Wannier function approach to electronic excitation spectra

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We present an efficient scheme for calculating the optical absorption spectra of condensed matter systems including electron hole interactions. A modern computational approach to photoexcitation consists of the following three steps. We first compute quasiparticle wavefunctions in the local density approximation of density functional theory. In the next step, the many-body correction in the GW approximation is added to quasiparticle energies. Although the GW band gap is quite accurate in many materials, the optical absorption spectrum from the independent quasiparticle picture deviates from experiments significantly. This is because electron-hole interaction plays a crucial role in photoexcited states. In the third step, we solve the Bethe-Salpeter equation (BSE) to include electron-hole interaction effects. The method has been established as a powerful tool for predicting optical properties. However, large computational cost limits applications to relatively small systems.

In the present work, we propose a Wannier interpolation scheme for BSE. The most time-consuming part in the BSE method is computation of the electron-hole interaction kernel on a fine k-point mesh. In our approach, we first compute the kernel on a coarse k-point mesh. The kernel is then transformed to the Wannier gauge in which the Wannier function is maximally localized. Since the kernel is smooth as a function of k in the Wannier gauge, it is accurately interpolated to a fine mesh. The interpolated kernel is transformed to the Hamiltonian gauge and put into the BSE. A similar interpolation technique is used also for the Berry connection to evaluate the optical transition matrix on a fine k mesh. We will discuss the detail of the scheme and present an application to silicon.