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GW/Bethe-Salpeter calculations for charged and model systems from real-space DFT DAVID A. STRUBBE, Department of Physics, University of California, Merced — GW and Bethe-Salpeter (GW/BSE) calculations use mean-field input from density-functional theory (DFT) calculations to compute excited states of a condensed-matter system. Many parts of a GW/BSE calculation are efficiently performed in a plane-wave basis, and extensive effort has gone into optimizing and parallelizing plane-wave GW/BSE codes for large-scale computations. Most straightforwardly, plane-wave DFT can be used as a starting point, but real-space DFT is also an attractive starting point: it is systematically convergeable like plane waves, can take advantage of efficient domain parallelization for large systems, and is well suited physically for finite and especially charged systems. The flexibility of a real-space grid also allows convenient calculations on non-atomic model systems. I will discuss the interfacing of a real-space (TD)DFT code (Octopus, www.tddft.org/programs/octopus) with a plane-wave GW/BSE code (BerkeleyGW, www.berkeleygw.org), consider performance issues and accuracy, and present some applications to simple and paradigmatic systems that illuminate fundamental properties of these approximations in many-body perturbation theory.

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