Emergence of the Hidden Order State from the Fano Lattice
Electronic Structure of the Heavy-Fermion Material URu$_2$Si$_2$

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Kondo Lattice & Heavy Fermions
Kondo Effect

$T \gg T_K$

$T \ll T_K$

$T_K$: characteristic Kondo temperature

$$T_K \propto \exp\left(-\frac{1}{\rho J}\right)$$

Below $T_K$ impurity spin is progressively screened: Kondo singlet
Heavy Fermion Effects in f-electron Lattices

- Lattice of certain f-electrons (most Ce, Yb or U) in metallic environment
- La\(^{3+}\): 4f\(^0\), Ce\(^{3+}\): 4f\(^1\) (J = 5/2), Yb\(^{3+}\): 4f\(^3\) (J = 7/2)
- partially filled inner 4f/5f shells → localized magnetic moment

\[ T^* \sim 5 - 50 \text{ K} \]

localized moments + conduction electrons
moments bound in spin singlets
Interactions bring $f$ level close to $E=0$ and result in a $d$-$f$ hybridization and a sharp $DOS(E)$ resonance.
Heavy Fermion Effects in Kondo Lattices

\[ \varepsilon_k^\pm = \varepsilon_k^f + \varepsilon_k \pm \sqrt{(\varepsilon_k^f + \varepsilon_k)^2 + 4|V_k|^2} \]

High temperature

Low temperature
Challenge: atomically resolved image of d-f electron hybridization and heavy band formation?

- Many-body resonance $\varepsilon_f$ just above $E=0$
- Hybridization energy region $\Gamma$ surrounding $\varepsilon_f$
- Light d-band beyond $\Gamma$ from $\varepsilon_f$
- High DOS and heavy f-band within $\Gamma$ from $\varepsilon_f$
Heavy Fermion Spectroscopic Imaging STM
Spectroscopic Imaging STM

Conductance(ns)
Spectroscopic Imaging STM Systems

Ultra low vibration lab.
Underground Concrete Vibration Isolation Vault
Internal Acoustic Isolation Chamber

Ultra low vibration cryostat.

vacuum lines
pump box
six air springs
30 Ton concrete inertial block
lead-filled legs
three air springs
lead-filled table

6 m
Spectroscopic Imaging STM Systems

Ultra low vibration cryostat.
Spectroscopic Imaging STM Systems


10 mK / 9 Tesla / SI-STM
Heavy Fermion QPI Example: Sr$_3$Ru$_2$O$_7$

1% Ti atoms on Ru sites

Spectroscopic Image $g(\vec{r}, E)$
Heavy Fermion QPI Example: $\text{Sr}_3\text{Ru}_2\text{O}_7$

1% Ti atoms on Ru sites

Spectroscopic Image $g(\vec{r}, E)$

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Heavy Fermion QPI Example: Sr$_3$Ru$_2$O$_7$
QPI identification of heavy d-electron ($\alpha_2$) band

Nature Physics 5, 800 (2009)
Can we explore Kondo-Lattice Heavy Fermions similarly?
Single Adatom Kondo Effect
Single Magnetic Adatom Kondo Resonance

Single Magnetic Adatom Kondo Resonance

Co on Au(111)

'Fano Spectrum' of Kondo Resonance

Physical Significance of Fano Signature

\[ g(r, E) \propto \frac{(q + E')^2}{E'^2 + 1}; \quad E' = \frac{(E - \varepsilon_0)}{\Gamma / 2} \]

\( \varepsilon_0 \) energy of many-body state screening spin

\( \Gamma \) width of resonance (simple Kondo \( 2k_B T_k \))

\( q \) Ratio of matrix elements linking tip state to resonance and to continuum

\[ q(r) = \frac{\text{Re} \, G(r) + t(r)}{\text{Im} \, G(r)} \]

\[ t(r) = t_0 e^{-\frac{d(r)}{\alpha}} \]
Kondo Lattice system: Perhaps one might expect a 'Fano Lattice'?
‘Fano Lattice’ Theories


URu$_2$Si$_2$
URu$_2$Si$_2$ is a modestly heavy fermion system

\[ \gamma = 100 \text{ mJ/mol K}^2 \quad m^*/m_e \sim 25 \]

\[ a_0/\sqrt{2} = 2.91\text{Å} \]

out-of-plane U-U distance: 5.61Å

Step height: 4.79Å

(same as CeCu$_2$Si$_2$ with U and Ru instead of Ce and Cu);

\[ a = 4.124\text{Å}; \ c = 9.582\text{Å} \ (PRL65-3189) \]
URu$_2$Si$_2$ is a modestly heavy fermion system $T^* \sim 55$K
$\text{URu}_2\text{Si}_2$ is a modestly heavy fermion system $T^* \sim 55\text{K}$ with an additional ‘Hidden Order’ phase transition at 17.5K.
Why URu$_2$Si$_2$?

- Heavy fermion system
- Perfect cleave surface
- Lattice of f-atoms at surface
- Scattering interference

\[ \gamma = 100 \text{ mJ/mol K}^2 \quad m^*/m_e \approx 25 \]

\[ a_0/\sqrt{2} = 2.91\text{Å} \]

Out-of-plane U-U distance: 5.61Å

Step height: 4.79Å
Si-layer termination

40nm x 40nm Si surface topography (70619)
Fano-like spectrum at every Si atom

40nm x 40nm topography

\[ g(r, E) \propto \frac{(q + E')^2}{E'^2 + 1}; \quad E' = \frac{(E - \varepsilon_0)}{\Gamma / 2} \]

\( \varepsilon_0 \) energy of many-body state screening spin

\( \Gamma \) width of resonance (simple Kondo \( 2k_B T_K \))

\( q \) Ratio matrix elements linking tip state to resonance and continuum

\[ q(r) = \frac{\text{Re} \ G(r) + t(r)}{\text{Im} \ G(r)} \quad t(r) = t_0 e^{-\frac{d(r)}{\alpha}} \]
'Fano Lattice' Electronic Structure ($T>T_O$)

URu$_2$Si$_2$ 'Hidden Order' State
'Hidden Order' Transition $T_o=17.5$K
'Hidden Order' Transition $T_o=17.5K$

- Heavy fermion material
- Superconductor below $T_c \sim 1.5K$
- Energy-gap $\sim 10^{+2} \text{ mV}$ (Photo, INS, $C_p$)

Palstra, T.T.M., Menovsky, A.A., & Mydosh, J.A.


**FIG. 1.** Specific heat of URu$_2$Si$_2$ plotted as $C/T$ vs $T^2$ (above) yielding $\gamma$ and $\Theta_D$, and as $C/T$ vs $T$ (below) showing the entropy balance.
‘Hidden Order’ Transition $T_o=17.5K$

‘Conventional’ Density Wave


‘Altered’ Kondo Effect


Emergence of 'Hidden Order' DOS(E) from the Heavy Fermion Fano Spectrum
Alterations in Fano signature at HO Transition

Si-layer Quasiparticle Interference Imaging

Rotated to overlap with 4.2K map
QPI inversion to identify bands was unachievable.

Rotated to overlap with 4.2K map
$U_{0.99}Th_{0.01}Ru_2Si_2$

40nm x 40nm Topography
(70619)

Signature of HO near $E=0$ on $dI/dV$ spectrum at U-layer

$T \ll T_{HO}$

T = 1.9 K
T=1.9K

- Extremely rapid $k(E)$ – heavy fermions
- Within range of hidden-order gap only
- Highly anisotropic QPI & gap structure
- Completely different $E<0 : E>0$
- No static $Q^*$ (density wave) at any energy

Extremely rapid $T$-dependence of band structure
'Hidden Order' splits light band into two heavy bands

Conclusions
Challenge: atomically resolved image of d-f electron hybridization and heavy band formation in Kondo lattice?
'Fano Lattice' Imaging: New approach to heavy fermion physics

'Hidden Order' Transition $T_o=17.5K$
HO transition in LDOS emerges from ‘Fano Lattice’ signature

Light d-band splits rapidly into two heavy bands below $T_o$.

- Conventional density wave, non-dispersive modulations at $Q^*$ should appear in the gap-edge states both above and below $E_F$. But the high-DOS gap-edge states of ‘hidden order’ state are at a completely different $k$-space locations.

- Instead, light band crossing $E_F$ near $k = 0.3(\pi/a_0)$ above $T_o$ which undergoes rapid temperature changes below $T_o$.

- The result is its splitting into two far heavier bands widely separated in $k$-space and with quite different anisotropies.

- The $k$-space hybridization gap and the DOS(E) changes detected in $r$-space occur within the same narrow energy range (consistent with the energy ranges deduced from thermodynamics and other spectroscopies).

‘Hidden order’ transition is caused primarily by a sudden alteration of the many-body state centered upon each U atom, with associated alterations to the $r$-space /$k$-space hybridization processes.