

# Reply to Comment by S. Friedemann *et al.* on “Zeeman-Driven Lifshitz Transition: A Model for the Experimentally Observed Fermi-Surface Reconstruction in YbRh<sub>2</sub>Si<sub>2</sub>”

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A reply to the comment by S. Friedemann *et al.* [arXiv:1207.0536] on our article [Phys. Rev. Lett. **106**, 137002 (2011), arXiv:1012.0303].

In the light of experimentally observed anomalies in the temperature–field phase diagram of the heavy-fermion metal YbRh<sub>2</sub>Si<sub>2</sub>, our Letter [1] proposed a Zeeman-driven narrow-band Lifshitz transition as an explanation which is alternative to the popular Kondo-breakdown scenario. This idea was qualitatively illustrated utilizing simple toy-model calculations for non-interacting electrons. The Comment by Friedemann *et al.* [2] argues that our ideas cannot apply to YbRh<sub>2</sub>Si<sub>2</sub> because of them contradicting experimental data. Below we provide a point-by-point reply in order to show that such contradictions do not exist.

First, we re-iterate [1] that various measurements on YbRh<sub>2</sub>Si<sub>2</sub> point to the existence of one or more small energy scales below the Kondo temperature, present even at the transition field  $B_c \approx 60$  mT: distinct crossovers at different temperatures below 0.5 K are seen in the thermal expansion, in  $\Gamma_{p,B}(T)$  [3, 4], the thermopower [5], and the thermal conductivity [6]. The existence of these crossover scales limits straightforward interpretations in terms of quantum criticality, and it partly motivated the proposal in Ref. 1.

Second, we note that, within the Lifshitz scenario, the small energy scale  $E_c \sim 5 \mu\text{eV}$  (or 50 mK) is actually *not* the total width of a narrow band, but the distance between the Fermi level and the bottom (or top) of the relevant band piece undergoing the Lifshitz transition, i.e., the depth of a Fermi pocket. The total width of the band piece may be much larger, and the resulting peak in the quasiparticle density of states (DOS) strongly asymmetric w.r.t. the Fermi level, see Fig. 1.

*A. Observability at elevated temperatures:* A central point of the scenario of Ref. 1 is that the properties for  $T \gg E_c$  are not that of the quantum critical regime of a Lifshitz transition, see Fig. 1 of Ref. 1. Instead, in this regime the Fermi pocket is “smeared”, and the Zeeman splitting of the narrow band piece leads to apparent non-Fermi liquid behavior and Schottky-like anomalies in thermodynamics. Nevertheless, in the Hall effect, a distinct crossover occurring at  $T_{\text{hall}} \propto B$  is still visible at temperatures  $T \gg E_c$ , as shown by explicit calculation in Fig. 3 of Ref. 1.

*B1. Entropy crisis:* This argument in Ref. 2 does not apply, as the energy scale  $E_c$  does not replace the Kondo

scale, but is an additional scale within the heavy-fermion band structure, as is clearly stated on pg. 2 of Ref. 1.

*B2/B3. Weight of the DOS peak:* The arguments in Ref. 2 aim at constraining the weight of the narrow band piece by a height (set by the specific heat coefficient  $\gamma$ ) and a width (set by  $E_c$ ). While such considerations are valid in principle, care is required: (i) Height: The narrow-band feature may well contribute a significant part of the  $T \rightarrow 0$   $\gamma$  value, which moreover is not known to good accuracy, because in our scenario it will only be attained below  $\approx 5$  mK. E.g.  $\gamma$  values of  $5 \text{ J/K}^2\text{mol}$  appear possible. (ii) Width: As noted above, the DOS peak can be strongly asymmetric w.r.t. the Fermi level, such that its width is much larger than  $E_c$  (Fig. 1), and only a fraction of the corresponding entropy is released at  $T = 50$  mK. Taken together, the weight estimate given in Ref. 2 can be off by an order of magnitude, and a weight corresponding to 1–2% of  $R \ln 2$  would be compatible with thermodynamic data.

The calculations in Ref. 1 were not intended to quantitatively match experiments (and hence did not take into account peak asymmetries etc.), and we believe that a detailed quantitative comparison is not appropriate at this stage, because correlation effects (e.g. the tendency towards ferromagnetism) are likely to significantly influence the results.

*C. Hall crossover:* Refs. [2, 7] interpret the evolution of the Hall coefficient in terms of a zero-temperature jump. This interpretation invokes an extrapolation to  $T = 0$ , which is problematic if small energy scales are present, see above. Also, sufficiently low temperatures have not been probed: At 20 mK, the crossover width is roughly 20 mT which is not small compared to  $B_c$ , i.e., even at the lowest investigated  $T$  the crossover is broad. In fact, Fig. 3d of Ref. 1 provided a proof of principle that a Lifshitz scenario can be consistent with the apparent linear-in- $T$  crossover width down to 20 mK (without jump at  $T = 0$ ), i.e., there is no inconsistency.

*D. Enhancement of specific heat:* Experimentally, the specific heat coefficient  $\gamma$  is large near  $B_c$  at the lowest  $T$ ; the claimed divergence is again based on a problematic  $T \rightarrow 0$  extrapolation. In our scenario, the large specific heat does *not* arise from the Lifshitz transition per se, but from the presence of the narrow piece of heavy-fermion

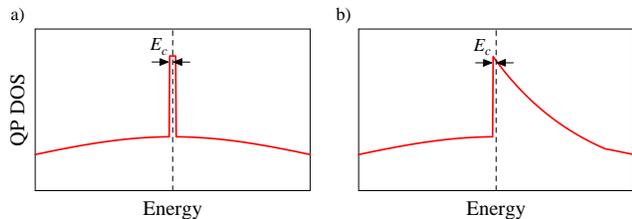


FIG. 1: Quasiparticle DOS (schematic), with a symmetric (a) or strongly asymmetric (b) narrow peak on top of the heavy-fermion background.  $E_c$  is the distance between the Fermi level (dashed) and the energy where the DOS strongly decreases (i.e. the bottom of the assumed weakly dispersing piece of band); in case (b) the effective width of the peak is much larger than  $E_c$ .

band which causes the peak in the quasiparticle DOS:  $\gamma$  keeps increasing upon lowering  $T$  until  $T$  becomes smaller than the energy scale on which the DOS varies – there is no inconsistency with experimental data for  $B \geq B_c$ .

In the narrow range  $B < B_c$  the detailed shape of the DOS peak becomes relevant, and an asymmetric peak could explain a decreasing  $\gamma$  upon lowering  $B$ . More importantly, the interplay with antiferromagnetism needs to be considered which is beyond the scope of Ref. 1.

We note that the weak singularities of a Lifshitz transition, alluded to in Ref. 2, will only be relevant at ultra-low temperatures (below 10 mK), see Fig. 1 of Ref. 1.

*E. Role of antiferromagnetism.* It is true that antiferromagnetism (AF) is not contained in the Lifshitz scenario, and is assumed to be secondary. We believe that

this assumption is not in contradiction to experiments. On the contrary: It has been shown that AF and the crossovers associated with the so-called  $T^*$  line [8] can be separated by doping [9]. This is most striking in recent data on  $\text{YbRh}_2\text{Si}_2$  with 5% Fe doping, where the  $T^*$  line signatures are seen disconnected from any AF transition [10]. A plausible idea would be that AF and the Lifshitz transition are two separate phenomena emerging from different portions of the Fermi surface.

In summary, we feel that the scenario of Ref. 1 continues to be viable candidate to explain salient features of the  $T - B$  phase diagram of  $\text{YbRh}_2\text{Si}_2$ . A more quantitative modeling needs to treat correlation effects beyond assuming effective quasiparticle band structures; initial work in this direction is in progress.

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- [1] A. Hackl and M. Vojta, Phys. Rev. Lett. **106**, 137002 (2011).
  - [2] S. Friedemann *et al.*, preceding comment, preprint arXiv:1207.0536.
  - [3] R. KÜchler *et al.*, Phys. Rev. Lett. **91**, 066405 (2003).
  - [4] Y. Tokiwa *et al.*, Phys. Rev. Lett. **102**, 066401 (2009).
  - [5] S. Hartmann *et al.*, Phys. Rev. Lett. **104**, 096401 (2010).
  - [6] H. Pfau *et al.*, Nature **484**, 493 (2012).
  - [7] S. Friedemann *et al.*, PNAS **107**, 14547 (2010).
  - [8] P. Gegenwart *et al.*, Science **315**, 969 (2007).
  - [9] S. Friedemann *et al.*, Nature Phys. **5**, 465 (2009).
  - [10] Y. Tokiwa and P. Gegenwart, unpublished results.