

# Constrained RPA calculations of the Hubbard U

F. Aryasetiawan

*Graduate School of Advanced Integration Science, Chiba University  
1-33 Yayoi-cho, Inage-ku, Chiba-shi, Chiba, 263-8522 Japan*

Recent development in materials science has revealed rich properties of materials containing 3d and 4f elements, notably when the 3d or 4f shells are partially filled, leading to strong on-site correlations. The LDA often fails qualitatively in treating these systems and the GW approximation, while able to partly improve the LDA, is not expected to cure most of the problems. However, due to the large number of degrees of freedom, it is very hard to improve upon the GW approximation using conventional diagrammatic method in order to be able to treat systems with strong on-site correlations. On the other hand, model approaches have been rather successful in treating strongly correlated materials, albeit not from first-principles.

It is therefore highly desirable to be able to construct reliable model Hamiltonians where the input parameters are computed from first-principles, thus avoiding adjustable parameters which may lead to misleading results. Here we propose a constrained random-phase approximation (cRPA) scheme [1] that allows for a systematic down folding of high energy screening channels resulting in a low-energy model Hamiltonian with a screened Coulomb interaction or the Hubbard U corresponding to an effective interaction among electrons residing in isolated and partially filled narrow 3d or 4f bands crossing the Fermi level. The model Hamiltonian can then be solved by sophisticated approaches such as dynamical mean-field theory (DMFT) scheme. We have applied the cRPA method to the 3d transition metal series and to a couple of 4f systems (Ce, Gd) as well as a perovskite SrVO<sub>3</sub>. Comparison with the constrained LDA method will also be discussed.

[1] F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein, Phys. Rev. B 70, 195104 (2004)