Finite temperature Green's function theories for periodic systems

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We perform periodic calculations with the Green's function second order (GF2) and GW method and discuss possible bottlenecks and remedies that can speed up these calculations. We evaluate momentum-resolved spectral functions and band gaps from bare and self-consistent second order perturbation theory for insulating periodic solids. We establish that, for systems with large gap sizes, both bare and self-consistent perturbation theory yield reasonable gaps. However, smaller gap sizes require a self-consistent adjustment of the propagator. In contrast to results obtained within a quasi-particle formalism used on top of bare second order perturbation theory, no unphysical behaviour of the band gap is observed. Our implementation of a fully self-consistent, -derivable and thermodynamically consistent finite temperature diagrammatic perturbation theory forms a framework on which embedding theories such as the dynamical mean field theory or self-energy embedding theories can be implemented.