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G0W0 implementation using Lanczos algorithm and Sternheimer equation JONATHAN LAFLAMME JANSSEN, NICOLAS BERUBE, GABRIEL ANTONIUS, MICHEL COTE, University of Montreal — The G0W0 approach is an accurate method to give a physical meaning to the eigenvalues obtained in adensity-functional theory (DFT) calculation.However, the calculation of such corrections with plane wave codes is currently prohibitive for systems with more than a few hundreds of electrons. What limits calculations to this system size is the need in current implementations to invert the dielectric matrix and the need to carry out summations over conduction bands. This talk presents a strategy to avoid both of these bottlenecks. In traditional plane wave implementations of G0W0, the dielectric matrix is expressed in a plane wave basis, which needs to be relatively big to properly describe the matrix. Here, we will explain how a Lanczos basis can be generated to substantially reduce the size of the matrix. Also, the number of conduction bands needed to reach convergence in the summations is usually an order of magnitude larger than the number of valence bands. Here, the calculation of the conduction states is avoided by reformulating the summations into linear equation problems (Sternheimer equations), which also substantially reduces the computation time. Preliminary results will be presented.

Jonathan Laflamme Janssen
University of Montreal

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