

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

GW approach to degenerate systems¹ JOHANNES LISCHNER, JACK DESLIPPE, STEVEN G. LOUIE, UC Berkeley — Many-body perturbation theory based on the GW approximation to the electron self energy describes accurately in first-principles calculations the electronic (quasiparticle) excited states of solids, clusters and molecules. However, despite the multitude of important systems with degenerate ground states, ranging from open-shell atoms and molecules to magnetic defects in solids, the GW approach has been applied almost exclusively to closed-shell systems. In this talk, we discuss some of the problems with existing GW calculations for degenerate systems, such as spin contamination, the multiplet problem, and the proper definition of the Green function in open-shell systems. Different formulations to overcome these problems are explored.

¹This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility

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Date submitted: 18 Nov 2010

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