Ghost Rotationally-Invariant Slave-Boson: An Efficient and Accurate Approach to Strongly Correlated Materials

Author: Tsung-Han Lee, National Chung Cheng University

Abstract:

The rotationally-invariant slave-boson (RISB) approach is a highly efficient method for simulating strongly correlated systems [1]. When combined with density functional theory (DFT+RISB), it becomes a powerful tool for studying strong correlation effects in materials [2,3]. However, despite its efficiency, the RISB method suffers from insufficient accuracy, leading to inaccurate descriptions of material properties, such as an overestimated effective mass of Sr_2RuO_4 [4] and a larger critical Coulomb interaction for Mott transitions [5].

In this talk, I will introduce a systematic way to enhance the accuracy of RISB by introducing auxiliary ghost orbitals, which we refer to as the ghost-rotationally-invariant slave-boson (g-RISB) method or equivalently ghost-Gutzwiller approximation [6]. I will first present examples of transition metal oxides where DFT+RISB necessitates the use of unrealistic Coulomb parameters, significantly deviating from first-principle calculated values, to reproduce the experimental observations [5]. Subsequently, I will demonstrate how DFT+g-RISB offers a systematic approach to improve the accuracy of DFT+RISB, enabling accurate descriptions of correlated materials with realistic Coulomb interactions [7,8]. Moreover, I will compare the accuracy and efficiency of g-RISB with the well-established dynamical mean-field theory (DMFT) and discuss the advantages and disadvantages of g-RISB over DMFT.

References:

[1] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, Phys. Rev. B 76, 155102 (2007)

[2] C. Piefke and F. Lechermann, physica status solidi (b) 248, 2269 (2011)

[3] Nicola Lanatà, Yongxin Yao, Cai-Zhuang Wang, Kai-Ming Ho, and Gabriel Kotliar, Phys. Rev. X 5, 011008 (2015)

[4] J. I. Facio, J. Mravlje, L. Pourovskii, P. S. Cornaglia, and V. Vildosola, Phys. Rev. B 98, 085121 (2018)

[5] Nicola Lanatà, Tsung-Han Lee, Yong-Xin Yao, Vladan Stevanović, Vladimir Dobrosavljević, npj Computational Materials 5 (1), 1-6 (2019)

[6] Nicola Lanatà, Tsung-Han Lee, Yong-Xin Yao, and Vladimir Dobrosavljević, Phys. Rev. B 96, 195126 (2017)

[7] Tsung-Han Lee, Nicola Lanatà, and Gabriel Kotliar, Phys. Rev. B 107, L121104 (2023)

[8] Tsung-Han Lee, Corey Melnick, Ran Adler, Nicola Lanatà, Gabriel Kotliar, arXiv:2305.11128 (2023)