Finite-temperature Green's functions for electronic correlations in solids

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Applying wavefunction based methods to address electronic correlations in solids is an arduous task. Imaginary-time/frequency Green's functions offer a viable alternative competitive with the traditional quantum-chemical approach. Imaginary-time Green's functions are fundamentally advantageous as they simultaneously include the effects of both electronic correlations and finite temperature; the latter is attaied without an explicit calculation of the excited states. Also, a self-consistent finite-temperature Green's function provides a direct access to the thermodynamic properties and can be continued to real frequencies yielding one-electron spectra. Finally, Green's functions are particularly convenient to develop various embedding techniques allowing for a multilevel self-energy approximation.

Perturbative approximation of the self-energy to the second order in a self-consistent Green's function (GF2) leads to a qualitatively correct behavior in important situations when its wavefunction counterpart — MP2 — fails: disappearance of the band gap and emergence of strong correlations. In this work we implement periodic GF2 and apply it to realistic crystalline systems without resorting to model Hamiltonians. We also embark on exploring routes beyond GF2 to a higher-level treatment of electronic correlations in solids via non-perturbative evaluation of the local self-energy.