2010 Summer Seminar, Sakai, Fukui
July 22-24, 2010
Echizensangoku

Hybridization wave as the ‘Hidden Order’ in URu_2Si_2

Yonatan Dubi and Alexander V. Balatsky, in preprint

July 24, 2010, 10:00~10:50

Kenichiro Hashimoto

Department of Physics, Graduate School of Science, Kyoto University

Outline

✓**Introduction of the heavy fermion compound URu_2Si_2**

✓**Recent key experimental results**

(i) Neutron-scattering

C. R. Wiebe et al., Nature Phys. **3**, 96 (2007).

✓**Incommensurate wave vectors $Q^* \sim 0.6, 1.4\ \pi/a_0$**

✓**Gap-like feature of $\Delta \sim 4$ meV**

(ii) Angle-resolved photoemission spectroscopy (ARPES)

A. F. Santander-Syro et al., Nature Phys. **5**, 637 (2009).

✓**A light conduction band and a heavy f-band**

(iii) Scanning tunneling microscopy (STM)

A. R. Schmidt et al., Nature. **465**, 570 (2010).

✓**Fano line-shape below the Kondo temperature develops a gap-like feature below $T_o = 17.5$ K.**

✓**The hole band develops a hybridization feature below the HO transition, corresponding to momentum $Q = 0.3\ \pi/a_0$.**

Incommensurate hybridization between the light and heavy fermion bands

✓**Hybridization wave as the hidden order**

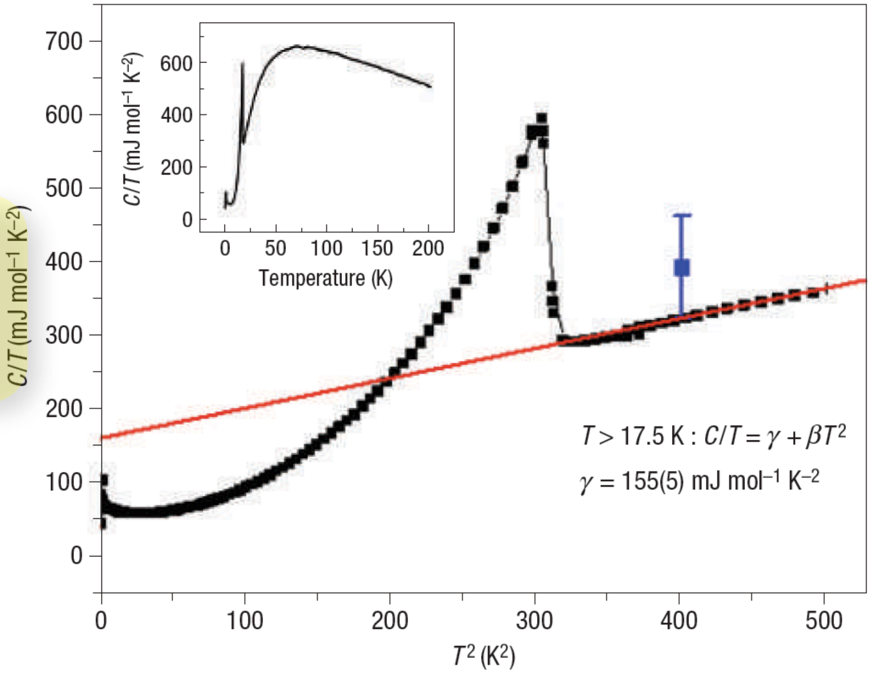
Yonatan Dubi and Alexander V. Balatsky, in preprint

‘Hidden Order’ in URu_2Si_2

Heavy fermion compound URu_2Si_2 (below ~ 70 K)

T_o = 17.5 K ‘hidden order’ state

Most of the Fermi surface disappear at the HO transition owing to partial gapping of the Fermi surface.



C. R. Wiebe et al., Nature Phys. **3**, 96 (2007).

Large entropy jump at T_o, but no magnetic ordering ($\mu \sim 0.02\ \mu_B/U$).

$\Delta C/T \sim 300\ \mathrm{mJmol^{-1}K^{-2}}$

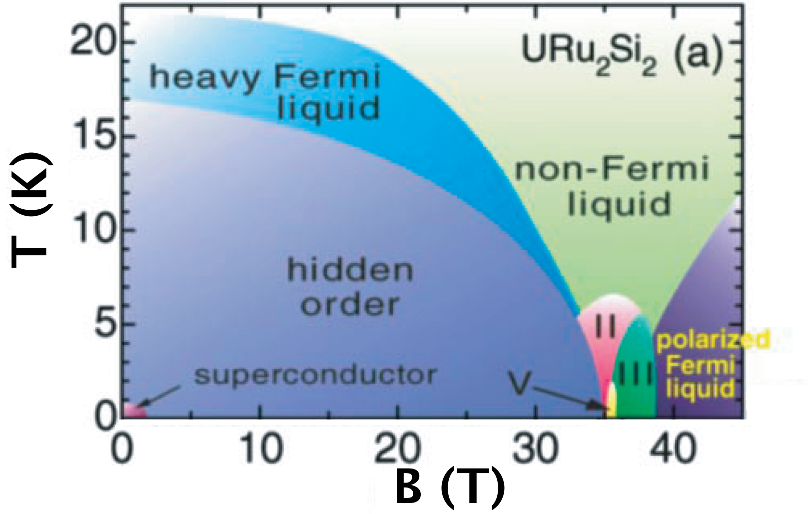
More than 20 models have been proposed for the hidden order parameter, but it is not identified yet.

A: Itinerant picture

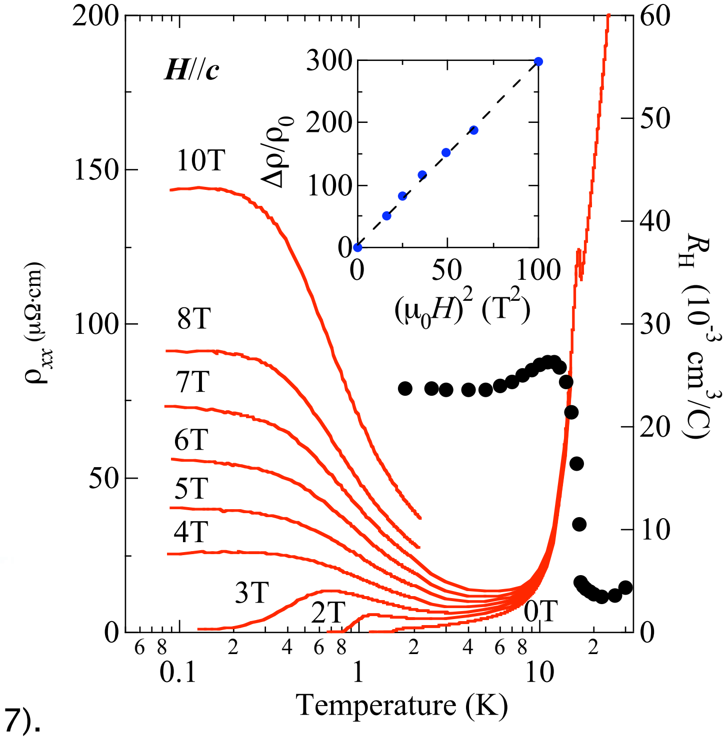
SDW	Mineev & Zhitomirsky (2001)
***d*-density wave**	Ikeda & Ohashi (1998) Virosztek *et al*. (2002)
Orbital current	Chandra *et al*. (2002)
Helicity order	Varma & Zhu (2006)

B: Localized picture

Quadrupole	Santini & Amoretti (1994) Santini (1998) Ohkawa & Shimizu (1999)
Octupole	Kiss & Fazekas (2005)

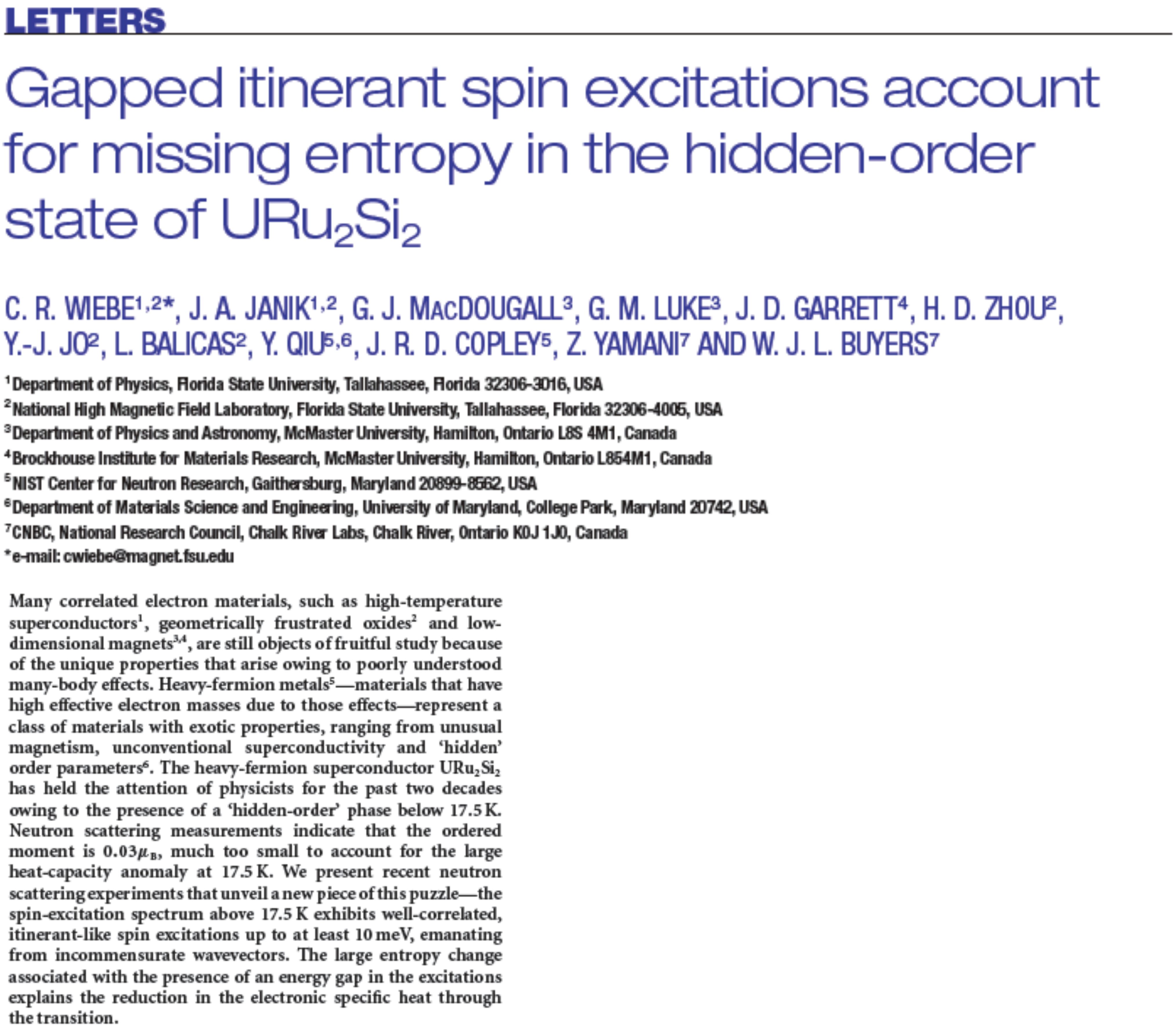


Y. S. Oh et al., Phys. Rev. Lett. **98**, 016401 (2007).



Y. Kasahara et al., Phys. Rev. Lett. **99**, 0116402 (2007).

Neutron-scattering



LETTERS

Gapped itinerant spin excitations account for missing entropy in the hidden-order state of URu_2Si_2

C. R. WIEBE[1,2*], J. A. JANIK[1,2], G. J. MACDOUGALL[3], G. M. LUKE[3], J. D. GARRETT[4], H. D. ZHOU[2], Y.-J. JO[2], L. BALICAS[2], Y. QIU[5,6], J. R. D. COPLEY[5], Z. YAMANI[7] AND W. J. L. BUYERS[7]

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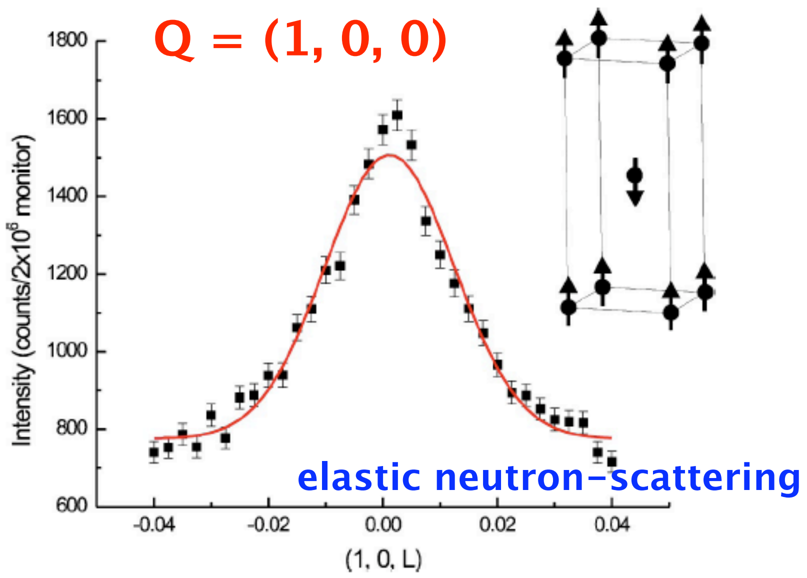
Many correlated electron materials, such as high-temperature superconductors[1], geometrically frustrated oxides[2] and low-dimensional magnets[3,4], are still objects of fruitful study because of the unique properties that arise owing to poorly understood many-body effects. Heavy-fermion metals[5]—materials that have high effective electron masses due to those effects—represent a class of materials with exotic properties, ranging from unusual magnetism, unconventional superconductivity and ‘hidden’ order parameters[6]. The heavy-fermion superconductor URu_2Si_2 has held the attention of physicists for the past two decades owing to the presence of a ‘hidden-order’ phase below 17.5 K. Neutron scattering measurements indicate that the ordered moment is $0.03\mu_B$, much too small to account for the large heat-capacity anomaly at 17.5 K. We present recent neutron scattering experiments that unveil a new piece of this puzzle—the spin-excitation spectrum above 17.5 K exhibits well-correlated, itinerant-like spin excitations up to at least 10 meV, emanating from incommensurate wavevectors. The large entropy change associated with the presence of an energy gap in the excitations explains the reduction in the electronic specific heat through the transition.

Inelastic Neutron-scattering

Antiferromagnetic order ?

$$\mu \simeq 0.02\mu_{\mathrm{B}}/\mathrm{U} \;\not\longleftrightarrow\; \Delta S \simeq 0.2R\ln 2$$

Small ordered moment of 0.02 μ_B/U cannot account for the large heat-capacity anomaly at the HO transition.



Below T_O = 17.5 K

(i) Antiferromagnetic wavevector

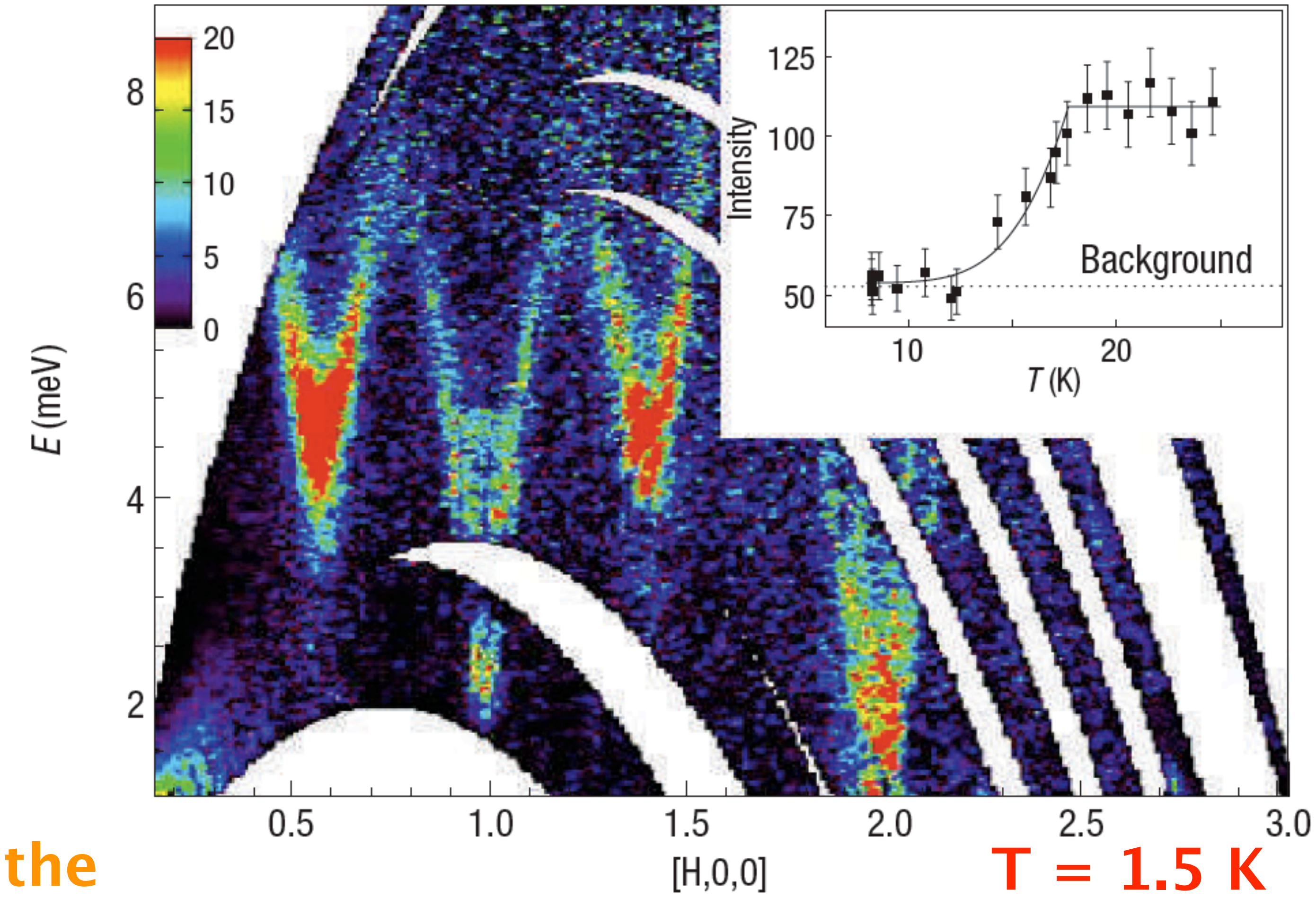
Q ~ (1, 0, 0)

Δ ~ 2 meV

(ii) Incommensurate wavevectors

Q* ~ (0.6, 0, 0), (1.4, 0, 0)

Δ ~ 4 meV



T = 1.5 K

The incommensurate excitations form the gap of ~ 4 meV through the HO transition.

C. R. Wiebe et al., Nature Phys. **3**, 96 (2007).

Inelastic Neutron-scattering

Above T_O = 17.5 K

(i) Antiferromagnetic wavevector

Q ~ (1, 0, 0)

Weak quasielastic spin fluctuations

(ii) Incommensurate wavevectors

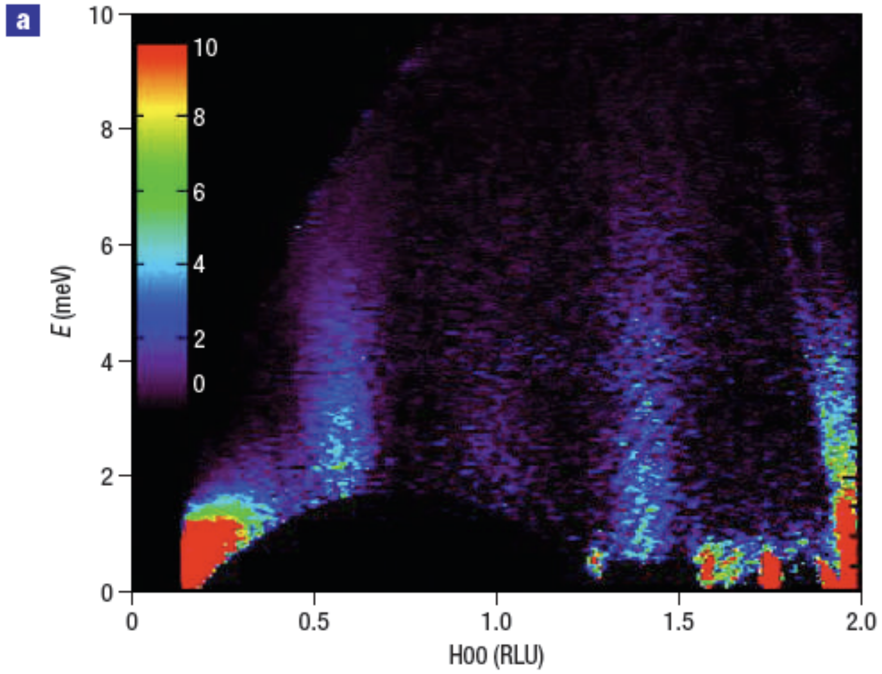
Q* ~ (0.6, 0, 0), (1.4, 0, 0)

Strong excitations

The incommensurate excitations have a well-defined structure. In short, the electrons are highly correlated above 17.5 K.

→ Not localized system but Itinerant system

T = 20 K



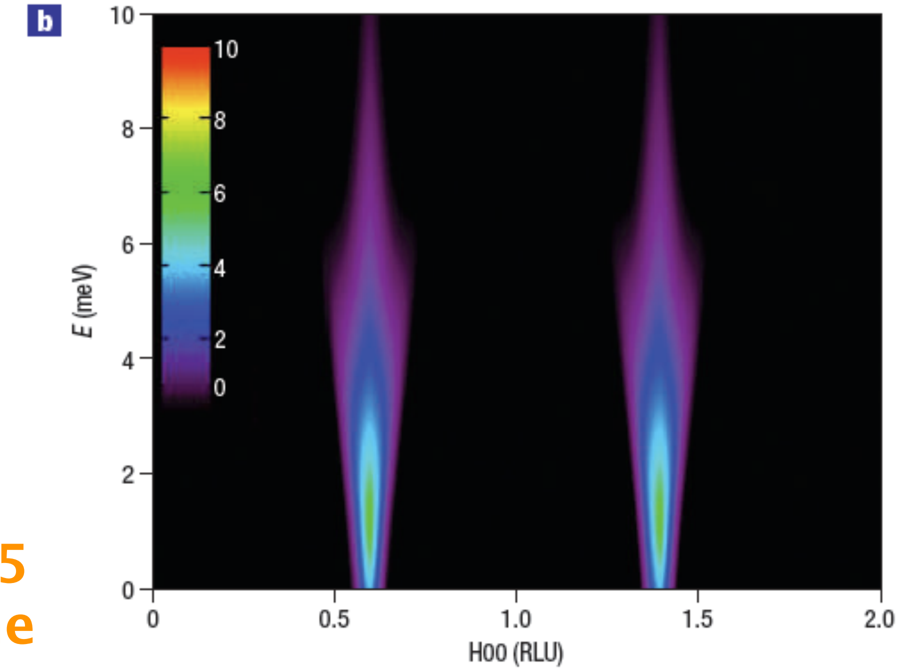
Chou model

$$S(q,\omega)=\frac{\hbar\omega}{1-\mathrm{e}^{-\hbar\omega/kT}}\frac{A}{\kappa^2+q^2}\left(\frac{\Gamma}{(\hbar\omega\pm\hbar\omega_q)^2+\Gamma^2}\right)$$

q = Q – δ (δ: incommensurate wavevector)
κ = ξ^{-1} (ξ: correlation length)
ω_q = cq (c: spin wave velocity)

ξ = 14 Å, c=45 meVÅ

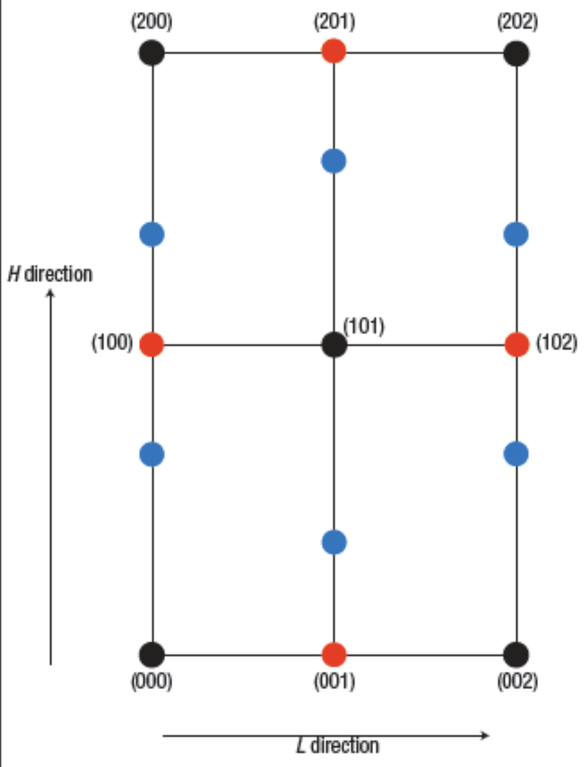
The estimated value is comparable to the Fermi velocity of ~35 meVÅ in the thermal conductivity measurements, indicating the itinerant nature of the excitations.



Inelastic Neutron-scattering

[H, 0, L]

Reciprocal space map

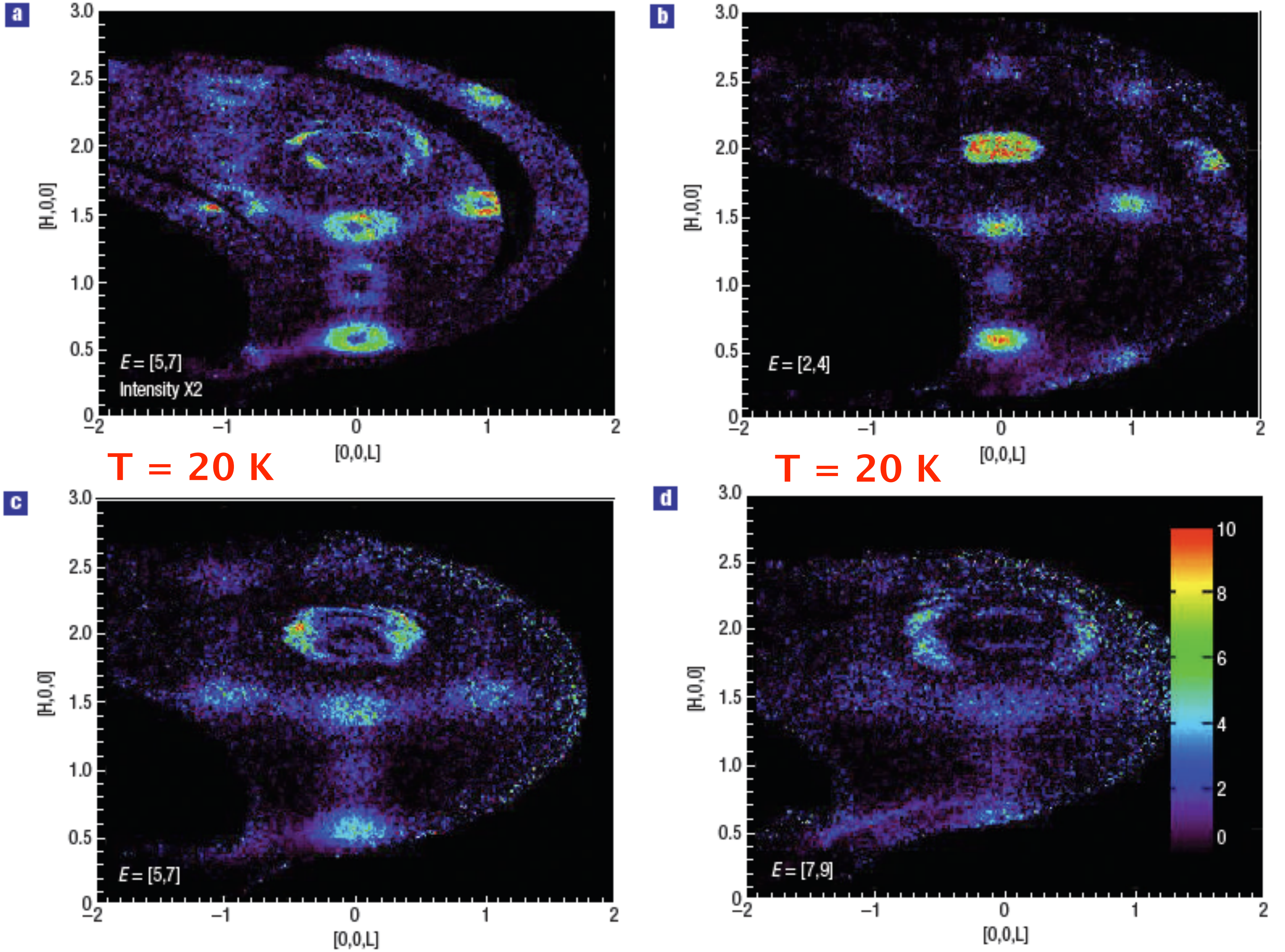


T = 1.5 K

T = 20 K

T = 20 K

T = 20 K



Inelastic Neutron-scattering

Electronic specific heat

$$C(T)=\frac{\partial}{\partial T}\frac{v_{\mathrm{a}}}{8\pi^3}\int_0^{\xi^{-1}}\mathrm{d}q4\pi q^2\int_0^{E_{\max}}\mathrm{d}E\rho_0 f(E)E$$

v_a : cell volume

ρ_0 : density of state

$f(E) = \coth(E/2k_BT)$

$E_{max} = k_BT$

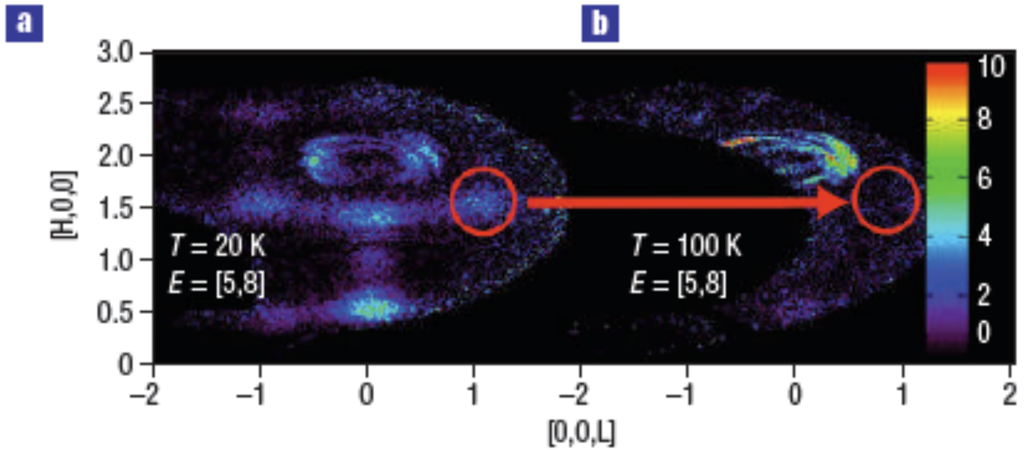
$\rho_0 = \Gamma^{-1}$ ($\Gamma = c\xi^{-1}$, Γ: damping)

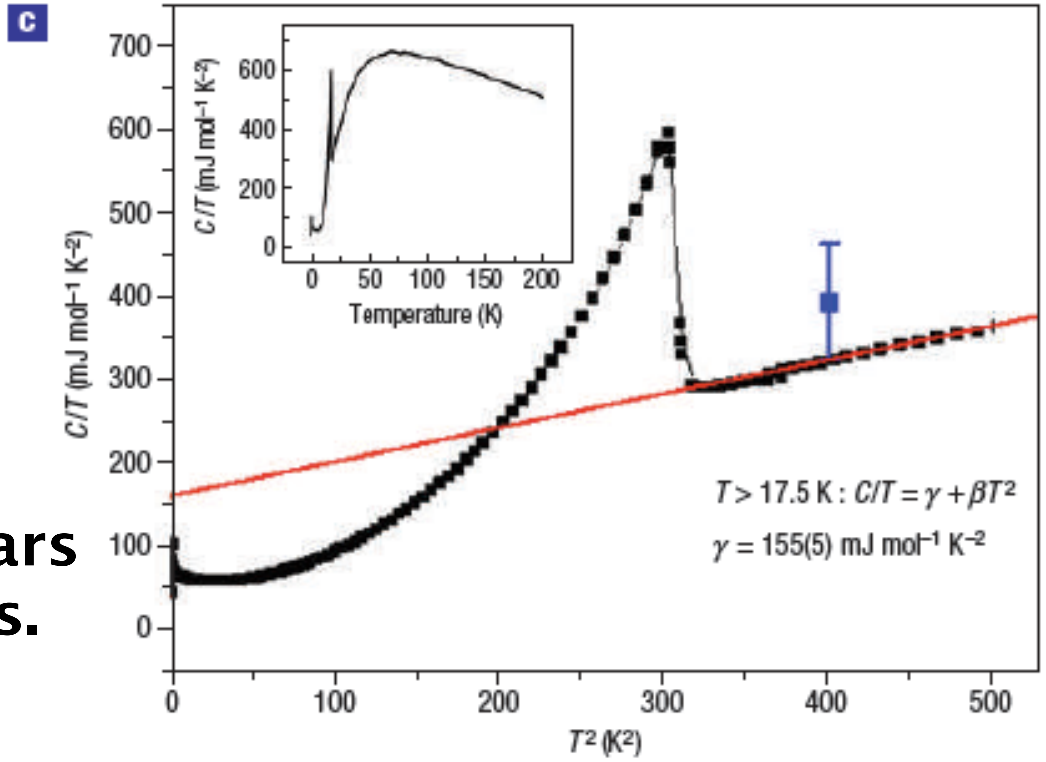
$$C_{\mathrm{v}}=\frac{v_{\mathrm{a}}\xi^{-2}}{3\pi^2 c}\times k_{\mathrm{B}}^2 T$$

ξ = 14 Å, c=45 meVÅ

γ = 220±70 mJmol^{-1}K^{-2}

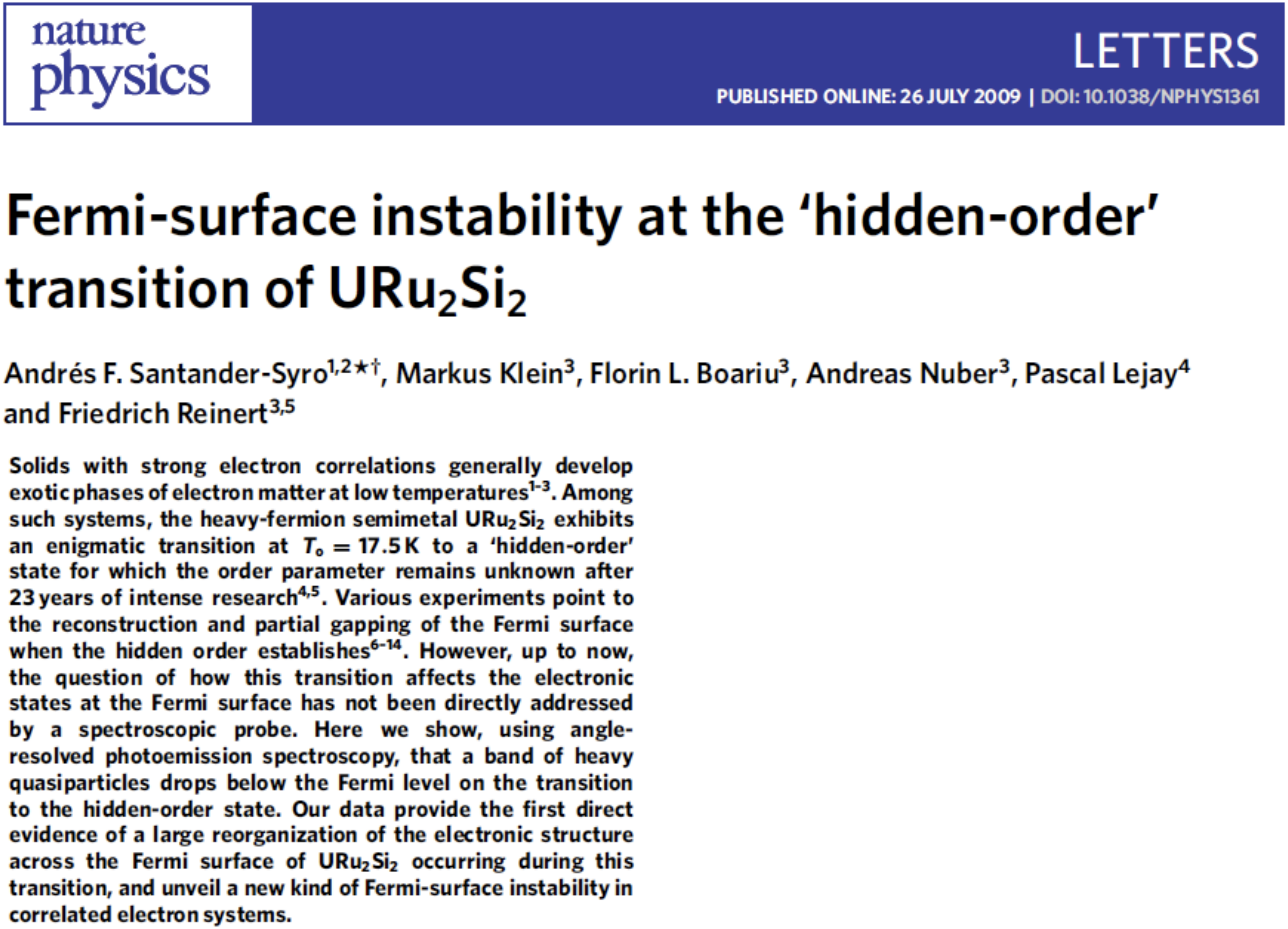
The incommensurate scattering at (1.6, 0, 1) disappears at 100 K, where heavy-quasiparticle formation occurs.





Itinerant picture

Angle-resolved photoemission spectroscopy (ARPES)



nature physics

LETTERS

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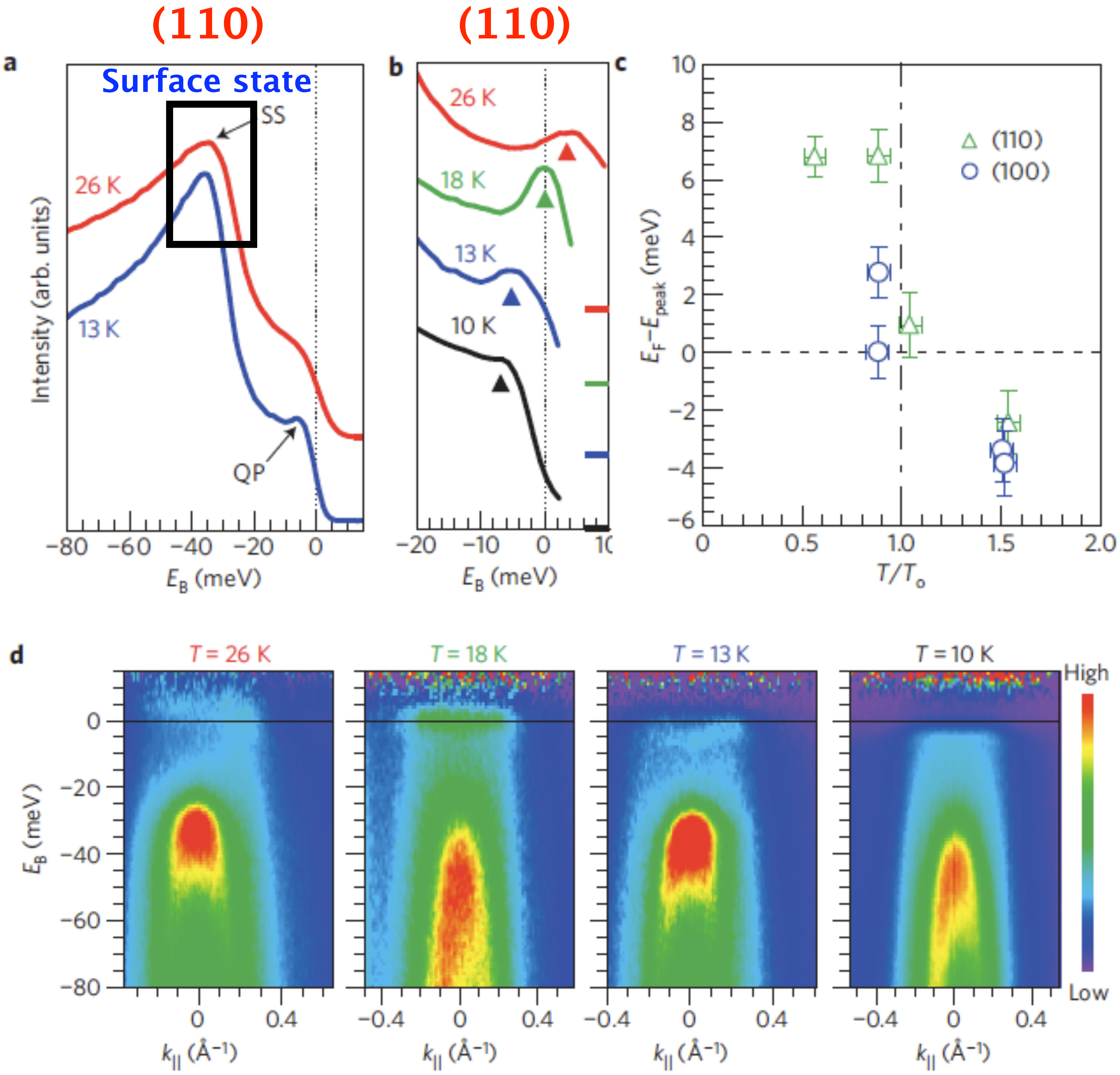
Fermi-surface instability at the ‘hidden-order’ transition of URu_2Si_2

Andrés F. Santander-Syro[1,2*†], Markus Klein[3], Florin L. Boariu[3], Andreas Nuber[3], Pascal Lejay[4] and Friedrich Reinert[3,5]

Solids with strong electron correlations generally develop exotic phases of electron matter at low temperatures[1-3]. Among such systems, the heavy-fermion semimetal URu_2Si_2 exhibits an enigmatic transition at $T_o = 17.5\,K$ to a ‘hidden-order’ state for which the order parameter remains unknown after 23 years of intense research[4,5]. Various experiments point to the reconstruction and partial gapping of the Fermi surface when the hidden order establishes[6-14]. However, up to now, the question of how this transition affects the electronic states at the Fermi surface has not been directly addressed by a spectroscopic probe. Here we show, using angle-resolved photoemission spectroscopy, that a band of heavy quasiparticles drops below the Fermi level on the transition to the hidden-order state. Our data provide the first direct evidence of a large reorganization of the electronic structure across the Fermi surface of URu_2Si_2 occurring during this transition, and unveil a new kind of Fermi-surface instability in correlated electron systems.

Angle-resolved photoemission spectroscopy (ARPES)



The quasiparticle band crosses E_F through the HO transition.

At 26 K and 18 K

A flat band above E_F and at E_F

Below T_O = 17.5 K

Heavy-quasiparticle band is located below E_F

A. F. Santander-Syro et al., Nature Phys. **5**, 637 (2009).

Angle-resolved photoemission spectroscopy (ARPES)

(110) direction

✓**Heavy quasiparticle band**

Band width W ~ 7 meV

$k_{\mathrm{LE}} = \pm 0.2\ \text{Å}^{-1} = 0.3\,\pi/a_0$

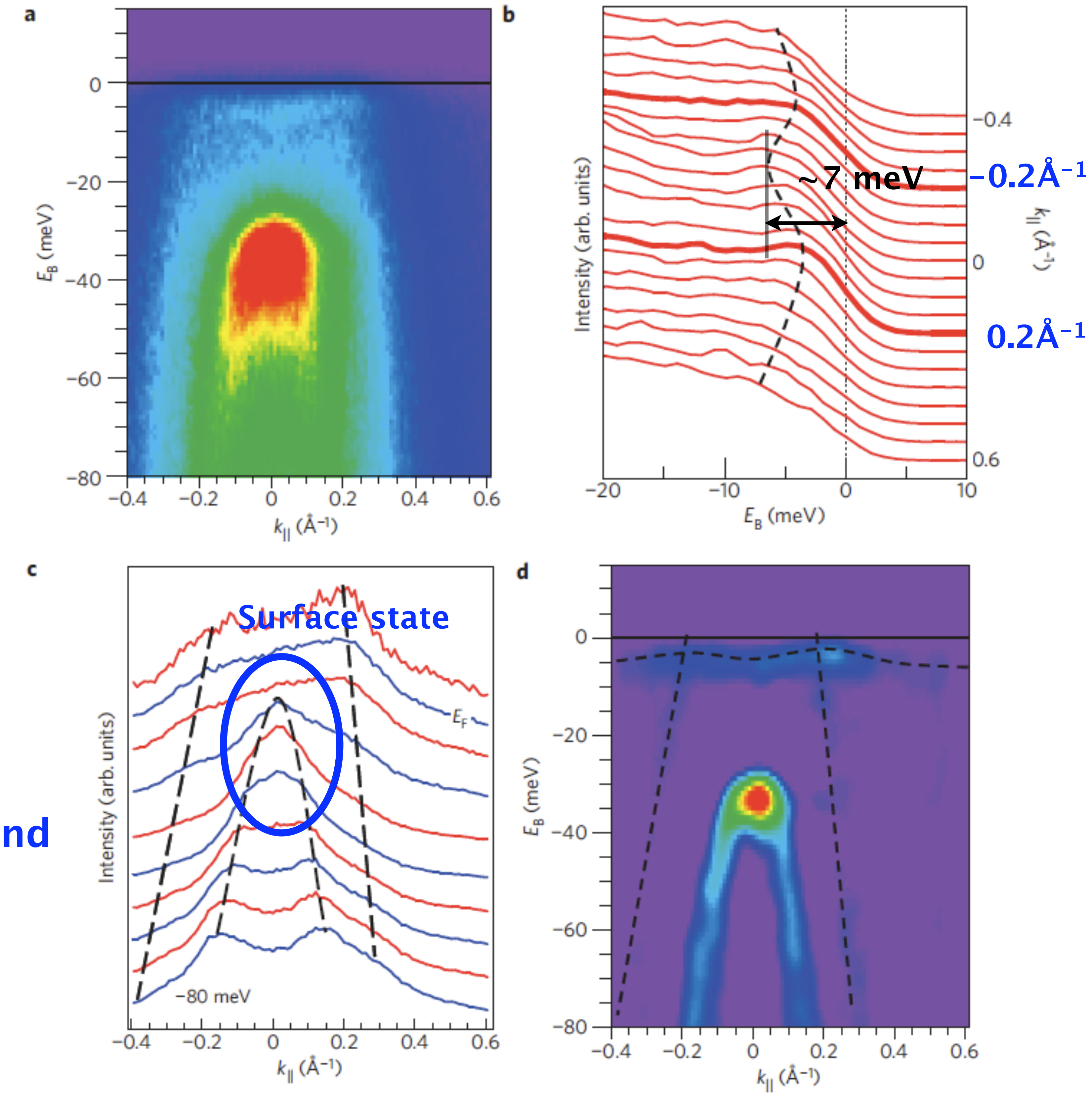
$$W = -\hbar^2 k_{\mathrm{LE}}^2/2m^\star$$

➡ $m^* \sim 22m_e$

✓**A light-hole-like conduction band**

$m^* \sim 1.4m_e$

T = 13 K

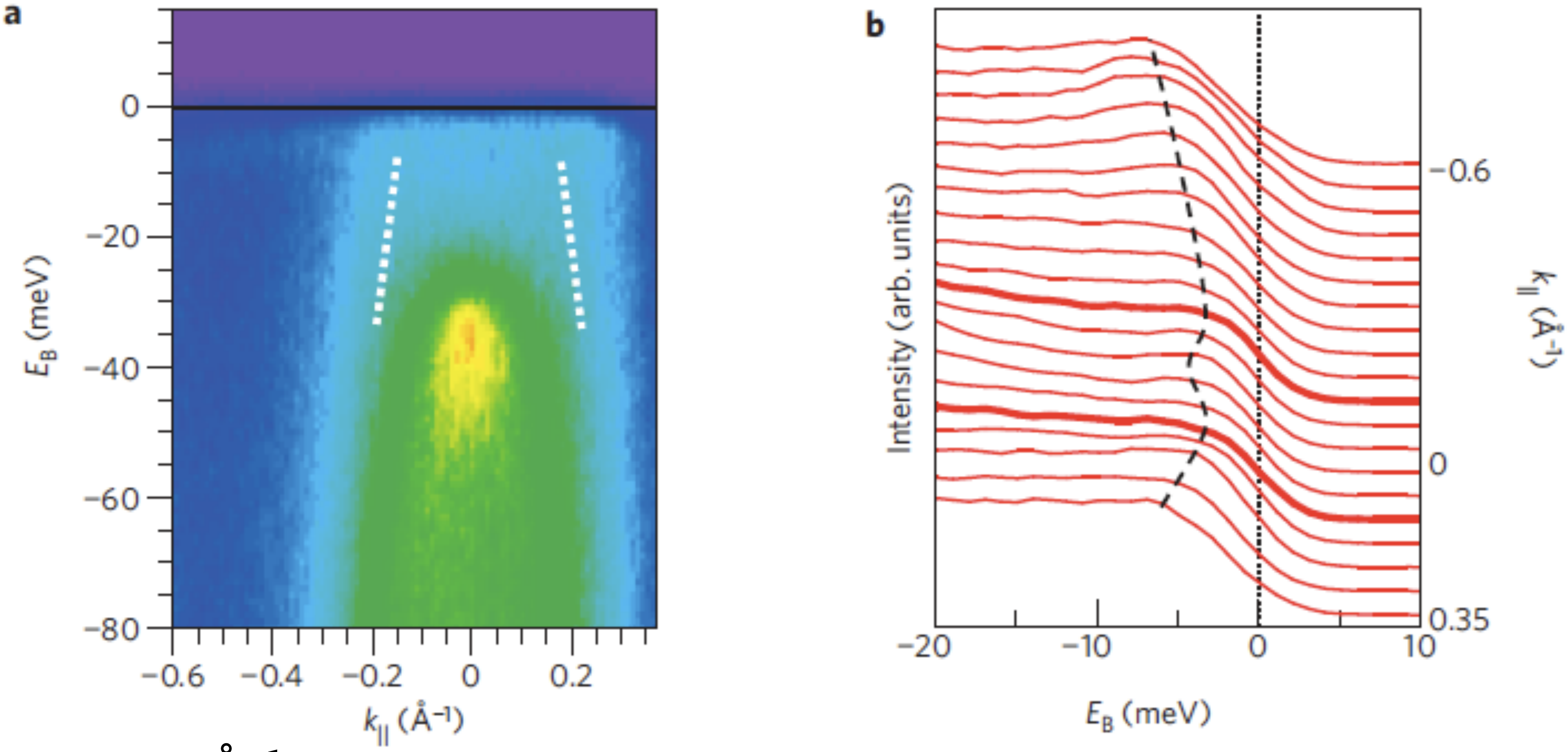


The heavy-quasiparticle band spreads beyond $|k_{\mathrm{LE}}|$.

Angle-resolved photoemission spectroscopy (ARPES)

(100) direction

T = 15 K

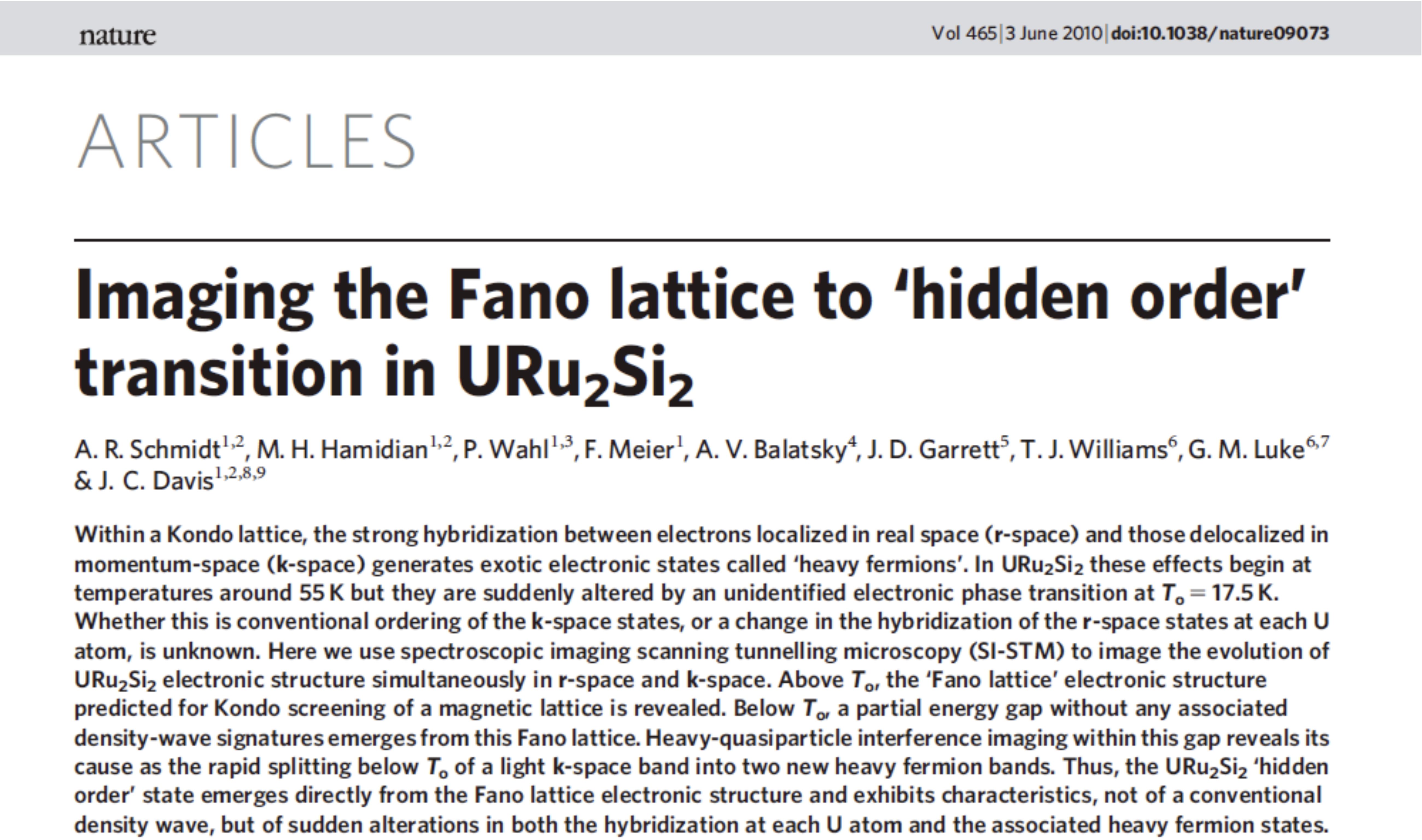


$k_{LE} = \pm 0.15$ Å^{-1}

The Fermi wavevectors along the (100) and (110) directions are small and different, proving the existence of anisotropic small-sized Fermi-surface pockets around the Γ point.

→ Fermi surface with multi-band compensated structure

Scanning tunneling microscopy (STM)



nature

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ARTICLES

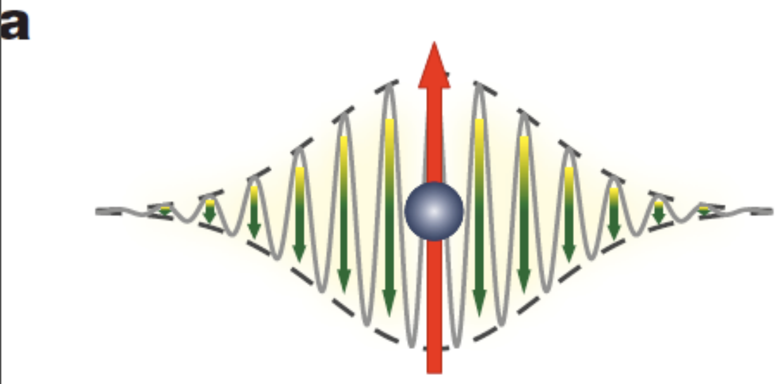
Imaging the Fano lattice to 'hidden order' transition in URu_2Si_2

A. R. Schmidt[1,2], M. H. Hamidian[1,2], P. Wahl[1,3], F. Meier[1], A. V. Balatsky[4], J. D. Garrett[5], T. J. Williams[6], G. M. Luke[6,7] & J. C. Davis[1,2,8,9]

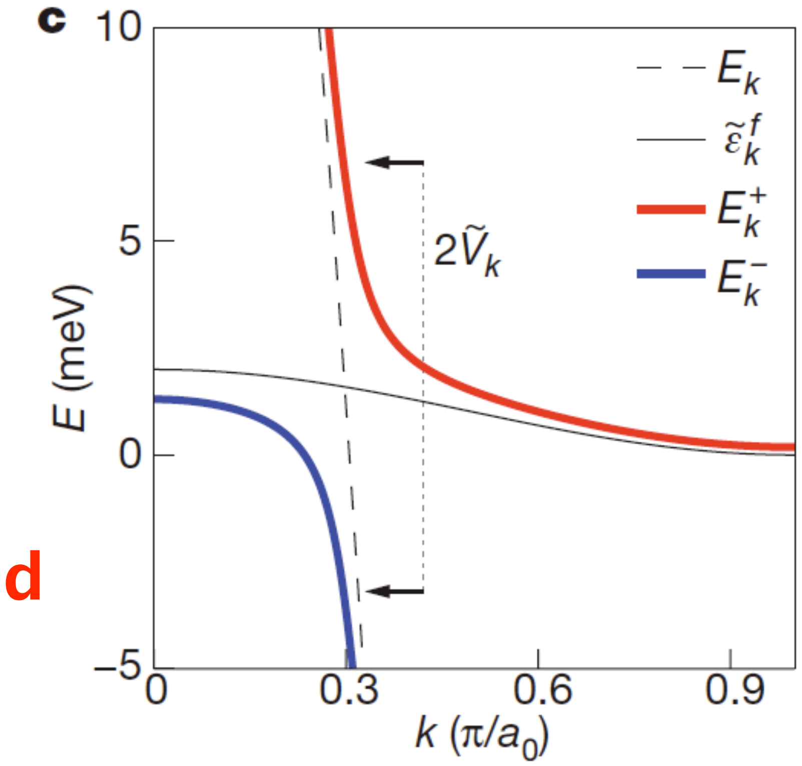
Within a Kondo lattice, the strong hybridization between electrons localized in real space (r-space) and those delocalized in momentum-space (k-space) generates exotic electronic states called 'heavy fermions'. In URu_2Si_2 these effects begin at temperatures around 55 K but they are suddenly altered by an unidentified electronic phase transition at $T_o = 17.5$ K. Whether this is conventional ordering of the k-space states, or a change in the hybridization of the r-space states at each U atom, is unknown. Here we use spectroscopic imaging scanning tunnelling microscopy (SI-STM) to image the evolution of URu_2Si_2 electronic structure simultaneously in r-space and k-space. Above T_o, the 'Fano lattice' electronic structure predicted for Kondo screening of a magnetic lattice is revealed. Below T_o, a partial energy gap without any associated density-wave signatures emerges from this Fano lattice. Heavy-quasiparticle interference imaging within this gap reveals its cause as the rapid splitting below T_o of a light k-space band into two new heavy fermion bands. Thus, the URu_2Si_2 'hidden order' state emerges directly from the Fano lattice electronic structure and exhibits characteristics, not of a conventional density wave, but of sudden alterations in both the hybridization at each U atom and the associated heavy fermion states.

Scanning tunneling microscopy (STM)

Kondo effect



$$E_k^{\pm} = \frac{\tilde{\varepsilon}_k^f + E_k \pm \sqrt{\left(\tilde{\varepsilon}_k^f - E_k\right)^2 + 4|\tilde{V}_k|^2}}{2}$$



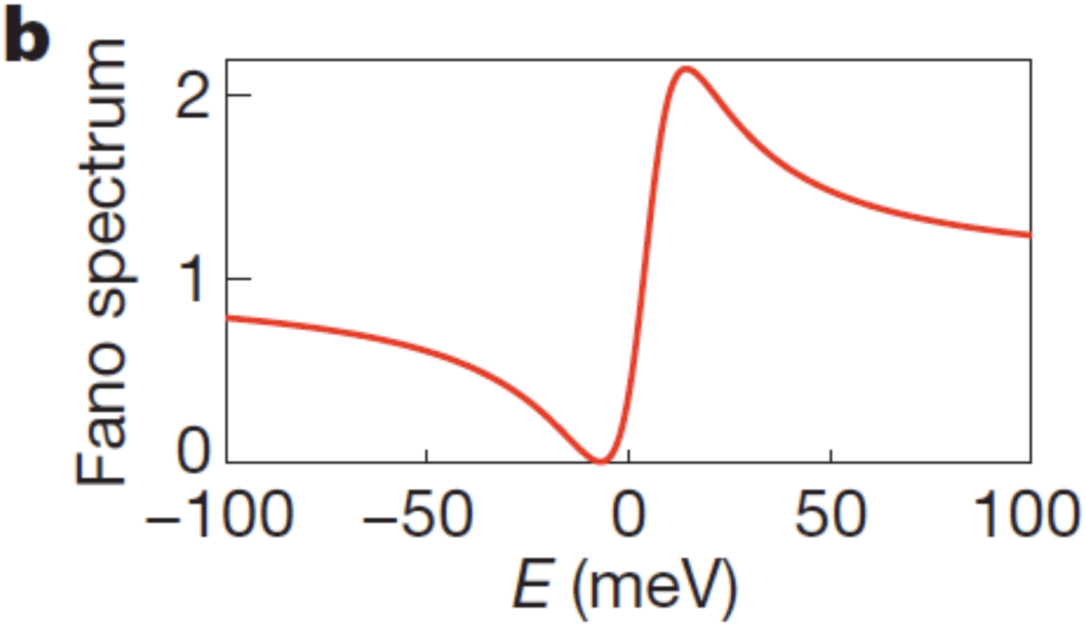
hybridization between the conductance and f-band

Asymmetric differential conductivity

$$g(\mathbf{r},\ E) \propto \frac{(\varsigma + E')^2}{E'^2 + 1} \text{ where } E' = \frac{(E - \varepsilon_0)}{\Gamma/2}$$

$$\Gamma = \pi N(E_F)\langle|\tilde{V}_k|^2\rangle$$

ζ : t_f/t_c
ε_0 : Kondo resonance energy
Γ : Kondo resonance width



A. R. Schmidt et al., Nature. **465**, 570 (2010).

Scanning tunneling microscopy (STM)

Above T_O = 17.5 K

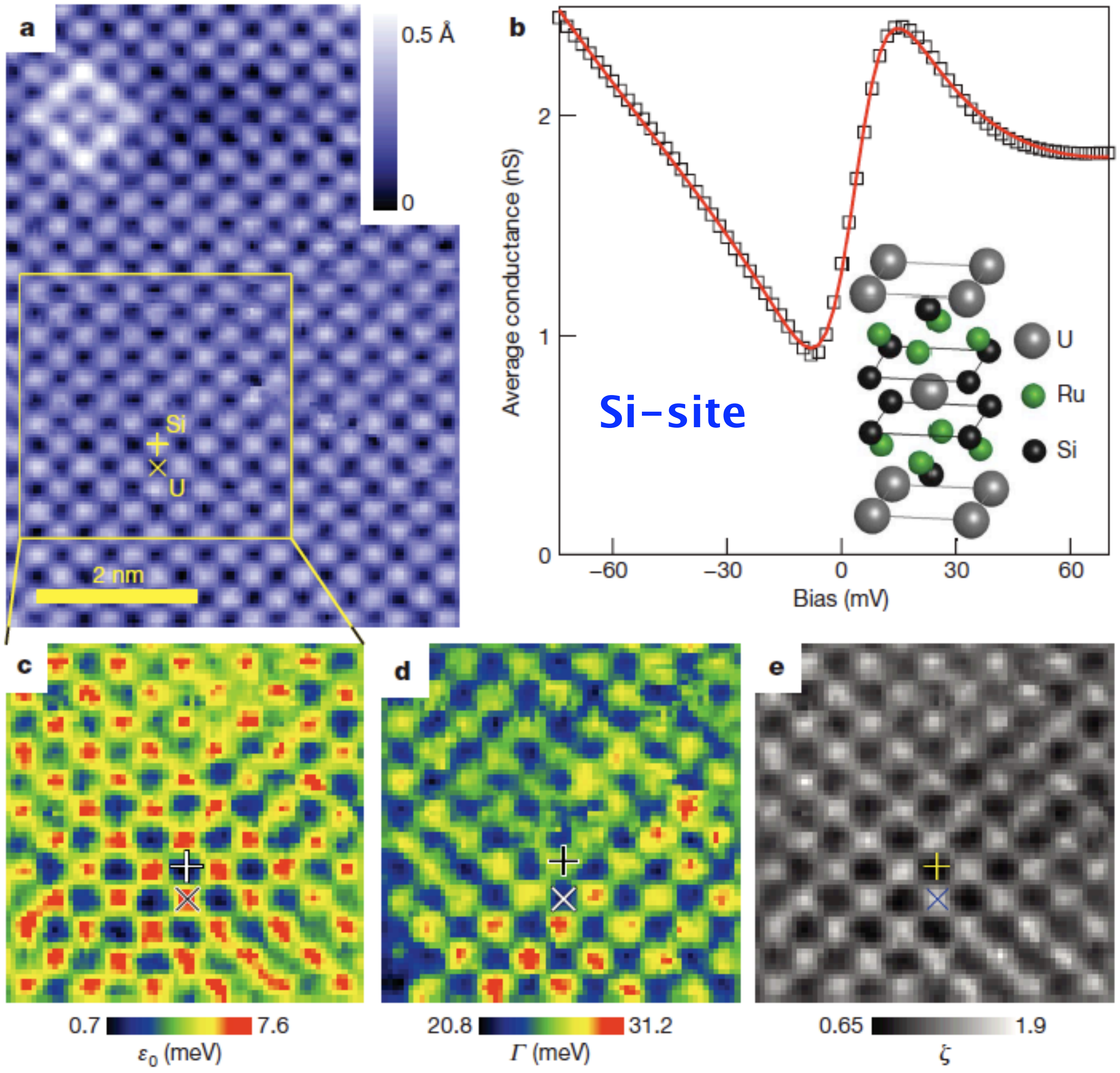
Si-site: d-electron

U-site: f-electron

Below 120 K, a Fano line-shape in the DOS is observed.

Strong evidence for the formation of the Kondo lattice in URu_2Si_2

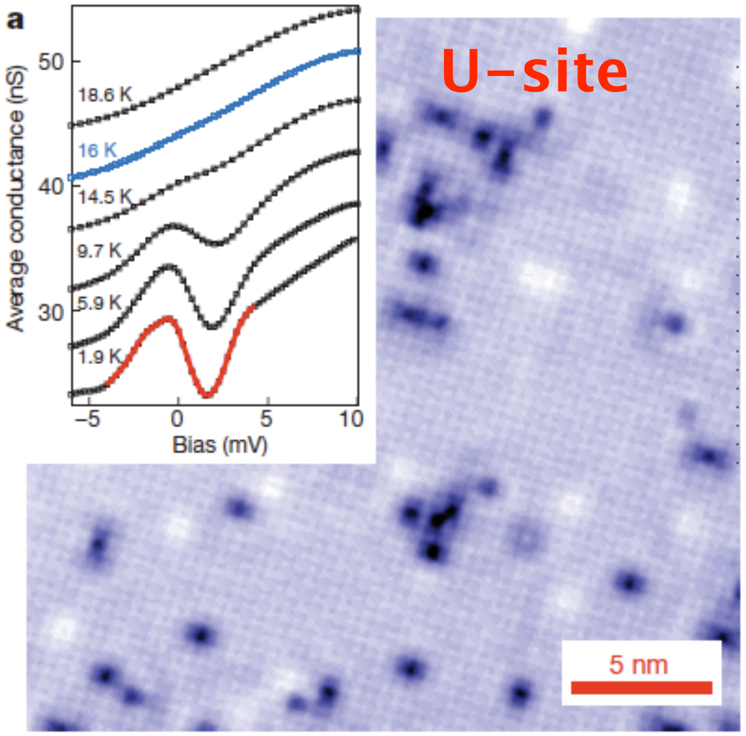
$$E_k^{\pm} = \frac{\tilde{\varepsilon}_k^f + E_k \pm \sqrt{\left(\tilde{\varepsilon}_k^f - E_k\right)^2 + 4|\tilde{V}_k|^2}}{2}$$

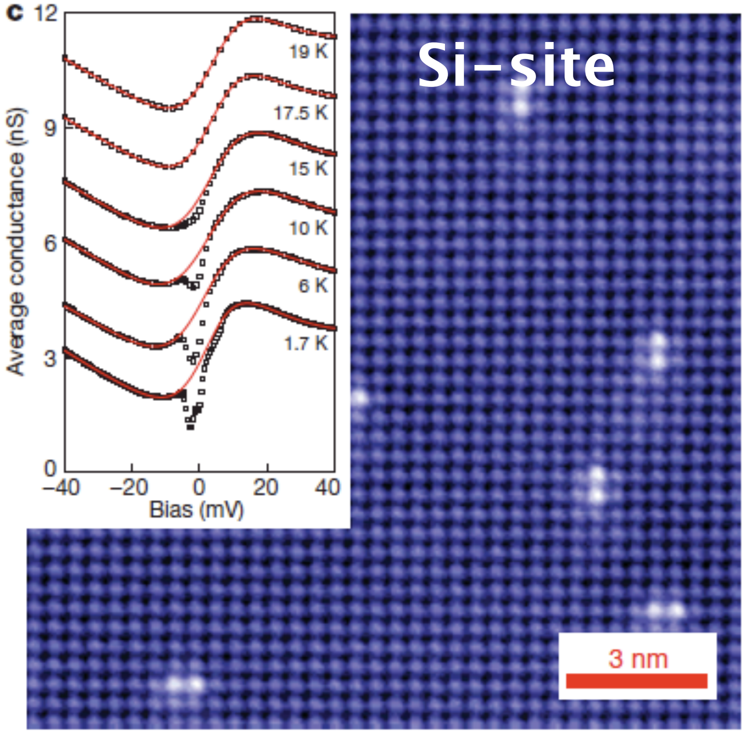


A. R. Schmidt et al., Nature. **465**, 570 (2010).

Scanning tunneling microscopy (STM)

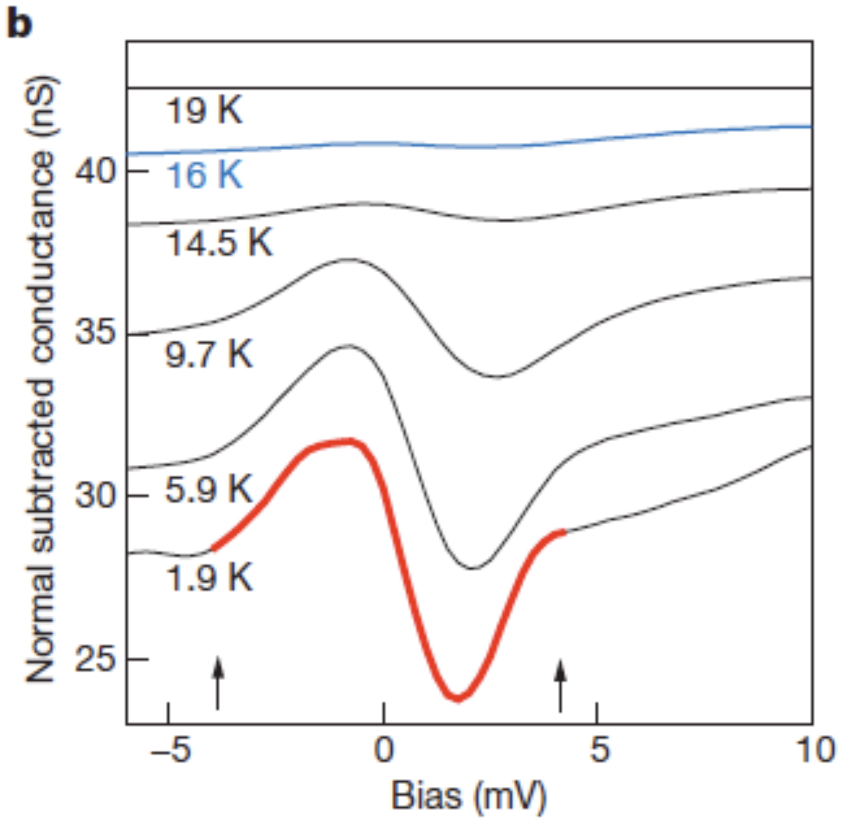
Below $T_O = 17.5$ K

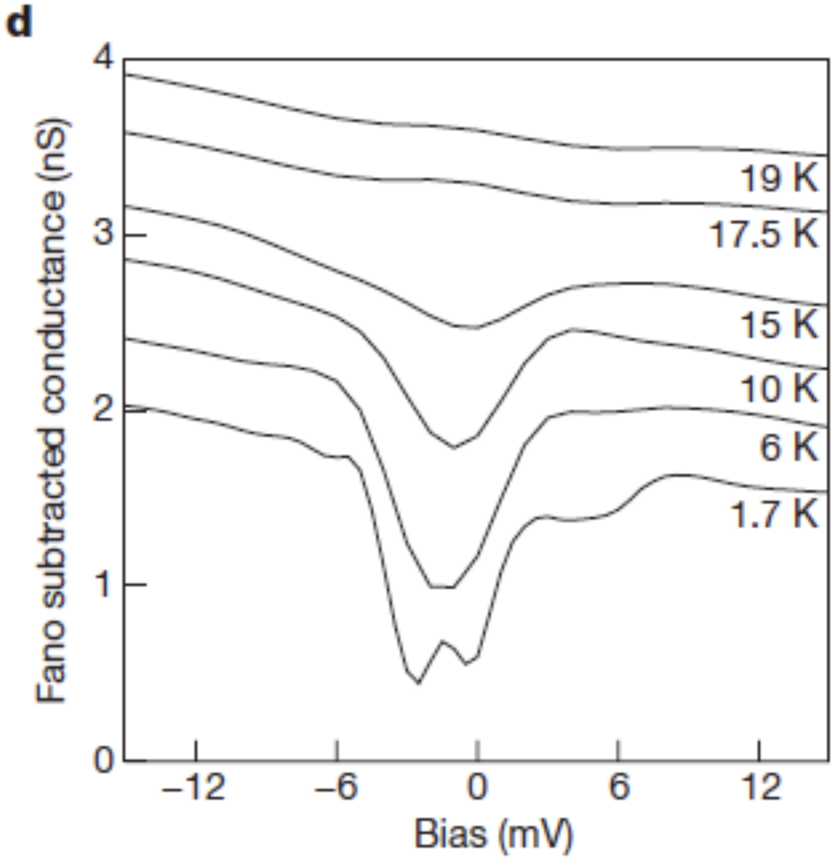




(i) Below To, the bottom of the Fano line-shape develops a gap-like feauture.

(ii) Both the Fano parameters and the gap structure depend on the STM tip positions (U- or Ru-site).



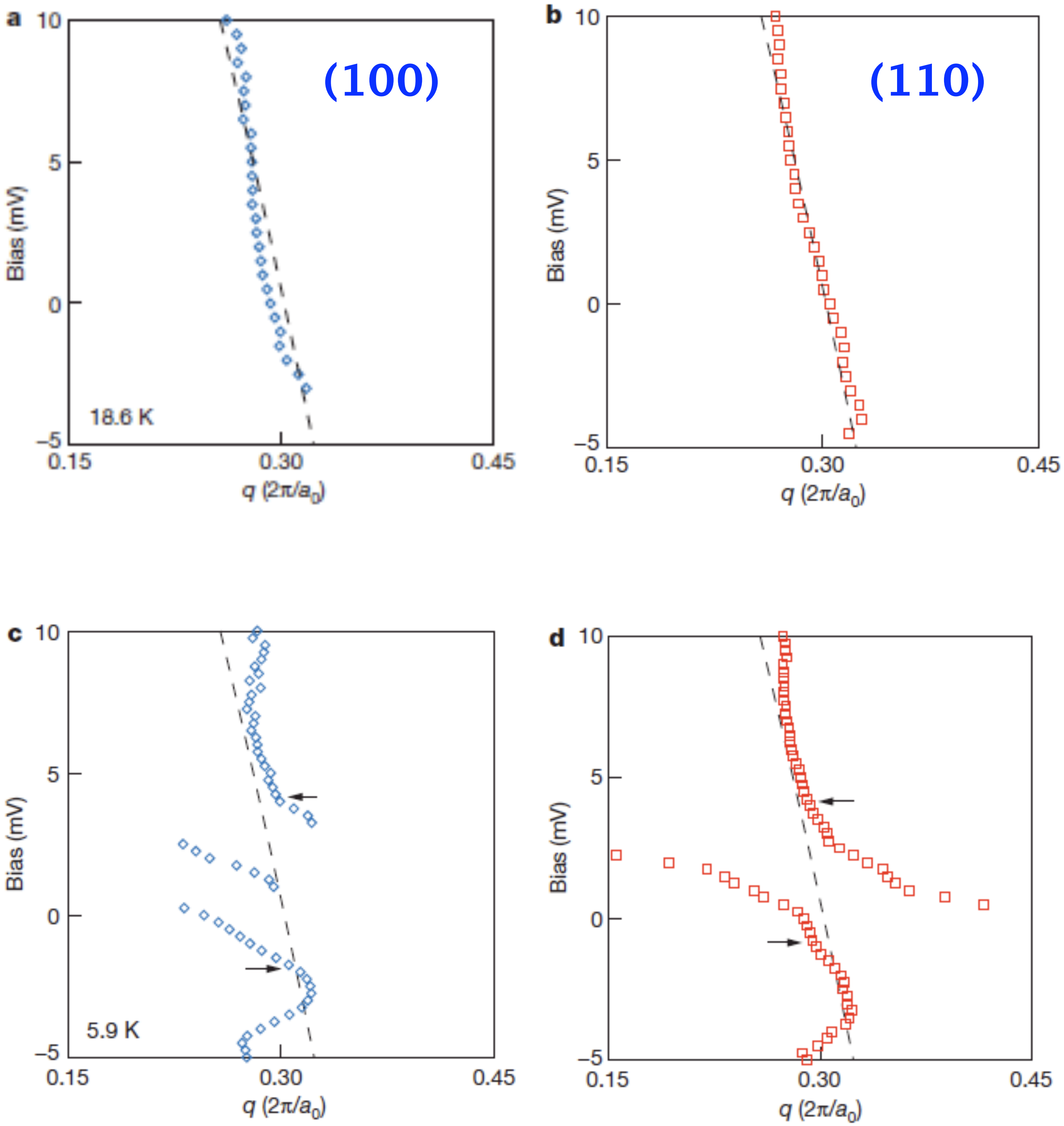


Scanning tunneling microscopy (STM)

Quasiparticle Interference (QPI)

✓The hole band develops a hybridization feature below T_0, corresponding to $Q = 0.3\ \pi/a_0$.

✓Rapid splitting of the light band into two heavy bands which become well separated.



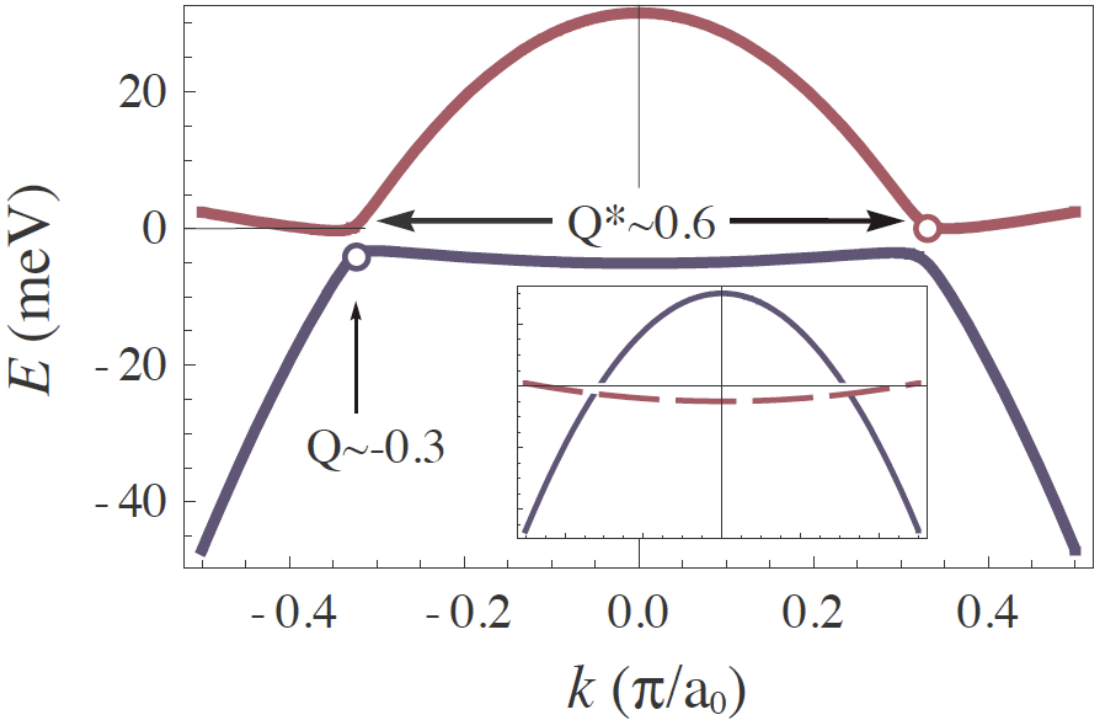
Hybridization wave in the HO

A light d-band and a heavy f-band cross at Q = ±0.3.

$$H = \sum_k \epsilon_k^{(c)} c_k^\dagger c_k + \sum_k \epsilon_k^{(f)} f_k^\dagger f_k + H_F$$

$$H_F = V_0 \sum_{k,r} c_k^\dagger f_r + h.c.$$

Hybridization between the d- and f-band



$$g_{k,k'} = g_k^{(0)} \delta_{k,k'} + \frac{V_0^2}{\omega - \epsilon_0 - V_0^2 \chi_0} g_k^{(0)} g_{k'}^{(0)}$$

$$f_0 = \frac{1}{\omega - \epsilon_0 - V_0^2 \chi_0}$$

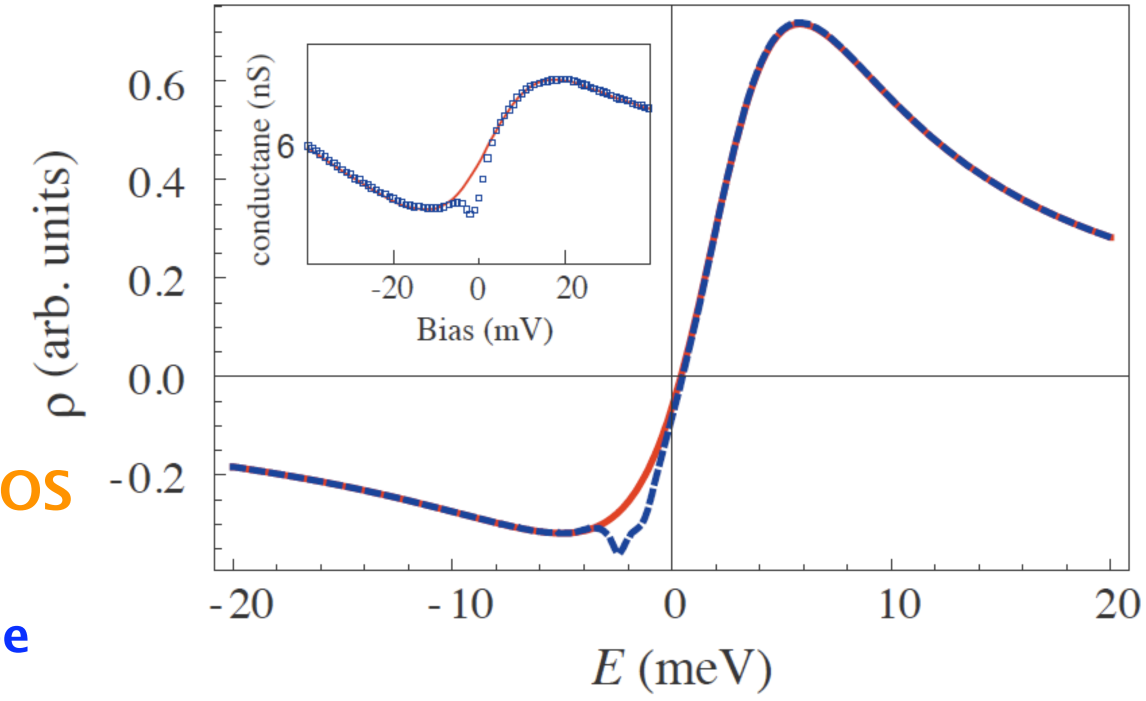
$g_{k,k'}$: Green function of the d-electron

f_0: Green function of the f-electron

$$\chi_0 = \sum_k g_k^{(0)} = -\Gamma_0 (i + q)$$

Γ_0 is proportional to the bare-d-band DOS

$\rho = -\frac{1}{\pi} \Im \sum_{k,k'} g_{k,k'}$ ➡ **Fano line-shape in the LDOS**



$\Gamma_1 = V_0^2 \Gamma_0$ **Γ_1: Band width of the Fano line-shape**

The holes first hybridizes with the local part of the f-electrons.

Hybridization wave in the HO

Below the HO transition

$$H_{I,MF} = V c^{\dagger}_{-Q} f_Q + h.c.$$

Q = 0.3 π/a$_0$

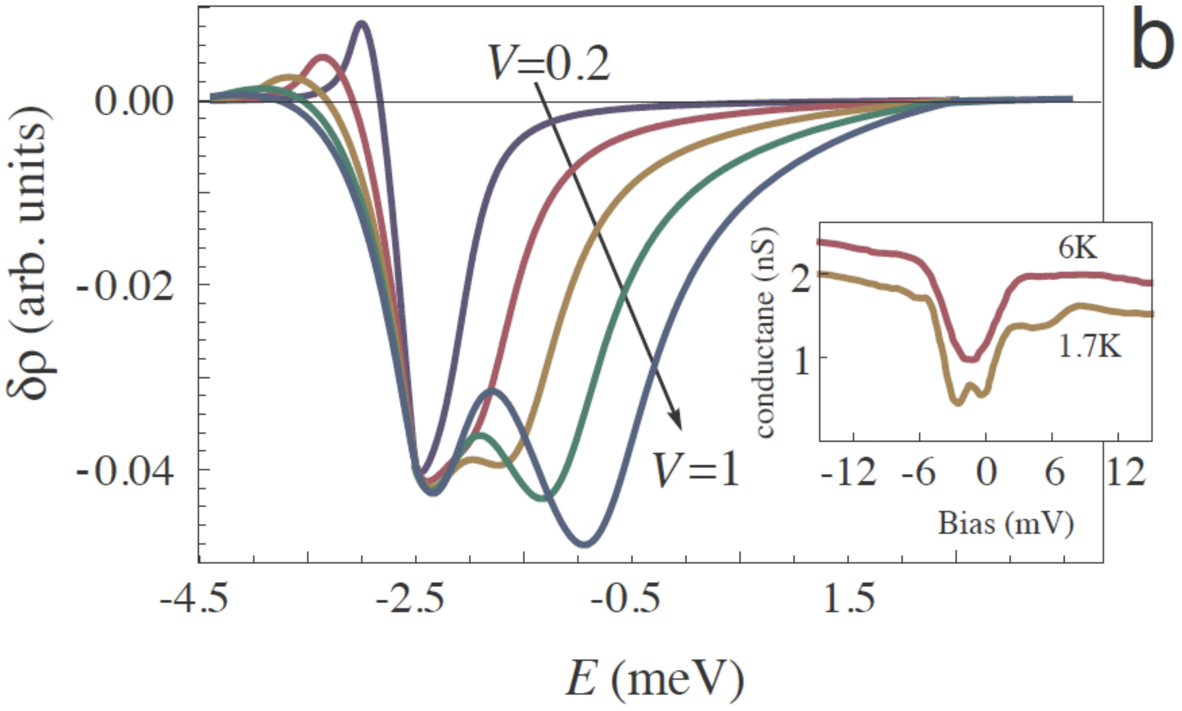
V: Hidden order parameter

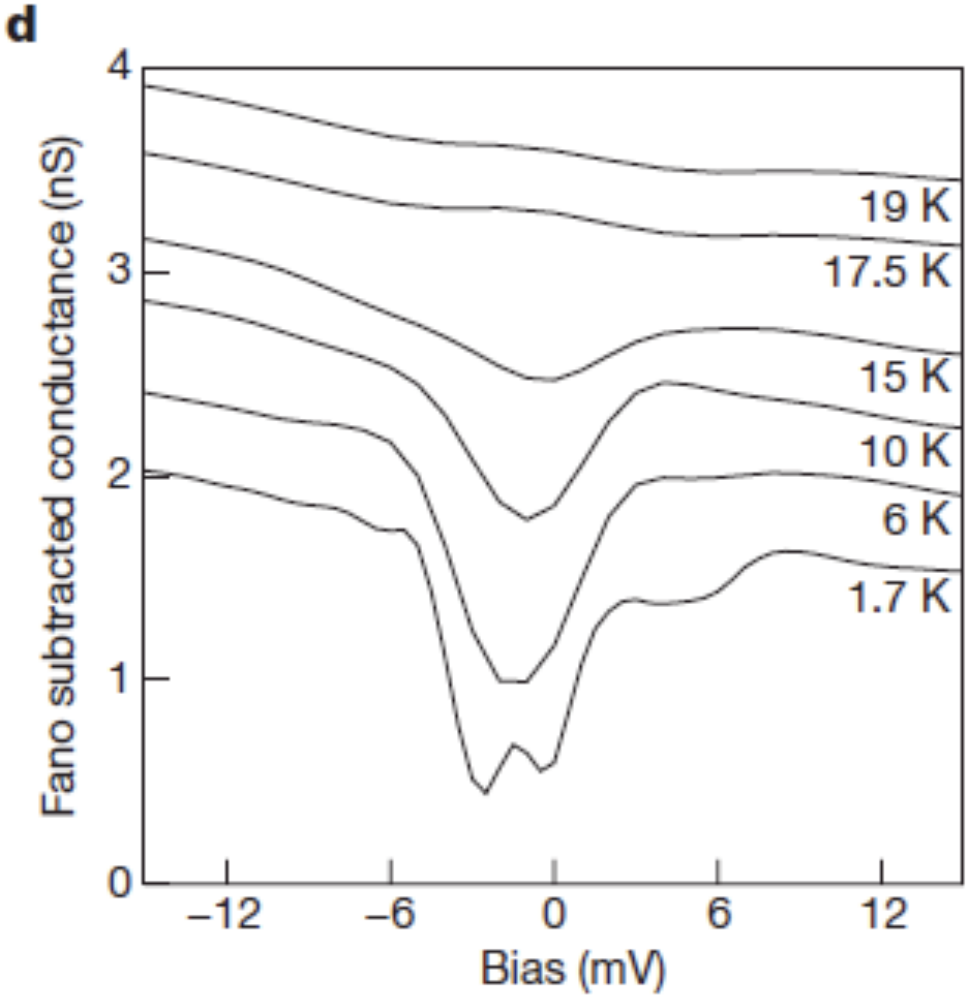
If H$_{I,\,MF}$ operate on the bare hamiltonian, no correction will be observed.

$$G_{k,k'} = g_{k,k'} + \frac{V^2 g_{k,-Q} g_{-Q,k'}}{\omega - \varepsilon_Q - V^2(g_{-Q,-Q} + G_{-Q,-Q})}$$

$$G_{-Q,-Q} = \frac{1 - \sqrt{1 - 4V^2 f_Q^{(0)} g_{-Q,-Q}}}{2V^2 f_Q^{(0)}} .$$

LDOS $\rho = \sum_{k,k'} G_{k,k'}$





(i) The gap-like feature develops as a function of V. Its width and position depend on V.

(ii) The additional peak appears at the bottom of the gap.

Hybridization wave in the HO

In the mean-field approximation,

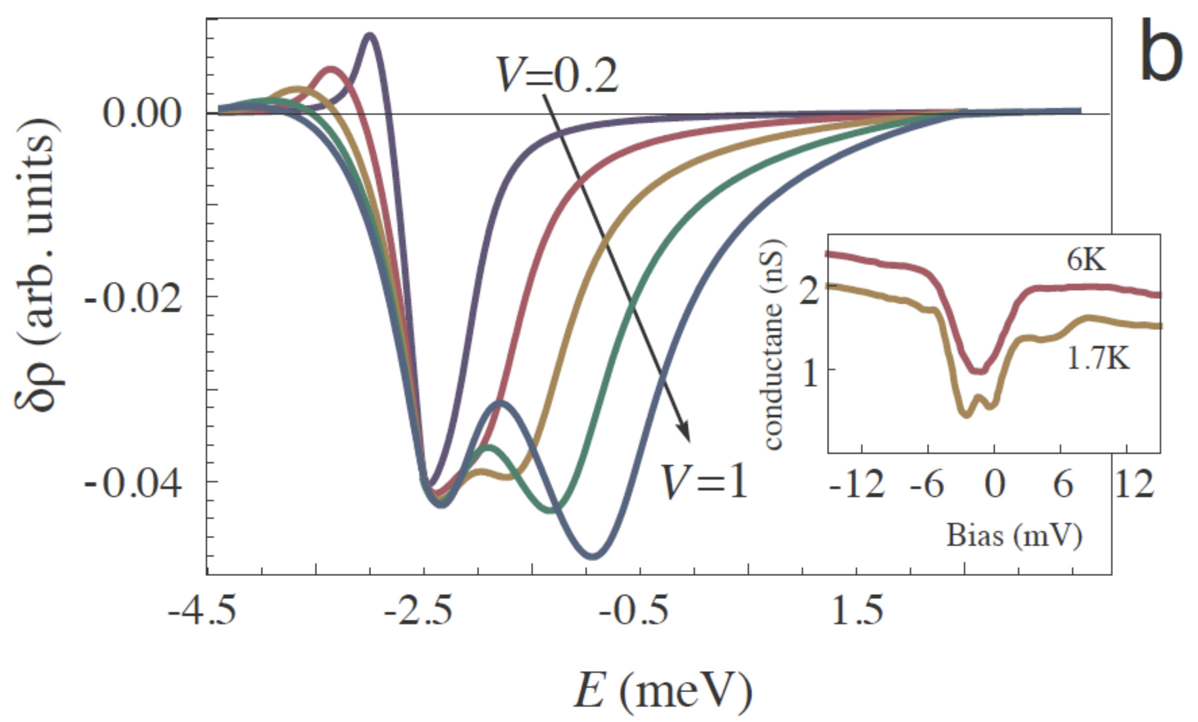
$$V^2 \propto (T_{HO} - T)$$

(i) E_{min}

independent on the temperature

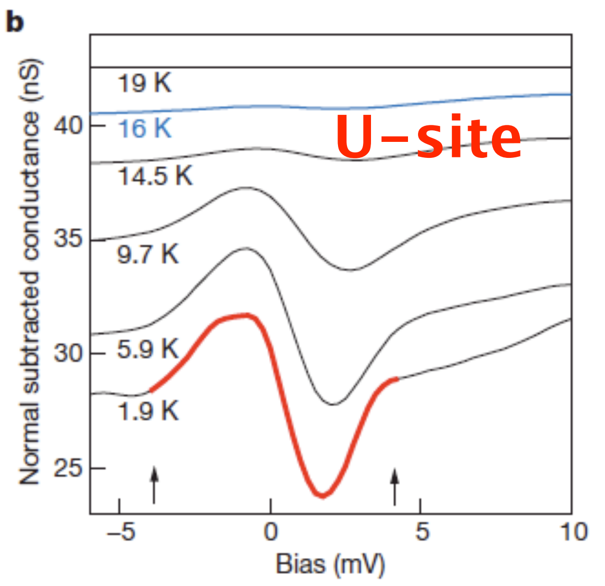
(ii) E_{peak}: additional peak structure

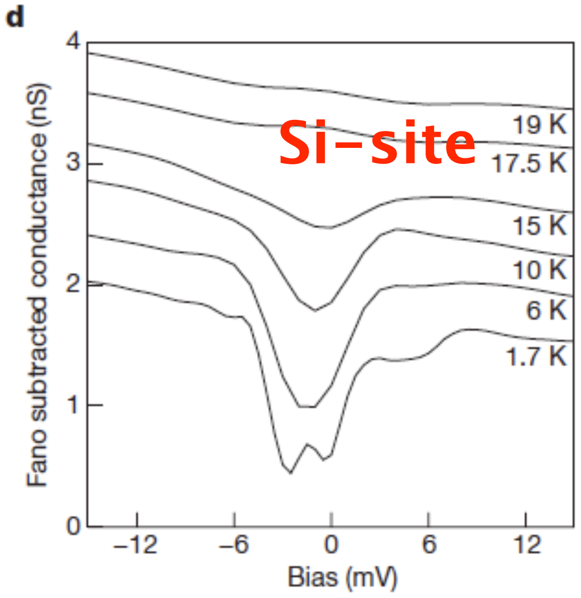
dependent on the temperature

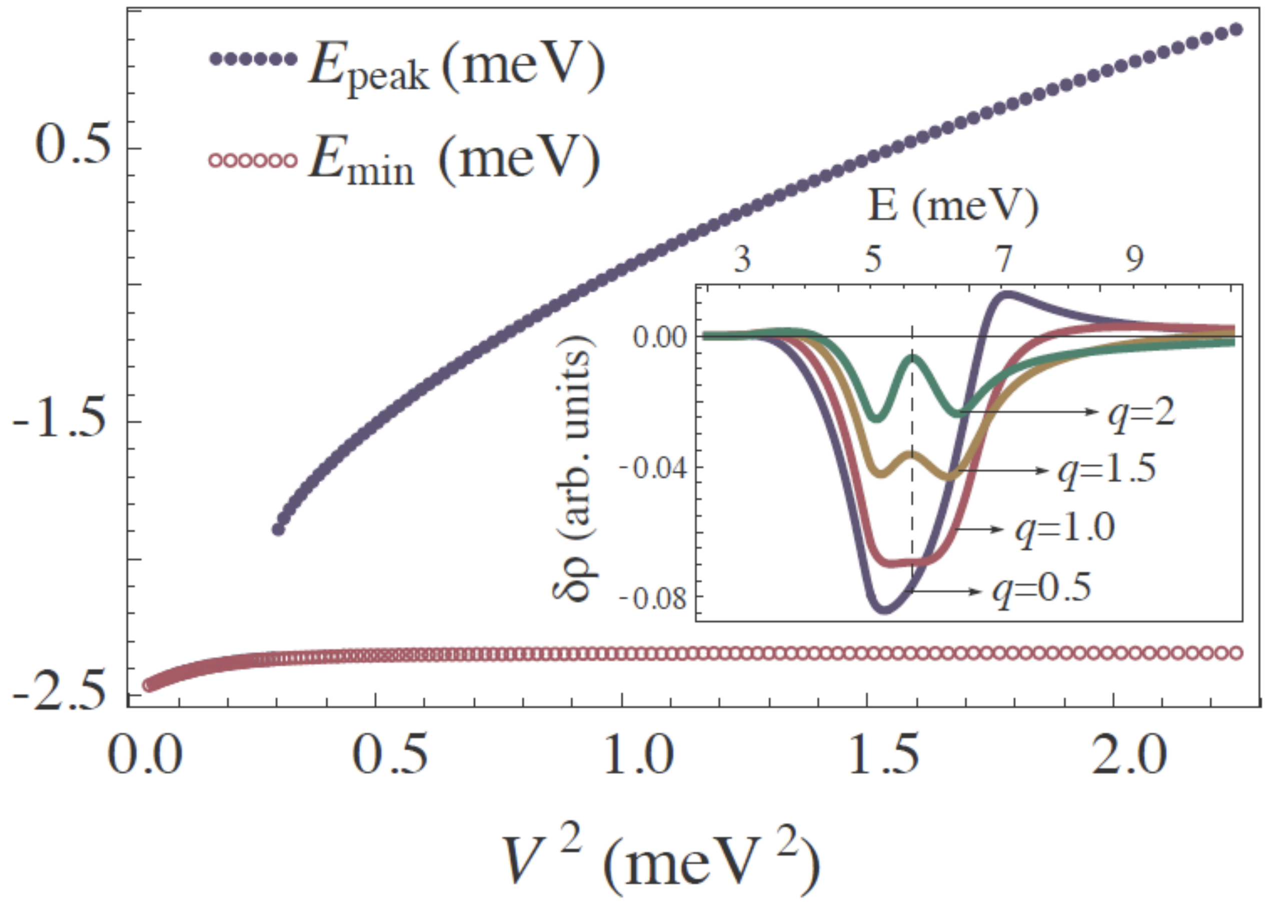


✓q-dependence of the

When the tip is above the Si site, it has better coupling to the d-band, which effectively increases the Fano factor.







Hybridization wave in the HO

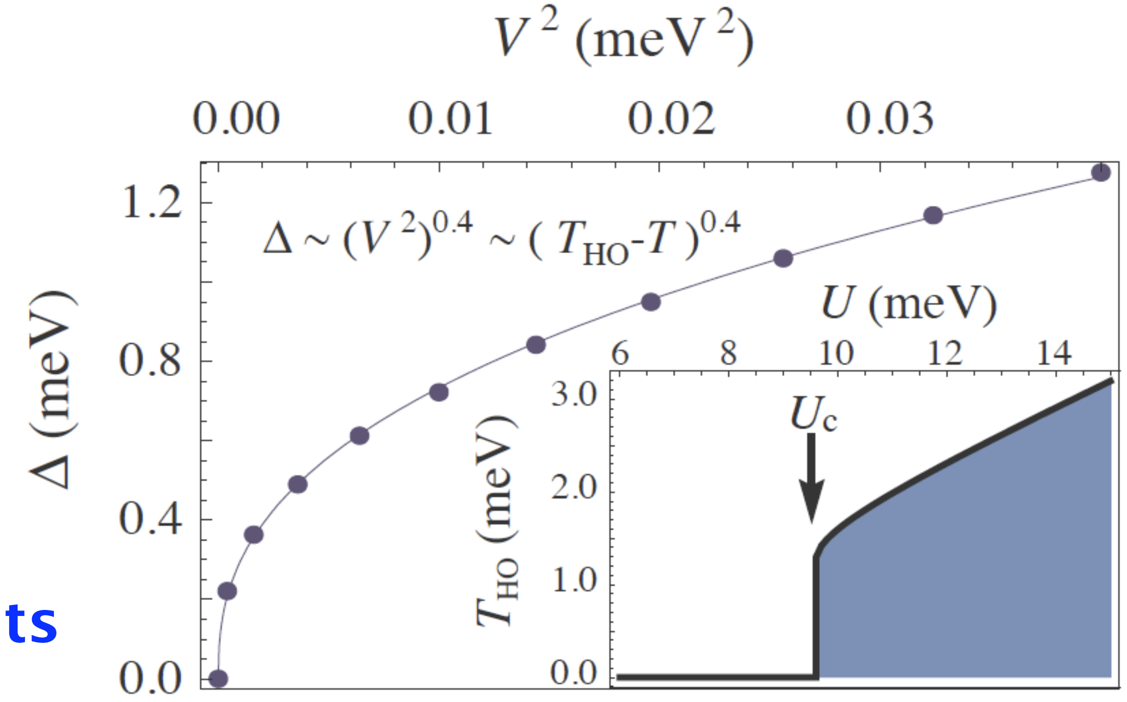
✓**Temperature dependence of the gap**

$$V^2 \propto (T_{HO} - T)$$

$$\rightarrow \quad \Delta \propto (T_{HO} - T)^{\nu}$$

$\nu = 0.4$

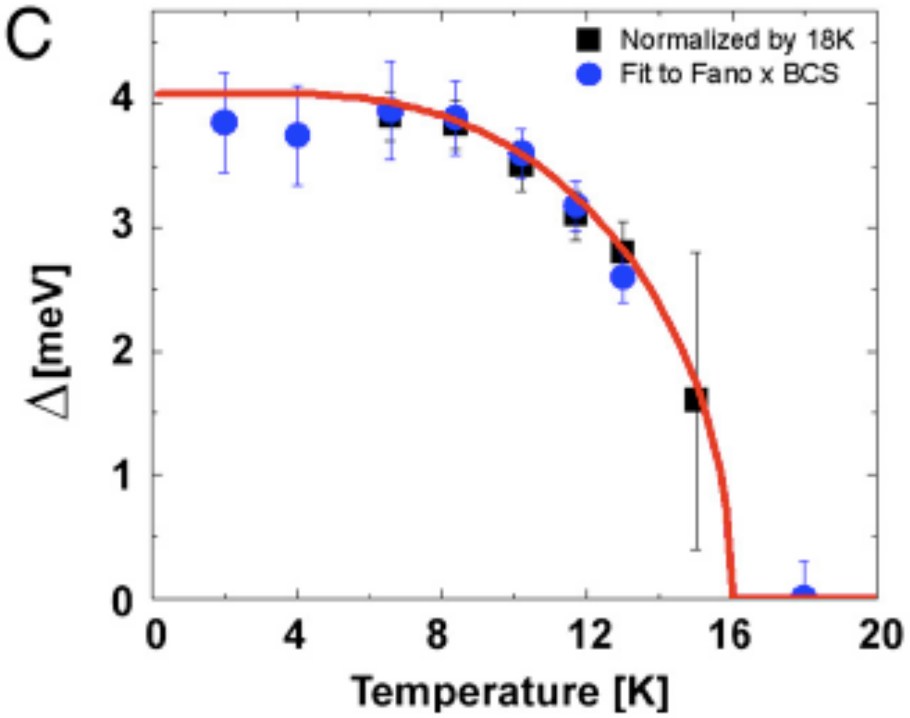
In good agreement with the experimental results



✓**Temperature of the HO transition**

$$-\frac{1}{U_{-Q,Q}} = T_{HO} \sum_{i\omega_n} f_Q(i\omega_n, Q) g_{-Q}(i\omega_n)$$

U below a certain value U$_c$, the equation does not have a solution, due to the compact nature of the interaction in momentum space.



Summary

(i) Neutron-scattering

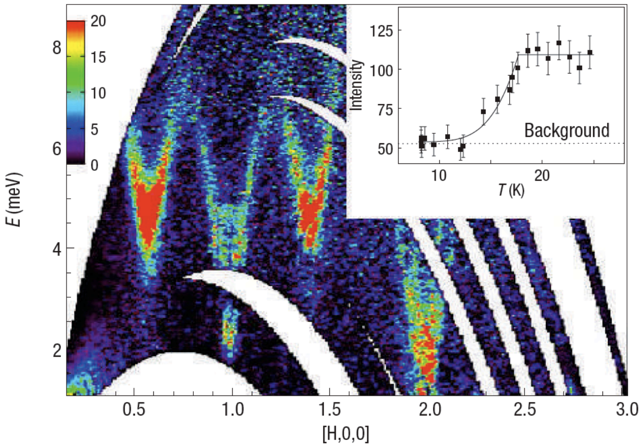
$Q \sim 0.6, 1.4\ \pi/a_0$

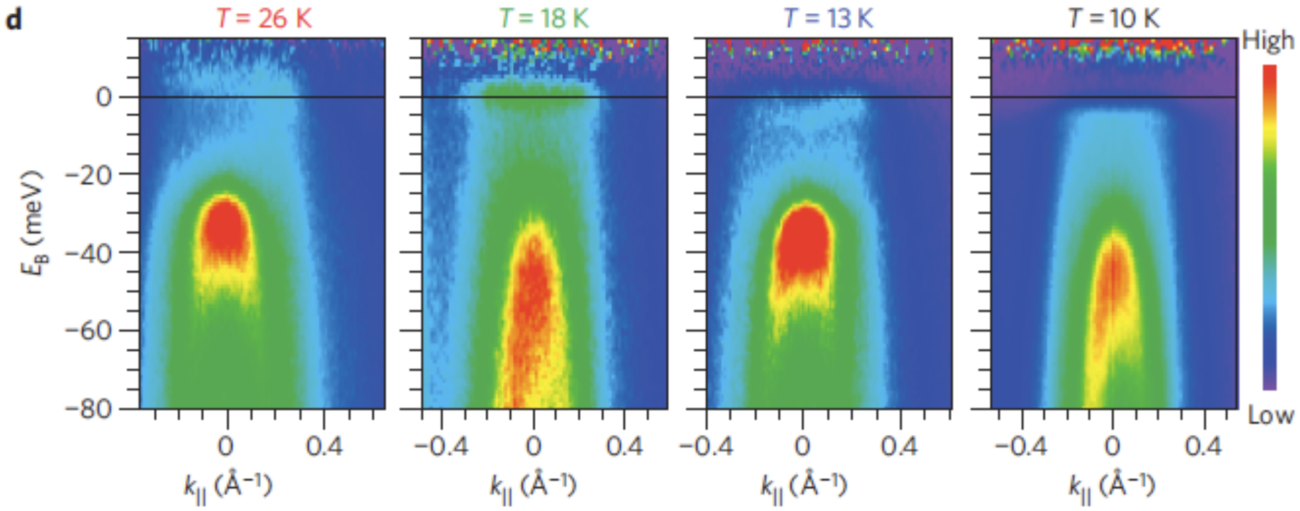
(ii) ARPES

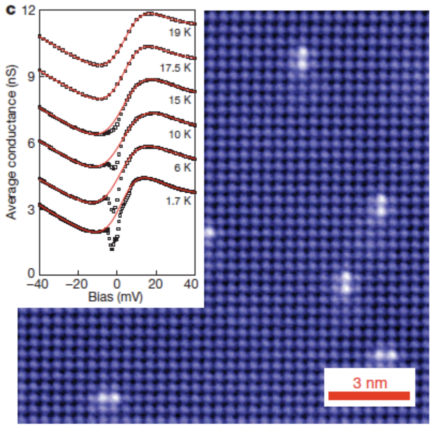
Heavy f-band

(iii) STM

Fano line-shape with a gap-like feature below T_o







✓A light d-band and a heavy f-band cross at $Q = \pm 0.3$.

✓Above T_o, the hole first hybridizes with the f-band.

→ Fano line-shape in the LDOS

✓Below T_o, the band structure gives rise to enhanced hybridization between the electron with Q and hole with -Q.

→ The resulting electron-hole coherence is the HO parameter.