The Modulated Spin Liquid: a new paradigm for URu2Si2

C. Pépin (IPhT, CEA-Saclay + IIP, Natal)

M. Norman (Argonne)

S. Burdin (Bordeaux, France)

A. Ferraz (IIP, Natal)

CP, M. Norman, S. Burdin and A. Ferraz, preprint 2010

Pohang, Sept. 8th 2010
Custers et al (CP), Nature 2003

Resistivity linear on 3 decades of energy

$\rho(T) \sim T^\epsilon$

Ginzburg-Landau type of itinerant electron QCP is ruled out!
URu2Si2 is a compensated metal

U. Matsuda, Unpublished

A very old mystery!

T. Palstra et al, PRL (85)
A very old mystery!

T. Palstra et al, PRL (85)

B. Maple et al, PRL (86)
Tiny magnetic moment $0.03\mu B$
that the hidden-order ground state switches at $T_{sc}$ unconventional superconductivity at occurrence of a tiny ordered moment $M/H_2O$ order have been proposed. The long standing debate on the occurs at as transport measurements, indicate clearly that nesting surface is not deeply modified through the transition line nature of the hidden order state. For example, the previous in the heavy fermion system URu$_2$Si$_2$, multipolar ordering exist on quite different proposals such as orbital hidden order the discovery of unexpected new order parameters. Debates materials, which belong often to the rich class of strongly ordering between localized and itinerant.

Up to now, there is no direct convincing microscopic evidence of the sharp low energy excitation at the wave vector $Q_0=(1,0,0)$, which disappears in the bulk at $T_X$; above $T_{sc}$ a unique nuclear magnetic resonance current" in cuprate superconductors. Due to the dual character of the $P$ phase diagram of URu$_2$Si$_2$ from previous neutron scattering experiments under pressure and stress, a unique simultaneous neutron scattering and thermal expansion measurements on the heavy-fermion superconductor $A$. Villaume, F. Bourdarot,* E. Hassinger, S. Raymond, V. Taufour, D. Aoki, and J. Flouquet. The remarkable feature is that below $T_0$ both excitations are cause of the Ising character along the $c$ axis of the magnetic excitations, they have been measured at the equivalent position $Q_0$ for $P=0$, two main inelastic magnetic responses of neutron scattering response for both ordered phases. At $P=4.5$ meV. Furthermore their temperature evolutions exist of dipolar origin. The order parameter is not yet determined: hidden order label reflects the fact that this order may not be small. How-
that the hidden-order ground state switches at unconventional superconductivity at $T_{sc}$.

The long standing debate on the nature of the hidden order state. For example, the previous proposal of orbital antiferromagnetism is not demonstrated.24

The elucidation of the nature of a hidden order in exotic correlated electronic systems, is a hot subject as it can lead to the possibility of multipolar ordering,8–11 or—of dipolar origin. The order parameter is not yet determined:

Due to the dual character of the 5d electrons in URu$_2$Si$_2$ the proposal of residual Si NMR linewidth22 has been rejected;15,23 never no evidence is found even in NMR experiments.15

Institut Nanosciences et Cryogenie, SPSMS/MDN, CEA-Grenoble, 38054 Grenoble, France

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PHYSICAL REVIEW B

A. Villaume et al, PRB (2008)

Pressure studies

B. Maple et al, PRL (2007)
Pressure studies

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Itinerant Gap

FIG. 1: Temperature dependence of the quasi-particle band in URu$_2$Si$_2$.

a, Raw photoemission spectra integrated within ±0.2 Å$^{-1}$ along the (110) direction at 13 K (blue) and 26 K (red). Below $T_o = 17.5 K$, a quasi-particle (QP) peak appears below $E_F$. For all temperatures, a surface state (SS) at $E_B < -35$ meV is observed.

b, Spectra integrated within ±0.2 Å$^{-1}$ along the (110) direction and normalized by the Fermi-Dirac distribution, at various temperatures around $T_o$: 26 K (red), 18 K (green), 13 K (blue) and 10 K (black). The zero-intensity level of each spectrum is indicated by the color bars in the right axis. The triangle markers give the peak position.

c, Energy of the QP peak in the integrated spectra (with respect to $E_F$) as a function of $T/T_o$ for cuts along the (110) (triangles) and (100) (circles) directions. The error bars in $T$ are due to thermal instabilities during the experiment. The error bars in the peak energy are calculated from the peak positions in spectra integrated over different momentum windows around $k_\parallel = 0$.

d, Angle-resolved spectra along the (110) direction for the same temperatures as in b, over an extended energy range. The intense hole-like feature dispersing below $E_B \sim -35$ meV is the surface state displayed in panel a.

FIG. 2: Heavy quasi-particle band in the hidden-order state and hybridisation with a conduction band along the (110) direction.

a, ARPES intensity map along the (110) direction at 13 K. The map shows a heavy quasi-particle band dispersing down to $\sim 7$ meV below $E_F$.

b, EDCs of the intensity map in (a) in the region close to $E_F$. The EDCs whose leading edge is closest to $E_F$ are drawn in bold.

c, MDCs from the intensity map in (a). Each MDC is normalized to its area. The two central peaks correspond to the hole-like surface state, and two lateral shoulders to a light conduction band that disperses through $E_F$.

d, Average of second derivatives along the energy and momentum axes (see methods), showing the heavy-QP band, the surface state, and the hole-like conduction band. In all panels, the dashed lines are guides to the eye for the dispersions of the different bands.

D. Bonn et al, PRL (88)

Itinerant Gap

D. Bonn et al, PRL (88)


Carriers disappear at the transition

K. Behnia et al, PRL (2005)
Inelastic signal at $Q = (1,0,0)$
Summary of experiments

Mysterious transition at 17.5 K in pure compound
Summary of experiments

Mysterious transition at 17.5 K in pure compound

↓

Big amount of entropy quenched at the transition 0.3 of RLn2
Summary of experiments

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Optical gap of order of 7 me V, seen in ARPES

↓

STM: see further in the talk
Itinerant theories

V. Barzykin, L. Gorkov, PRL (93) and (95)
Multi-Spin Correlations
Valence Admixture

A. Ramirez, PRL (92)
H. Ikeda, PRL (98)
Spin Density Wave

P. Santini, PRB (98)
Ohkawa & Shimizu JPCM (99)
quadrupolar order

Haule & Kotliar Nature (2009)
Hexadecapolar order
Arrested Kondo effect

Localized theories

Kiss & Fasekas, PRB (2005)
K. Hanzawa JMMM (2007)
Octupolar Order

P. Santini, PRB (98)
Jahn-Teller distorsion

T. Kasuya, JPSJ (97)
Over-screened Kondo effect

V. VMineev, PRB (2005)
SDW + Induced moments

D. Cox, PRL (87)

A. Balatsky, PRB (2009)
Charge Density Wave

C. Varma, PRL (2006)
Lifshitz transition

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CP, Norman, Burdin, Ferraz (2010)

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The Modulated Spin Liquid

Original idea of Resonant Valence Bond

\[ H_0 = \frac{J}{4} \sum_{\langle i, j \rangle, \sigma} \chi_i^\dagger \chi_i \chi_j \chi_j^\dagger \]

\[ \varphi_{ij} = \sum_{\sigma} \langle \chi_i^\dagger \chi_j \rangle \quad \Delta_{ij} = \frac{1}{\sqrt{2}} \left( \chi_i^\dagger \chi_j - \chi_i \chi_j^\dagger \right) \]

\[ S_i^Q = \sum_{\alpha\beta} \langle \chi_{i\alpha}^\dagger \sigma_{\alpha\beta} \chi_{i\beta} e^{iQ \cdot r_i} \rangle \]

P. Fazekas & P.W. Anderson, SSC (74)
P. Anderson, Science (87)
Baskaran, Z. Zou & P.W. Anderson, SSC (87)
Affleck & Marston, PRL (87)
The Modulated Spin Liquid

Original idea of Resonant Valence Bond

\[ H_0 = \frac{J}{4} \sum_{\langle i,j \rangle, \sigma} \chi^{\dagger}_{i\sigma}\chi_{i\bar{\sigma}}\chi^{\dagger}_{j\bar{\sigma}}\chi_{j\sigma} \]

\[ \varphi_{ij} = \sum_{\sigma} \langle \chi^{\dagger}_{i\sigma}\chi_{j\sigma} \rangle \quad \Delta_{ij} = \frac{1}{\sqrt{2}} \left( \chi^{\dagger}_{i\sigma}\chi_{j\bar{\sigma}} - \chi^{\dagger}_{i\bar{\sigma}}\chi_{j\sigma} \right) \]

\[ S^Q_i = \sum_{\alpha\beta} \langle \chi^{\dagger}_{i\alpha}\chi_{i\beta}e^{iQ\cdot r_i} \rangle \]

\[ \varphi^Q_{ij} = \sum_z \varphi_0 \delta_{r_i, r_j + z} e^{iQ\cdot (r_i + r_j)/2} \]

Staggered flux Phase

Affleck & Marston, PRL (87)
Only One Spin Liquid: it is modulated!

\[ \mathcal{L}_0 = \sum_{\langle i,j \rangle, \sigma} \left[ \chi_{i\sigma}^\dagger \left( \delta_{ij} (\partial_\tau + \lambda_i) + \sum_m \varphi_{ij}^m + S_i^Q \cdot \sigma \right) \chi_{j\sigma} \right] \]

\[ - \sum_i \lambda_i + \sum_{\langle i,j \rangle} \left[ \sum_m \frac{1}{J_{SL}} (\varphi_{ij}^m)^2 + \frac{1}{J_{AF}} S_i^Q \cdot S_j^Q \right] \]

\[ J \equiv J_{SL} + J_{AF} \]

\[ \varphi_{ij} = \varphi_{\mathbf{r}_i-\mathbf{r}_j, (\mathbf{r}_i+\mathbf{r}_j)/2} = \sum_q e^{i\mathbf{q} \cdot (\mathbf{r}_i+\mathbf{r}_j)/2} \varphi_{\mathbf{r}_i-\mathbf{r}_j, q} \rightarrow \{ q = \mathbf{0}, q = \mathbf{Q} \} \]
Only One Spin Liquid: it is modulated!

\[ \mathcal{L}_0 = \sum_{\langle i,j \rangle, \sigma} \chi^\dagger_{i\sigma} \left( \delta_{ij} (\partial_\tau + \lambda_i) + \sum_m \varphi_{ij}^m + S_i^Q \cdot \sigma \right) \chi_{j\sigma} \]

\[ - \sum_i \lambda_i + \sum_{\langle i,j \rangle} \left[ \sum_m \frac{1}{J_{SL}} (\varphi_{ij}^m)^2 + \frac{1}{J_{AF}} S_i^Q \cdot S_j^Q \right] \quad J \equiv J_{SL} + J_{AF} \]

\[ \varphi_{ij} = \varphi_{\mathbf{r}_i - \mathbf{r}_j, (\mathbf{r}_i + \mathbf{r}_j)/2} = \sum_q e^{i\mathbf{q} \cdot (\mathbf{r}_i + \mathbf{r}_j)/2} \varphi_{\mathbf{r}_i - \mathbf{r}_j, q} \rightarrow \{ q = \mathbf{0}, q = \mathbf{Q} \} \]

\[ J=10, \quad t'=0.8, \quad T=0, \quad nk=100 \]
MSL vs AF decoupling

\[ F = \frac{1}{2} \sum_{k,i} \ln(1 + e^{-\beta \omega_i(k)}) + \frac{4}{J_{SL}} (\phi_0^2 + \phi_Q^2) + \frac{4}{J_{AF}} S_Q^2 \]

\[ \omega_i(k) = \frac{\phi_0}{2} (\epsilon_k + \epsilon_{k+Q} - 2\mu_f) \]
\[ \pm \sqrt{\phi_0^2 (\epsilon_k - \epsilon_{k+Q})^2 + (\phi_Q \epsilon_k - \phi_{Q/2} \pm S_Q)^2} \]

\[ \epsilon_k = -2(\cos(k_x a) + \cos(k_y a)) - 4 \frac{t'}{t} \cos(k_x a) \cos(k_y a) \]
First order transition between MSL and AFM: they compete!
Similarity of the dispersions: similar entropy quenched at the transition

Breaks Z4 symmetry

Band structure interpretation

AFM

MSL

that the hidden-order ground state switches at unconventional superconductivity at $T_{sc}$ occurs from the paramagnetic moment occurrence of a tiny ordered moment orbital antiferromagnetism,1 chiral spin state,12 and helicity order13 have been proposed. The long standing debate on the spin or charge density wave,5–7 multipolar ordering,8–11 or hidden order label reflects the fact that this order may not be nature of the hidden order state. For example, the previous in the heavy fermion system URu$_2$Si$_2$,1 multipolar ordering the discovery of unexpected new order parameters. Debates variety of experiments.4 At zero pressure, a phase transition between localized ordered phase leading to the possibility of multipolar order.17–19 Reveal an interesting phase diagram The elucidation of the nature of a hidden order in exotic.Institut Nanosciences et Cryogenie, SPSMS/MDN, CEA-Grenoble, 38054 Grenoble, France.
A. Villaume, F. Bourdarot,* E. Hassinger, S. Raymond, V. Taufour, D. Aoki, and J. Flouquet

$J_{AF}(V) = 10 + 0.7(V - 52)$
$J_Q(V) = 10 - 0.7(V - 52)$

C.P., M. Norman, S. Burdin & A. Ferraz preprint

A. Villaume et al, PRB (2008)
Summary of this part

$\text{MSL} = \text{RVB} + \text{Modulations in the dual lattice}$
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\[ \text{MSL} = \text{RVB} + \text{Modulations in the dual lattice} \]

\[ \downarrow \]

Breaks Z4 symmetry: 2nd order phase transition instead of a cross-over
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\[ MSL = RVB + \text{Modulations in the dual lattice} \]

Breaks Z4 symmetry: 2nd order phase transition instead of a cross-over

It is a spin liquid, a gauge symmetry breaking: simple reason why it is "hidden" for so long
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MSL = RVB + Modulations in the dual lattice

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Striking similarity with AFM phase, same dispersions, same order of magnitude for entropy quenching
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- MSL is the RVB-parent of the AFM order
Summary of this part

MSL = RVB + Modulations in the dual lattice

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MSL is the RVB-parent of the AFM order

Delocalization transition at $T_0$: the spins are freed for $T > T_0$
Localization of the f-electrons
Extended Anderson lattice model

\[ H = \sum_{\langle i,j \rangle \sigma} \left( c_{i\sigma}^\dagger t_{ij} c_{j\sigma} + f_{i\sigma}^\dagger (\alpha t_{ij} + E_0 \delta_{ij}) \tilde{f}_{j\sigma} \right) \]

\[ + \sum_{i,\sigma} \left( V f_{i\sigma}^\dagger c_{i\sigma} + h.c. \right) + \sum_{\langle i,j \rangle} J \tilde{S}_{f,i} \cdot \tilde{S}_{f,j} \]

\[ + \sum_{i} U \tilde{n}_{f,i,\uparrow} \tilde{n}_{f,i,\downarrow} \]

tool U(1) slave boson formulation

Case of 3He bi-layers

\( (\tilde{f}, \tilde{f}^\dagger) \rightarrow \text{first layer} \)

\( (c, c^\dagger) \rightarrow \text{second layer} \)

\( \tilde{f}_{i\sigma} \rightarrow f_{i\sigma} b_{i}^\dagger \), \quad \tilde{f}_{i\sigma}^\dagger \rightarrow f_{i\sigma}^\dagger b_{i} \)

\( n_{f,i} + n_{b,i} = 1 \)

\((b, b^\dagger)\) are the holons in the impurity sites
**Kondo Breakdown Theory**

\[
H_{\text{Coulomb}} = U \sum_i n_f^{\uparrow} n_f^{\downarrow}
\]

\[
H_{\text{Kinetic}} = - \sum_{\langle ij \rangle} f_i^{\dagger} t_{ij} f_j
\]

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**Diagram**

- **T** vs. **x**
  - Spin liquid
  - Super conductor
  - Fermi liquid
  - Anti ferromagnet
  - Mott transition

- **T** vs. **V**
  - Spin liquid
  - Anti ferromagnet
  - Heavy Fermi liquid
  - Mott transition
  - Anderson lattice

**High Tc**

**Anderson lattice**
``Selective'' Mott transition ... around the Fermi surface of cuprates

Platé 05  Photo emission

Le Tacon 08  Raman scattering

Civelli 08  DMFT

Ferraz 08  2 loops RG
``Selective” Mott transition ... in heavy fermions f-electrons localize, conduction electrons itinerants

\[ V^* = 0.58 \]

De Leo, Civelli, Kotliar 07

Cluster-DMFT studies

\[ t_c = -0.15; t_f = -0.015 \]
\[ U = 0.25 \mu = 0.2 \]
\[ \beta = 2000 V = 0.05 \]

M.Ferrero, O. Parcollet, CP (10)
Entropic considerations

Ce : $4f^1$
- $S=1/2$, $L=3$
- Spin Orbit: $J = |L-S| = 5/2$
- AF singlets

Yb : $4f^{13}$
- $S=1/2$, $L=3$
- Spin Orbit: $J = |L+S| = 7/2$
- Spin Liquid

U : $5f^2$
- $S=1$, $L=3+2$
- Spin Orbit: $J = |L-S| = 4$
- Kondo screening

Cooper pairs
Entropic considerations

Ce : $4f^1$
S=1/2  L=3
Spin Orbit : $J=|L-S|=5/2$

Yb : $4f^{13}$
S=1/2  L=3
Spin Liquid

U : $5f^2$
S=1  L=3+2

S O : $J=|L+S|=7/2$

Ce : Yb : U :
\[ S=1/2 \quad L=3 \quad S=1/2 \quad L=3 \quad S=1 \quad L=3+2 \]

Spin Orbit : $J=|L-S|=5/2$

Spin Liquid

Kondo screening

Yang, Pines, Fisk, Thompson, 2008

AF singlets

Spin Liquid

Kondo screening

Cooper pairs

KB

RKKY quenching

Kondo quenching

T0

Spin liquid

heavy Fermi liquid

Fermi liquid

QCP

Local moments

Anomalies

(4p)_s = 0.35

Kondo liquid

Kondo screening

0.0
0.1
0.2
0.3
0.4

0.0
0.01
0.01
0.01
0.01

0.0
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0.01
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Fig. 2: Tentative phase diagram of the Kondo Breakdown QCP in the presence of magnetism. The third axis represented on this diagram is the axis of “frustration”. It can be any external parameter which competes with the AF long range order. When the frustration parameter is strong enough, AF disappears, revealing the Kondo Breakdown QCP. Within this 3D phase diagram, one observed a line of Kondo Breakdown QCPs, which are uncorrelated with the magnetic order. The crossing of the two critical lines of AF LRO and Kondo Breakdown is accidental. In the Kondo Breakdown theory, the compound YbRh$_2$Si$_2$ is situated at the crossings; CeRhIn$_5$ would be situated somewhere on the frustration axis, URu$_2$Si$_2$ would be deep in the heavy Fermi liquid phase (with a super-conducting instability at low temperatures) and CeCu$_{5.9}$Au$_{0.1}$ is located at the AF QCP of itinerant character. This phase diagram suggests that the Kondo Breakdown QCP is a generic feature of any heavy fermion phase diagram; it is a universal fixed point, of non magnetic character, whose influence on transport properties dominates other scattering mechanisms in the quantum critical regime. Note that another phase diagram has been proposed [48] where the crossing of the Kondo breakdown line and the AF line has a finite width.
Imaging the hybridization gap by STM

P. Aynajian et al, PNAS (2010)

Our interpretation: Imaging the **hybridization gap**!

KB prediction: **No spatial modulations**

( hole-like bands hybridize )
Conclusions

• MSL is a serious candidate for explaining the "Hidden Order Phase" of URu2Si2

• Few experimental tests and predictions:
  STM, no modulations in the hybridization
  Neutrons, harmonics of the (1,0,0)-resonance at (2,0,0)
  Recent torque-experiment shows breaking of tetragonal symmetry
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  - STM, no modulations in the hybridization
  - Neutrons, harmonics of the (1,0,0)-resonance at (2,0,0)
  - Recent torque-experiment shows breaking of tetragonal symmetry

\[ (1 - \frac{T}{T_H}) \]

\[ c = 1.93 \pm 0.41 \]
\[ c' = 0.31 \pm 0.06 \]

**FIG. 3:** R. Okazaki et al.

**U. Matsuda, Unpublished**