Extracting Kondo temperature of strongly-correlated systems from the inverse local magnetic susceptibility

A. A. Katanin

ARISING FROM X. Deng et al. Nature Communications https://doi.org/10.1038/s41467-019-10257-2 (2019)

The temperature scales of screening of local magnetic and orbital moments are important characteristics of strongly correlated substances. In a recent paper, Deng et al. using dynamic mean-field theory (DMFT) have identified temperature scales of the onset of screening in orbital and spin channels in some correlated metals from the deviation of temperature dependence of local susceptibility from the Curie law. We argue that the scales obtained this way are in fact much larger than the corresponding Kondo temperatures, and, therefore, do not characterize the screening process. By reanalyzing the results of this paper we find the characteristic (Kondo) temperatures for screening in the spin channel \( T_K = 100 \text{ K} \) for \( \text{V}_2\text{O}_3 \) and \( T_K \approx 350 \text{ K} \) for \( \text{Sr}_2\text{RuO}_4 \), which are almost an order of magnitude smaller than those for the onset of the screening estimated in the paper (1000 K and 2300 K, respectively); for \( \text{V}_2\text{O}_3 \) the obtained temperature scale \( T_K \) is therefore comparable to the temperature of completion of the screening, \( T^{\text{emp}} \approx 25 \text{ K} \), which shows that the screening in this material can be described in terms of a single temperature scale.

Deng et al. have performed a detailed analysis of the temperature dependence of orbital and magnetic local susceptibilities of two strongly correlated materials, \( \text{Sr}_2\text{RuO}_4 \) and \( \text{V}_2\text{O}_3 \) within DMFT. At high temperatures, the susceptibilities obey the Curie law, \( \chi(T) \sim 1/T \). The temperatures \( T^{\text{ons}} \) of the onset of screening of spin- and orbital local moments are obtained from the deviation of \( T\chi(T) \) from a constant value. Corresponding temperature scales \( T^{\text{ons}} \) are found to be much larger than the scales, corresponding to the completed screening (onset of the Fermi-liquid behavior) \( T^{\text{emp}} \approx 25 \text{ K} \).

In the following, we argue however that the temperatures \( T^{\text{ons}} \), obtained by the authors, do not correspond to the temperature scales of the spin screening. Indeed, instead of considering the quantity \( T\chi(T) \), we plot inverse spin susceptibility \( \chi^{-1}(T) \) for both considered compounds, \( \text{Sr}_2\text{RuO}_4 \) and \( \text{V}_2\text{O}_3 \) on the basis of the data of the paper (see Fig. 1). For \( \text{Sr}_2\text{RuO}_4 \) (see Fig. 1a) we do not find any peculiarity at the onset temperature \( T^{\text{ons}} = 2300 \text{ K} \) suggested by the authors. Instead, at all considered temperatures the local susceptibility follows the Curie–Weiss law:

\[
\chi(T) = \frac{C}{T + \theta}
\]

with a positive temperature \( \theta \approx 500 \text{K} \) (in agreement with the earlier result of ref. and experimental data). Following Wilson’s result for the local spin \( s = 1/2 \) Kondo problem, the temperature \( \theta \approx \sqrt{2}T_K \) yields the temperature scale of screening of the local moment (Kondo temperature) \( T_K \). Since the dependence \( \chi(T)/\chi(0) \) is almost universal for different values, the abovementioned relation between \( \theta \) and \( T_K \) is also expected to hold approximately for arbitrary local spin \( s \). Therefore, for \( \text{Sr}_2\text{RuO}_4 \) we find the temperature scale of spin screening \( T_K \approx 350 \text{ K} \), which is much smaller than \( T^{\text{ons}} \), obtained by the authors. We also note that very similar linear dependence of the inverse susceptibility is observed in the other Hund metals: \( \alpha \)-iron \( (T_K = 50 \text{ K} \) for density–density interaction and \( T_K = 320 \text{ K} \) for Kramers–Kronig interaction\)), \( \gamma \)-iron \( (T_K \approx 700 \text{ K} \)\), nickel \( (T_K \approx 850 \text{ K} \)\), etc.

For \( \text{V}_2\text{O}_3 \) the situation is more complex, since the inverse susceptibility shows at \( T \sim 600 \text{ K} \) a crossover (see Fig. 1b) from the Curie behavior \( (\theta \approx 0) \) to Curie–Weiss behavior with \( \theta \approx 150 \text{ K} \). This crossover, however, is likely not related to the screening, but reflects passing from a crossover regime to metallic one in the vicinity of Mott metal–insulator transition for this compound. To confirm this viewpoint, we present in the inset of Fig. 1b the temperature dependence of the inverse local spin susceptibility of the single-band half-filled Hubbard model on the square lattice with nearest-neighbor hopping \( t \) (on-site Coulomb repulsion \( U = 9t \) in the vicinity of Mott transition), showing that this dependence is qualitatively similar to the one, obtained for \( \text{V}_2\text{O}_3 \). Therefore, the screening scale of local magnetic moments in \( \text{V}_2\text{O}_3 \) is again given by the Kondo temperature \( T_K = \theta/\sqrt{2} \approx 100 \text{ K} \), extracted from the low-temperature part of the local susceptibility in
The inverse susceptibility, calculated from the data of ref. 1 for Sr$_2$RuO$_4$ is shown in the paramagnetic phase. The latter value is also much smaller than obtained by the authors and has the same order of magnitude as the temperature, at which the screening is completed, $T^{\text{cmp}} \sim 25$ K. This makes it reasonable to describe spin screening in V$_2$O$_3$ in terms of a single energy (or temperature) scale, as it should be for a screening process of a single impurity site, considered in DMFT. We note that rather large Weiss temperature in Sr$_2$RuO$_4$ and V$_2$O$_3$ (~200 K), observed experimentally in nuclear magnetic resonance studies, in the temperature range $T > 150$ K may be related to the impact of strong antiferromagnetic correlations on local susceptibility, which is absent in paramagnetic DMFT solution.

The observation that for V$_2$O$_3$ the Kondo temperature $T_K \sim T^{\text{cmp}}$ is in contrast to the above-described situation in Sr$_2$RuO$_4$, where $T_K \gg T^{\text{cmp}} \sim 25$ K. We note that such an inequality is also fulfilled for nickel$^{13}$, and in that case it was attributed to underscreened Kondo effect, since the Fermi level of nickel is close to the upper edge of the band. The origin of the strong difference between Kondo temperature and the temperature, corresponding to the completion of the screening in Sr$_2$RuO$_4$, requires further studies and clarification.

Data availability

The DMFT data for susceptibility of Sr$_2$RuO$_4$ and V$_2$O$_3$ analyzed here, are taken from ref. 1. The data on the single-band model are available within the present paper.

Received: 26 December 2019; Accepted: 7 September 2020; Published online: 04 March 2021

References

1. Deng, X. et al. Signatures of Mottness and Hundness in archetypal correlated metals. Nature Commun. 10, 2721 (2019).
2. Metzner, W. & Vollhardt, D. Correlated lattice fermions in $d = \infty$ dimensions. Phys. Rev. Lett. 62, 324 (1989).
3. Georges, A., Kotliar, G., Krauth, W. & Rozenberg, M. Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions. Rev. Mod. Phys. 68, 13 (1996).
4. Kotliar, G. & Vollhardt, D. Strongly correlated materials: insights from dynamical mean-field theory. Physics Today 57, 53 (2004).
5. Mravlje, J. & Georges, A. Thermopower and Entropy: Lessons from Sr$_2$RuO$_4$. Phys. Rev. Lett. 117, 036401 (2016).
6. Imai, T., Hunt, A. W., Thubner, K. R. & Chou, F. C. 17O NMR evidence for orbital dependent ferromagnetic correlations in Sr$_2$RuO$_4$. Phys. Rev. Lett. 81, 3006 (1998).
7. Wilson, K. R. The renormalization group: critical phenomena and the Kondo problem. Rev. Mod. Phys. 47, 773 (1975).
8. Mel’nikov, V. I. Thermodynamics of the Kondo problem. Soviet Phys. JETP Lett. 35, 511 (1982).
9. Tsvelick, A. M. & Wiegmann, P. B. Exact results in the theory of magnetic alloys. Adv. Phys. 32, 453 (1983).
10. Desgranges, H. U. Thermodynamics of the n-channel Kondo problem (numerical solution). J. Phys. C: Solid State Phys. 18, 5481 (1985).
11. Katanin, A. A. et al. Orbital-selective formation of local moments in α-iron: First-principles route to an effective model. Phys. Rev. B 81, 045117 (2010).
12. Igoshev, P. A., Efremov, A. V. & Katanin, A. A. Magnetic exchange in α-iron from ab initio calculations in the paramagnetic phase. Phys. Rev. B 91, 195123 (2015).
13. Hausoul, A. et al. Local magnetic moments in iron and nickel at ambient and Earth’s core conditions. Nat. Commun. 8, 16062 (2017).
14. Igoshev, P. A., Efremov, A. V., Poteryaev, A. I., Katanin, A. A. & Anisimov, V. I. Magnetic fluctuations and effective magnetic moments in γ-iron due to electronic structure peculiarities. Phys. Rev. B 88, 155120 (2013).
15. McWhan, D. B., Ment’ov, A., Remeika, J. P., Brinkman, F. & Rice, T. M. Metal-insulator transitions in pure and doped V$_2$O$_3$. Phys. Rev. B 7, 1920 (1973).
16. Poteryaev, A. I. et al. Enhanced crystal-field splitting and orbital-selective coherence induced by strong correlations in V$_2$O$_3$. Phys. Rev. B 76, 085127 (2007).
17. Hansmann, P. et al. Mott–Hubbard transition in V$_2$O$_3$ revisited. Phys. Status Solidi B 250, 1251 (2013).
18. Jones, E. D. Contributions to the V$_{51}$ nuclear magnetic resonance frequency shift and susceptibility in vanadium sesquioxide. Phys. Rev. 137, A978 (1965).
19. Rubinstein, M. Investigation of the metal-insulator transition in V$_2$O$_3$ by nuclear magnetic resonance. Phys. Rev. B 2, 4731 (1970).

Acknowledgements

The work is partly supported by the theme "Quant" AAAA-A18-118020190095-4 of Minobrnauki, Russian Federation.

Author contributions

A.K. is the sole author of this work and is responsible for the conception and design of the work.

Competing interests

The author declares no competing interests.

Additional information

Correspondence and requests for materials should be addressed to A.A.K.

Peer review information Nature Communications thanks the anonymous reviewer(s) for their contribution to the peer review of this work.

Reprints and permission information is available at http://www.nature.com/reprints

Publisher’s note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.