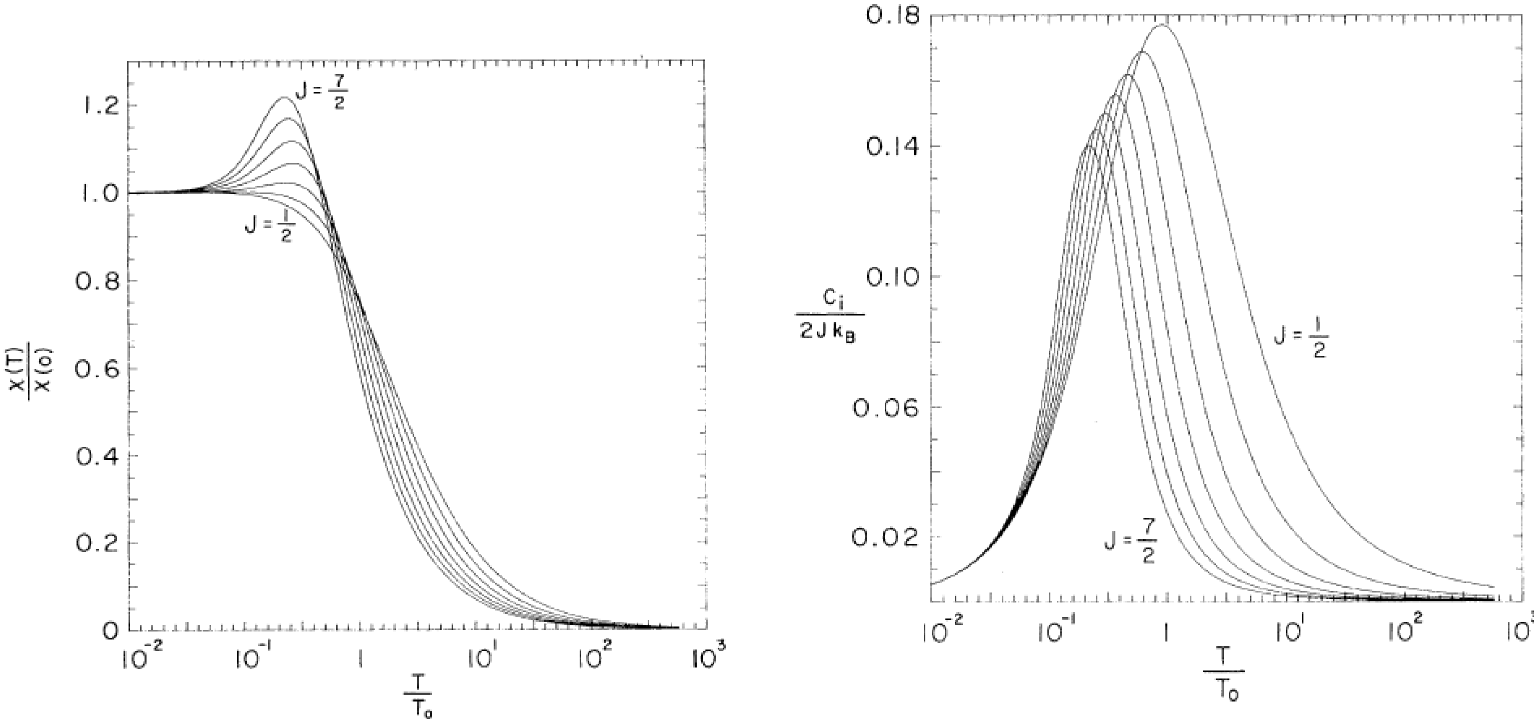
$$\chi_0 = (2J + 1)C_J / 2\pi T_K$$

- *Cox calculation of noncrossing approximation for neutron scattering cross section $\chi''(\Delta E)$[2]:*

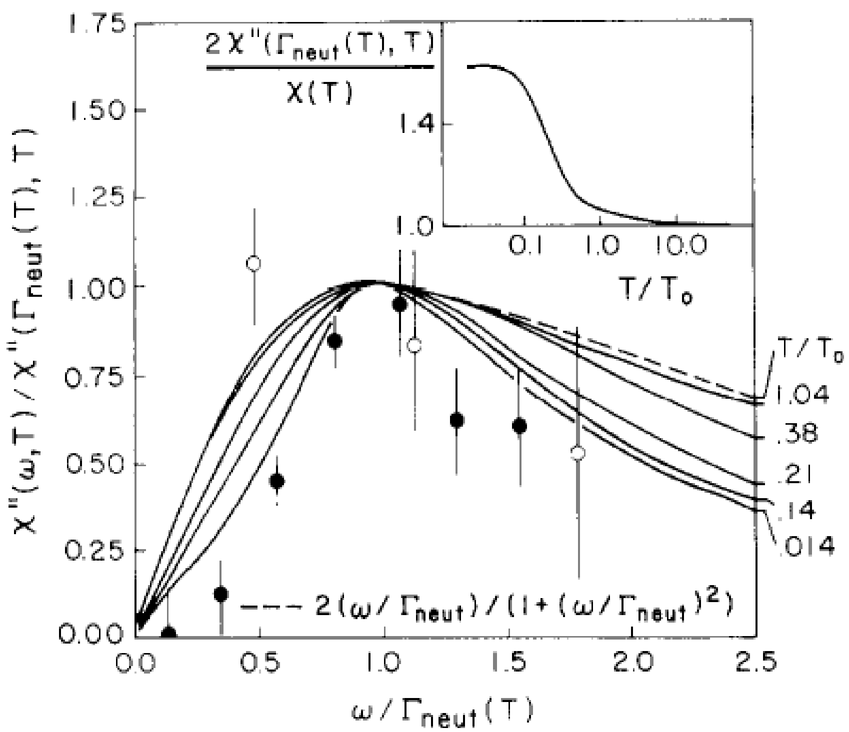
  The peak position E_{max} is roughly constant at low temperature as

$$E_{max} = 1.36T_o^{Cox} = 1.36T_K^{Rajan} / 1.15.$$

V. T. Rajan ey al., Phys. Rev. Lett., 51, 308 (1983).
D. L. Cox et al., J. Magn. Magn. Mater., 54, 333 (1986).

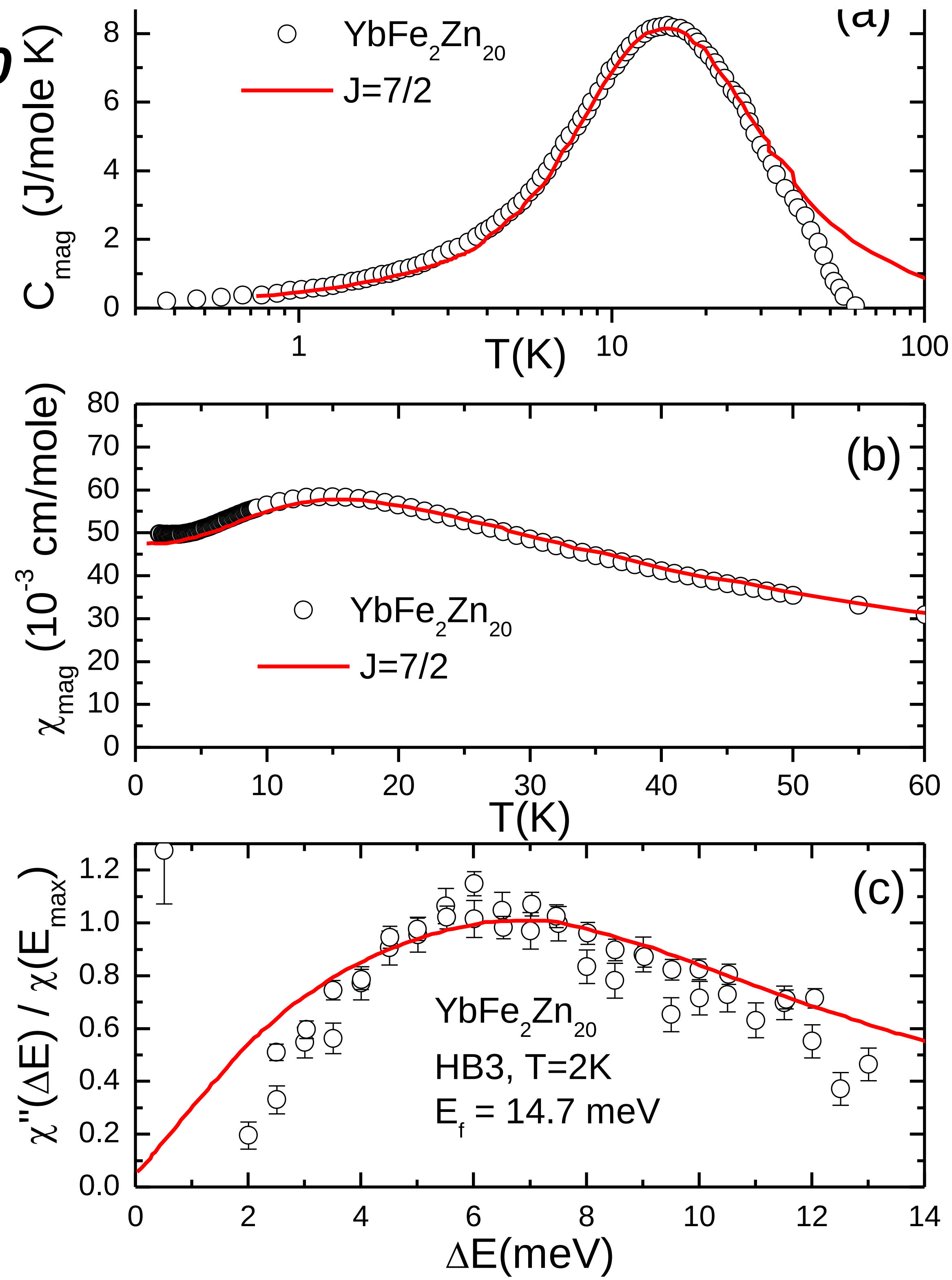


Temperature dependent behavior of χ and C_m for different J impurities[1]



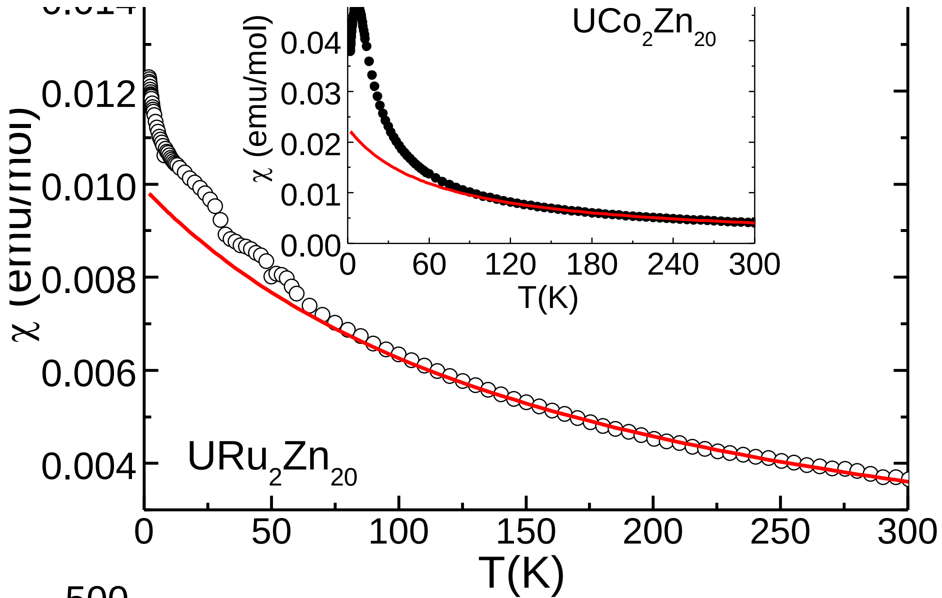
Energy dependent dynamic susceptibility behavior for different temprature. $\Gamma_{neutron}$ is the peak position[2].

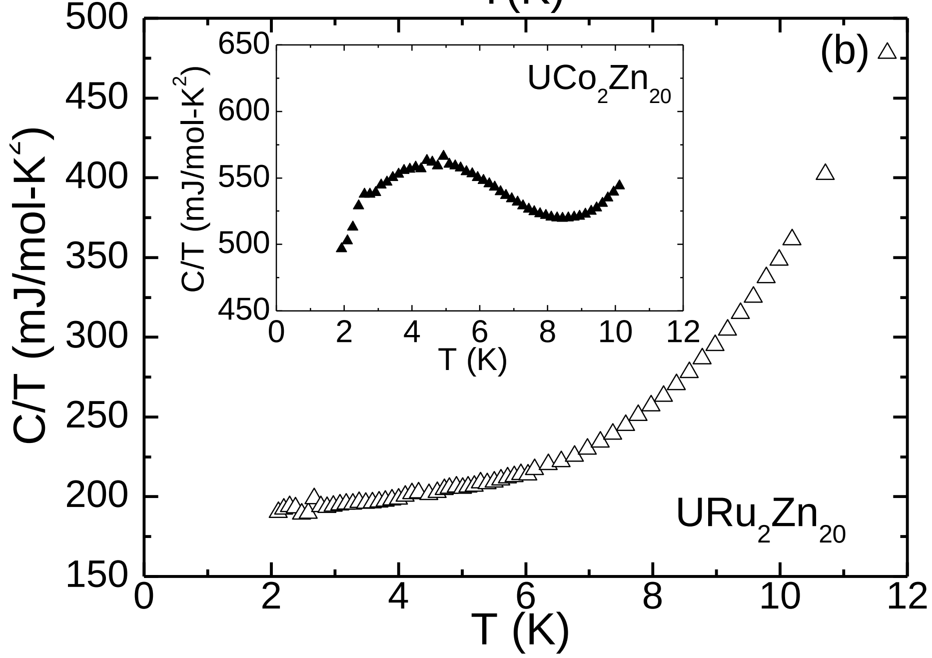
The validity of the AIM for the rare earth 4f compound $YbFe_2Zn_{20}$

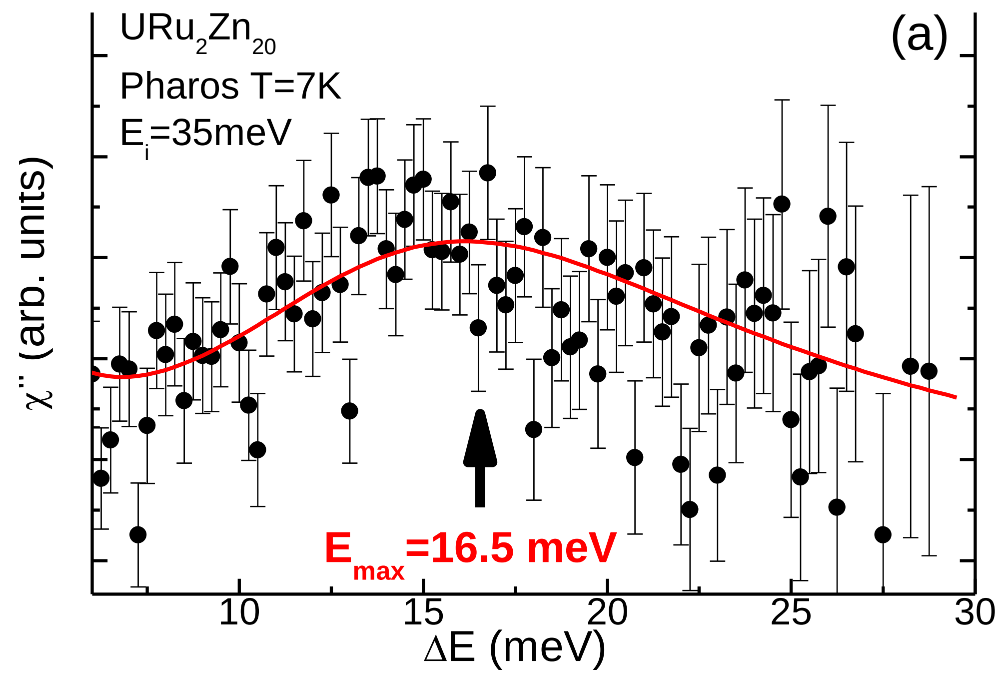


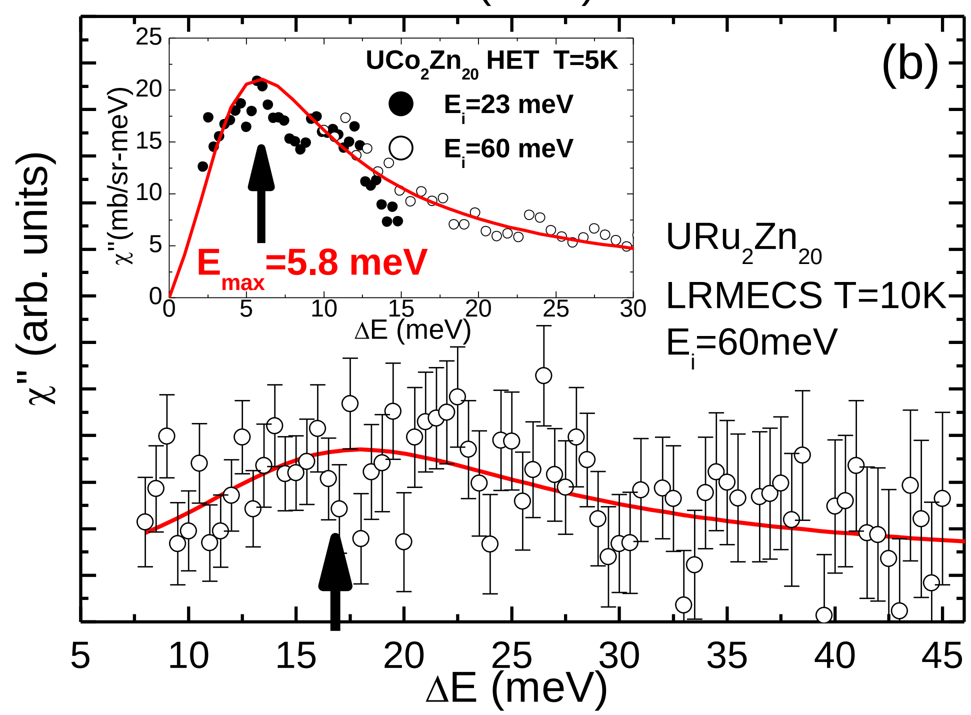
- ➢We compare the data for $C_{mag}(T)$ and $\chi(T)$ (The data are taken from Torikachvili *et al*[3]) with Rajan's predictions for the J=7/2 case.
- ➢The **only one** adjustable parameter is T_K, which we found out 69.2 K is the best value.
- ➢The peak position of the dynamic susceptibility at low temperature as $E_{max} = 1.36\ T_K^{Rajan} / 1.15 = 1.18\ T_K^{Rajan} = 82K = 7\ meV$.
- ➢The lineshape for $\chi''(\Delta E)/ \chi''(E_{max})$ was determined from figure 4 of Cox[2] by using the value of $E_{max} = 7\ meV$.

General scaling behavior:









$\gamma(2K)_{Co} / \gamma(2K)_{Ru} = 2.63$
$\gamma(Tmax)_{Co} / \gamma(2K)_{Ru} = 2.93$
$\chi(2K)_{Co} / \chi(2K)_{Ru} = 3.01,$
$E_{max}(Ru) / E_{max}(Co) = 2.84$

χ and γ scaling as $1/k_B T_{sf} = 1/E_{max}$.

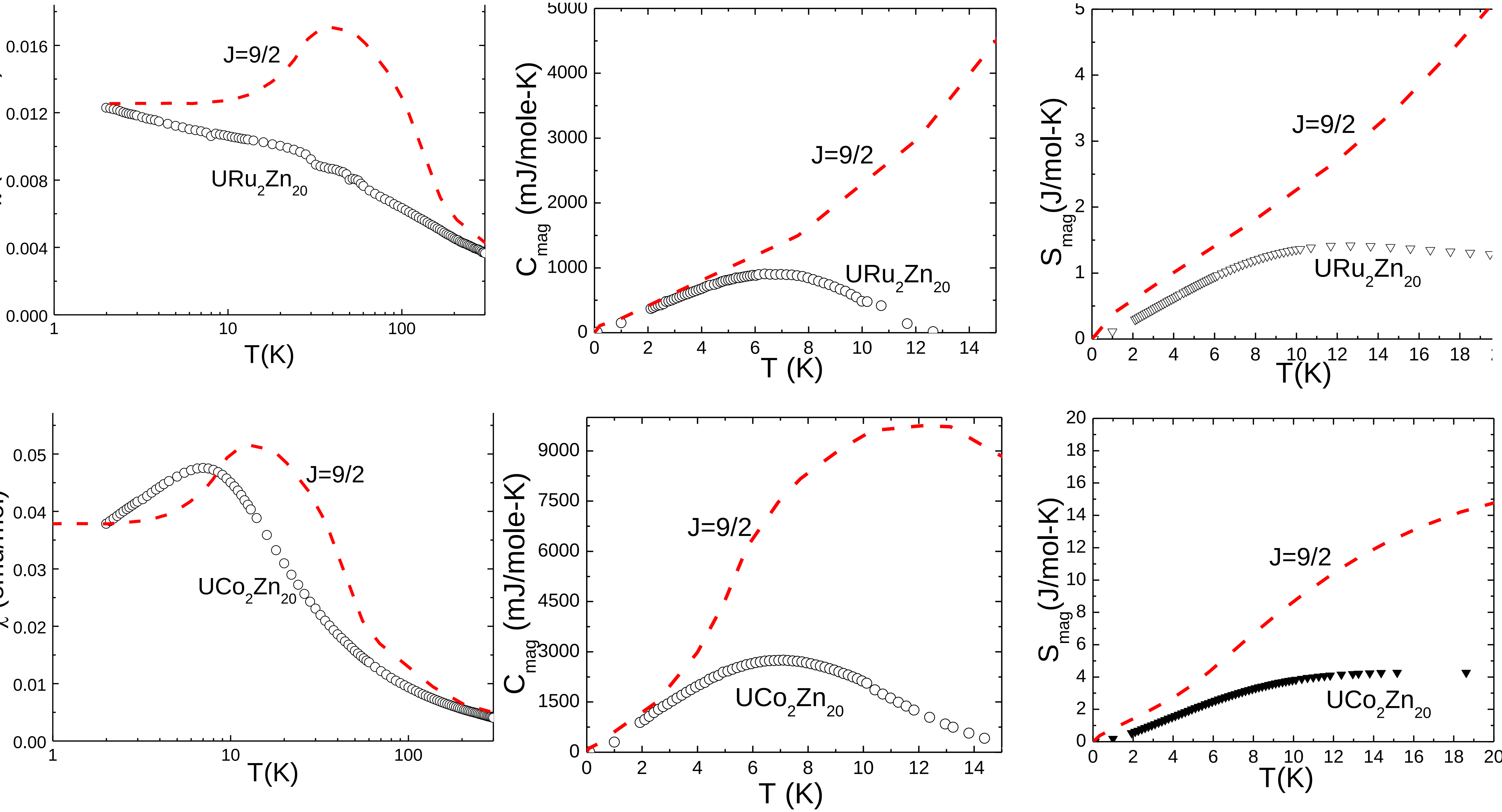
Scaling behavior in Anderson Impurity Frame:

- High temperature curie-weiss constants are close to free ion value.
- We took J=9/2.
- Estimate T_K from γ_0.
- Estimate χ_0 from this T_K and E_{max}.
- We also do the same calculation for J=5/2 and 1/2.

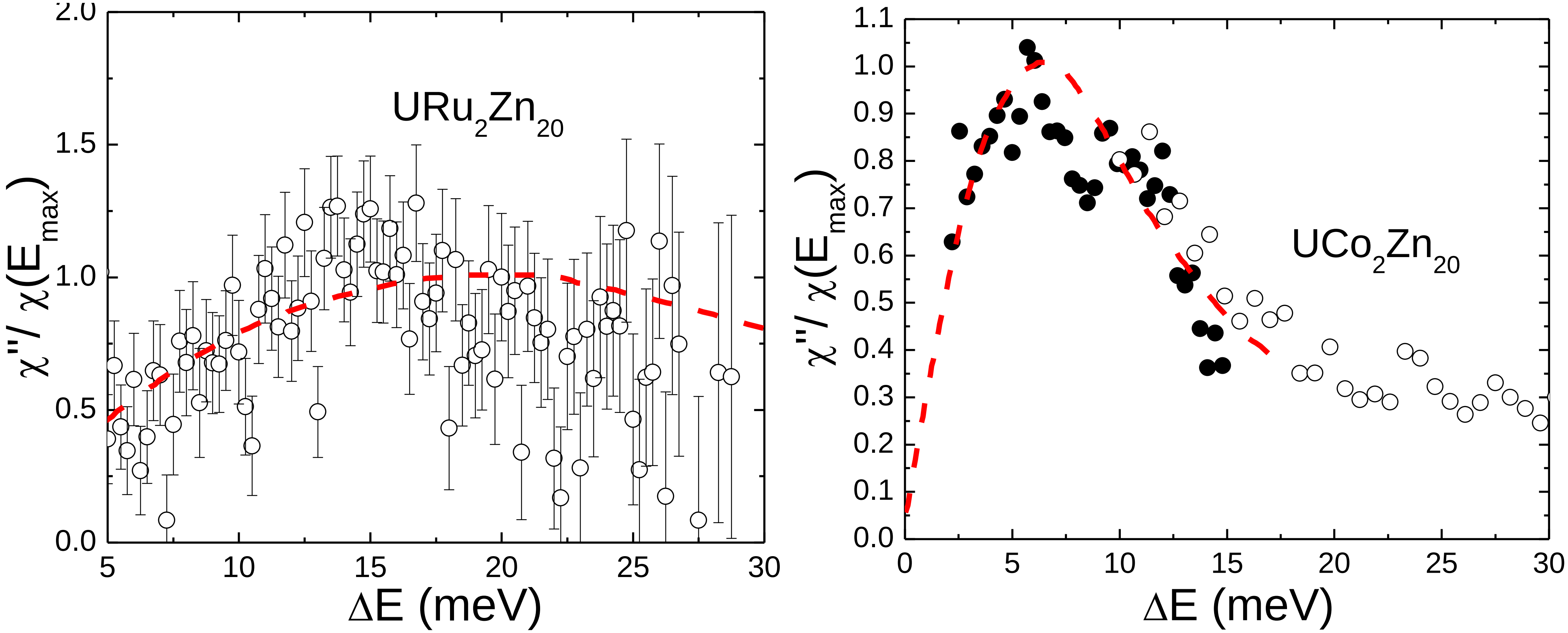
	T_K(K)		T^C_{max}(K)		$\chi_0(\frac{emu}{mole})$		$T^{\chi}_{max}(K)$		E_{max}(meV)	
	Ru	Co	Ru	Co	Ru	Co	Ru	Co	Ru	Co
experiment			6.8	7.1	0.0123	0.037		7	16.5	5.8
J=9/2	208	69	36.5	12.1	0.0125	0.0378	39.2	13.0	21.3	7.1
J=5/2	116	38	34	11	0.0135	0.0412	30	10	11.9	3.9
J=1/2	23	7.6	20	6.8	0.0245	0.0402			2.4	0.8

- **J=9/2** gives the estimated values of χ_0 and E_{max} which are closer to the experiment values.

AIM predictions for the temperature dependence of $\chi(T)$ $C_{mag}(T)$ and $S_{mag}(T)$ in the J = 9/2 case:



AIM predictions for the energy dependence of $\chi''(\Delta E)\,/\,\chi''(E_{max})$:



- We took J=9/2.
- **Only one** adjustable parameter T_K, which is determined from the low temperature specific heat coefficient γ_0.
- Expected values of T_{max} for both $\chi(T)$ and $C_{mag}(T)$ are much higher than observed in the experiment.
- Experimental entropy is *much* smaller than expected.

Conclusions

- We show that AIM works perfect for $YbFe_2Zn_{20}$.
- The scaling behavior exists in URu_2Zn_{20} and UCo_2Zn_{20}.
- AIM model works very well for the low temperature limit values of γ_0 and χ_0 and 18% to 25% error for peak position of dynamic susceptibility $\chi''(\Delta E)$.
- Experimental entropy is *much* smaller than expected.

Acknowledgements

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References

*[1] V. T. Rajan ey al., Phys. Rev. Lett., **51**, 308 (1983).*
*[2] D. L. Cox et al., J. Magn. Magn. Mater., **54**, 333 (1986).*
*[3] M. S. Torikachvili et al., PNAS, **104**, 9960 (2007).*