Neutron Scattering and Scaling Behavior in URu$_2$Zn$_{20}$

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*International Conference on Neutron Scattering, Knoxville, TN, May 3-7 (2009)*
Abstract

Cubic compounds $\text{URu}_2\text{Zn}_{20}$ and $\text{YbFe}_2\text{Zn}_{20}$ 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 $\sim 6\text{Å}$.

We measured time-of-flight ($\text{PHAROS}$ at $\text{LANSCE}$, $\text{LRMECS}$ at $\text{IPNS}$) spectra for $\text{URu}_2\text{Zn}_{20}$ and triple-axis ($\text{HB3}$, $\text{HFIR-ORNL}$) for $\text{YbFe}_2\text{Zn}_{20}$.

We observed a broad peak in dynamic susceptibility $\chi'\prime'(\Delta E)$ centered at 16.5 meV for $\text{URu}_2\text{Zn}_{20}$ and 7 meV $\text{YbFe}_2\text{Zn}_{20}$. Together with specific heat and susceptibility the, it is obviously that $\gamma$ and $\chi$ scale inversely with the characteristic energy for spin fluctuations, $T_{sf} = E_{\text{max}} / k_B$. Kondo impurity model describes the behavior of the $4f$ compound $\text{YbFe}_2\text{Zn}_{20}$ very well but works badly for the $\text{URu}_2\text{Zn}_{20}$, suggesting that the scaling behavior of the actinide compounds arises from spin fluctuations of itinerant $5f$ electrons.
Motivation

For 4f 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 occurrence 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\[1\]:
  
  \[ \gamma_0 = \pi J R / 3 T_K \]
  
  \[ \chi_0 = (2J + 1)C_J / 2 \pi T_K \]

- 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
  
  \[ E_{max} = 1.36 T_o^{Cox} = 1.36 T_K^{Rajan} / 1.15. \]

Temperature dependent behavior of $\chi$ and $C_m$ for different J impurities[1]

Energy dependent dynamic susceptibility behavior for different temperature. $\Gamma_{\text{neutron}}$ is the peak position[2].
The validity of the AIM for the rare earth 4f compound YbFe$_2$Zn$_{20}$

- We compare the data for $C_{\text{mag}}(T)$ 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 $E_{\text{max}} = 1.36 \frac{T_K^{\text{Rajan}}}{1.15} = 1.18 \frac{T_K^{\text{Rajan}}}{1.15} = 82K = 7 \text{ meV}$.
- The lineshape for $\chi''(\Delta E)/\chi''(E_{\text{max}})$ was determined from figure 4 of Cox[2] by using the value of $E_{\text{max}} = 7 \text{ meV}$.
General scaling behavior:

\[ \chi(T) \propto \frac{1}{k_B T_s} \]

\( \chi(T) \propto (T/k_B)^n \)

\( \gamma(T) \propto (T/k_B)^m \)

\[ \frac{\chi(2K)_{Co}}{\chi(2K)_{Ru}} = 2.63 \]

\[ \frac{\chi(T_{max})_{Co}}{\chi(2K)_{Ru}} = 2.93 \]

\[ \frac{\chi(2K)_{Co}}{\chi(2K)_{Ru}} = 3.01, \]

\[ \frac{E_{max}(Ru)}{E_{max}(Co)} = 2.84 \]

\( \chi \) and \( \gamma \) 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 $\gamma_0$.
- Estimate $\chi_0$ from this $T_K$ and $E_{\text{max}}$.
- We also do the same calculation for J=5/2 and 1/2.

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<th></th>
<th>$T_K$(K)</th>
<th>$T^C_{\text{max}}$(K)</th>
<th>$\chi_0$(emu/mole)</th>
<th>$T^x_{\text{max}}$(K)</th>
<th>$E_{\text{max}}$(meV)</th>
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<td></td>
<td>Ru</td>
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</table>

- **J=9/2** gives the estimated values of $\chi_0$ and $E_{\text{max}}$ 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 $\chi''(\Delta E) / \chi''(E_{\text{max}})$:

- We took $J=9/2$.
- **Only one** adjustable parameter $T_K$, which is determined from the low temperature specific heat coefficient $\gamma_0$.
- Expected values of $T_{\text{max}}$ for both $\chi(T)$ and $C_{\text{mag}}(T)$ are much higher than observed in the experiment.
- Experimental entropy is **much** smaller than expected.
Conclusions

- We show that AIM works perfect for YbFe$_2$Zn$_{20}$.
- The scaling behavior exists in URu$_2$Zn$_{20}$ and UCo$_2$Zn$_{20}$.
- AIM model works very well for the low temperature limit values of $\gamma_0$ and $\chi_0$ and 18% to 25% error for peak position of dynamic susceptibility $\chi''(\Delta E)$.
- Experimental entropy is much smaller than expected.

Acknowledgements

Work at UC Irvine was supported by the U.S. DOE Grant No. DE-FG03-03ER46036. Work at Los Alamos, Argonne and at Oak Ridge was supported by U.S. DOE.

References