Hund's metals: Beyond the Mott-Hubbard *U-t* physics

1. Orbital selectivity in Hund's metals: The iron chalcogenides, N. Lanatà, H. U. R. Strand, G. Giovannetti, B. Hellsing, L. de' Medici, and M. Capone, Phys. Rev. B **87**, 045122 (2013).
2. Strong electronic correlations from Hund's coupling, A. Georges, L. de' Medici, and J. Mravlje, arXiv:1207.3033; to appear in Annu. Rev. Cond. Mat. Phys. **4** (2013).

Recommended with a Commentary by Atsushi Fujimori, University of Tokyo

Strong electron correlation in transition-metal compounds has often been discussed using the single-orbital model, in which the ratio between the on-site Coulomb interaction U and the hopping integral t is the controlling parameter. As for the metallic *versus* insulating behaviors, there is a critical U value $U_{crit} = W \propto t$ (W: one-electron bandwidth) below which the system becomes metallic. In the case of high-T_c cuprates, owing to the fortunate combination of the d^9 electronic configuration of Cu and the strong crystal field which lifts the orbital degeneracy, the single-orbital model is realistic and has been used extensively.

The multi-orbital nature of transition-metal compounds was paid serious attention particularly when manganites and ruthenates became active research topics. In manganites such as $La_{1-x}Ca_xMnO_3$, various types of orbital ordering have been observed and extensively studied, while in ruthenates such as $Sr_{2-x}Ca_xRuO_4$, orbital-selective Mott transitions have been proposed and strongly debated. Different metallic *versus* insulating behaviors of the multi-orbital systems from the single-orbital systems arise from Hund's coupling between d electrons, which changes the band gap of the Mott insulating phase and hence the critical U value [1]: (i) For the half-filled d shell with the d-electron number $n = 5$, the Mott gap magnitude increases from $U - W$ to $U + 4J - W$, where J is Hund's exchange coupling constant, and hence $U_{crit} = W - 4J$. The insulating state is therefore stabilized and the metallic region shrinks; (ii) For $n \leq 4$ or ≥ 6, the Mott gap is reduced from $U - W$ to $U - J - W$ and therefore $U_{crit} = W + J$. Then the metallic region expands.

In the case of $n \leq 4$ or ≥ 6, in the region $U_{crit} - J < U < U_{crit}$, i.e., $W < U < W + J$, the system is metallic owing to Hund's coupling. In the paramagnetic metallic state, there is strong Hund's correlation in which the spins of electrons on the same atom tend to align in the same direction. Then, a low-energy electron can hop from one atom to a neighboring atom only at the instant when both atoms have nearly parallel spins. This constraint is particularly strong for $n = 4$ or 6 and considerably reduces the coherence of the quasi-particle (QP) and hence the spectral weight Z of the QP [2,3]. While electron correlation generally *reduces* Z, Hund's correlation on the contrary *increases* Z from zero to a small but finite value ($<<1$) in the region $W < U < W + J$, where the system would be insulating ($Z = 0$) if J were zero. (According to DMFT calculations, the metallic regime extends well above the mean-field value $U \sim W + J$ [3].) That U region is referred to as a "Janus-faced" regime by the authors of the recommended papers, Lanatà *et al.* and Georges *et al*.

Lanatà *et al.* have studied electron correlation in Fe chalcogenide superconductors, where $n \sim 6$ and the QP is known to be highly incoherent among the Fe-based superconductors, by applying the Gutzwiller approximation to the realistic electronic structure calculated using first-principles methods. The results explicitly show that the Hund's metal scenario is realized: An incoherent metallic state survives for U a few times larger than the band width W when J is large. Interestingly, in the Janus-face regime, different orbitals differently renormalized, which may lead to orbital-selective Mott transitions or at least to orbital-dependent electron correlation. The d_{xy} orbital is shown to be most strongly correlated among the five d orbitals.

The strong electron correlation caused by Hund's coupling is confined within a small energy region of $\sim J$ from the Fermi level. That is, correlation effect would be moderate in the valence-band region of several eV, as recent theoretical studied have explicitly demonstrated [4,5]. Hund's correlation may open a pseudogap [4] and/or may even induce a non-Fermi-liquid behavior but only the vicinity of the Fermi level is affected [5]. The formation of an instantaneous local moment in the paramagnetic state is predicted by Hund's correlation, and has indeed been observed through the exchange splitting of core-level photoemission spectroscopy [6].

Incoherent metallic states due to Hund's correlation have also been discussed for the ruthenate $Sr_{1-x}Ca_xRuO_3$, which is known as a "bad metal", by de'Medici *et al*. [3] and by Georges *et al.* in the second recommended paper, in addition to the Fe pnictides and chalcogenides [2-5]. The entire d-band width of the ruthernates as probed by photoemission spectroscopy is not narrow compared to band-structure calculations although the effective mass deduced from electronic specific heat measurements is enhanced by a factor of $1/Z \sim 5$. The high-temperature paramagnetic metallic phase

of manganites such as overdoped $La_{1-x}Sr_xMnO_3$ is highly incoherent [1], which would be at least partly due to Hund's correlation. There are many intermetallic compounds such as MnSi and $Y_{1-x}Sc_xMn_2$ that show enhanced effective masses in thermodynamic measurements but no appreciable band narrowing in photoemission spectra [7]. We may therefore consider that Hund's correlation governs the properties not only of ferromagnetic metallic states, as has already been pointed out in the history of itinerant ferromagnetism [8], but also of paramagnetic metallic phases in a wide variety of transition-metal compounds.

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