Green's function approach to *ab initio* band structures

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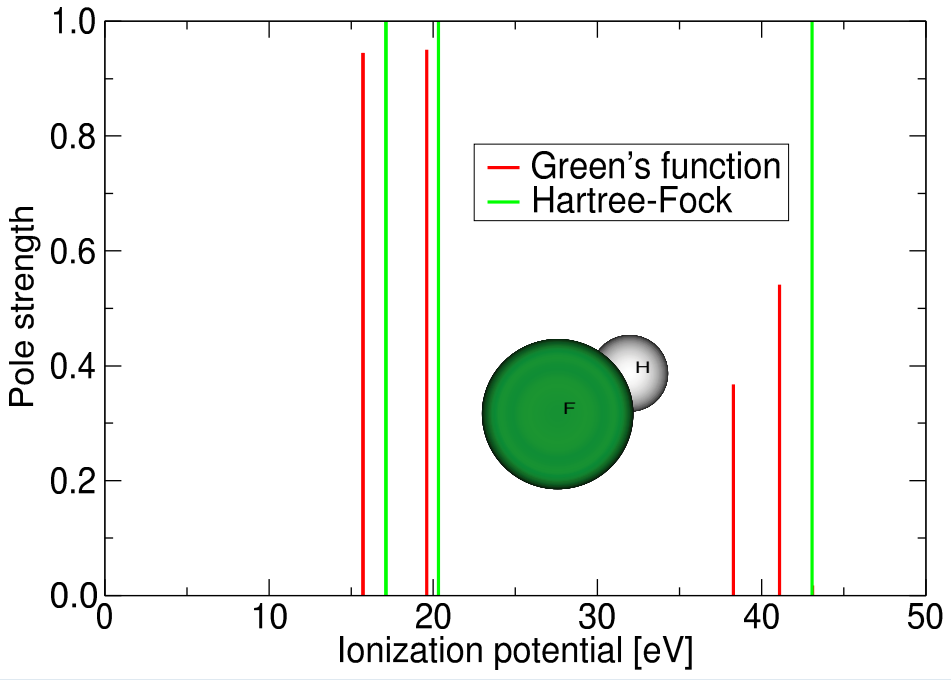
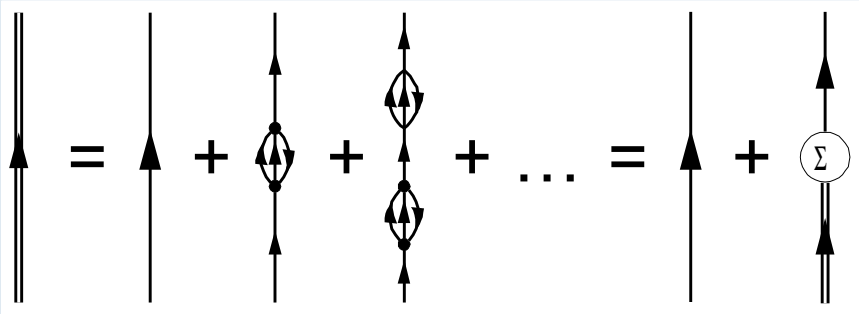
- There are many-body effects beyond the quasi-particle picture!



Crystal orbital algebraic diagrammatic construction

- One-particle Green's function
- Dyson equation



- *Intermediate* representation of $\mathbf{\Sigma}(\vec{k},\omega)$ in terms of Wannier orbitals
- Band structure from a Hermitian *eigenvalue problem*
- Configuration selection

Correlated band structures

- Band structure of
  - HF chains
  - LiF crystals
- Assessment of the perturbative treatment of off-diagonal Fock matrix elements