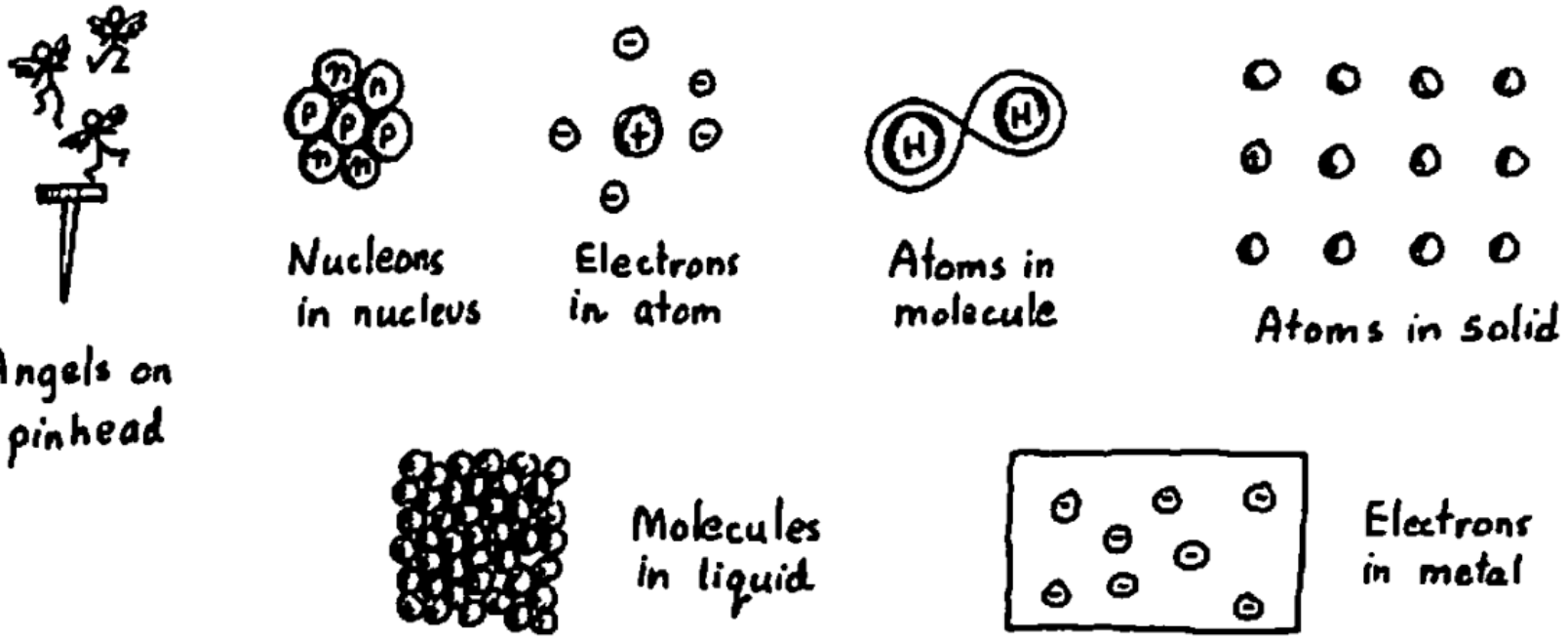
Finite-temperature Green's Function Methods for ab-initio Quantum Chemistry



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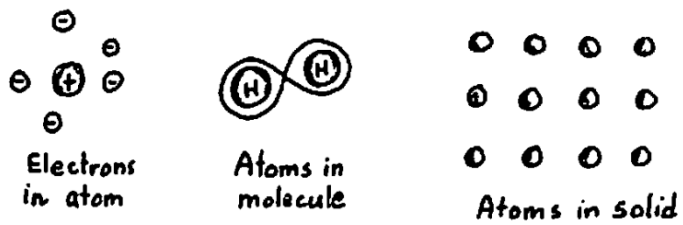
Electrons interaction is a **many-body problem**.

There are multiple bodies present.

There are interactions between the bodies.



We can't solve it **analytically** for real systems!

Strategies to deal with prohibitive computational cost

parallelism

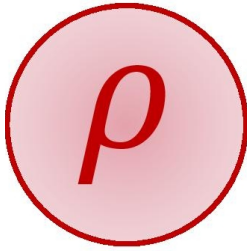
new theories & algorithms

Chemical theories with lower scaling such as DFT, low order perturbation theories.

Taking advantage of matrix sparsity for less storage/operations

Mattuck, Richard D. *A guide to Feynman diagrams in the many-body problem*. Courier Corporation, 1976.

Wavefunctions
Highly accurate
Unfavorable scaling



Density functional theory
Empirical parameters
Good scaling

Green's functions

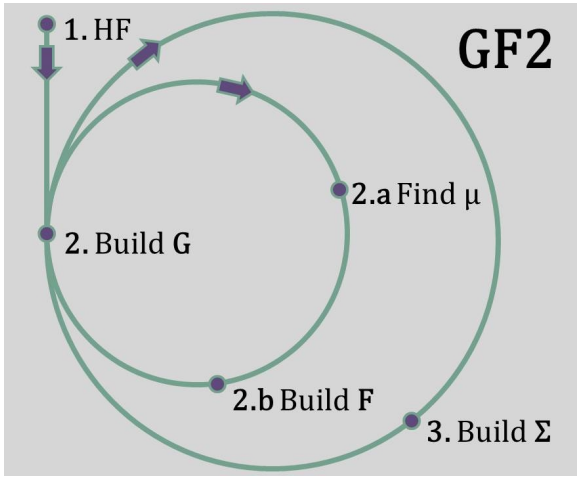
Controllable accuracy
Reasonable scaling
Temperature-dependent

Green's functions are not new in quantum chemistry, they were just more cumbersome than wavefunction methods or density functional theory.

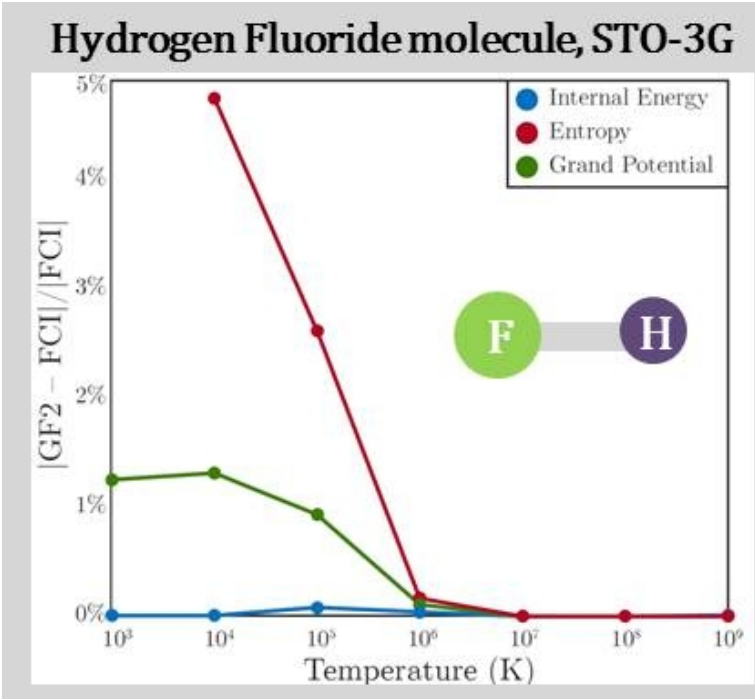
Advances in computing make Green's functions deserving of a resurgence.

My PhD work: Finite-temperature Green's function Methods for ab-initio Quantum Chemistry: Thermodynamics, Spectra, and Quantum Embedding

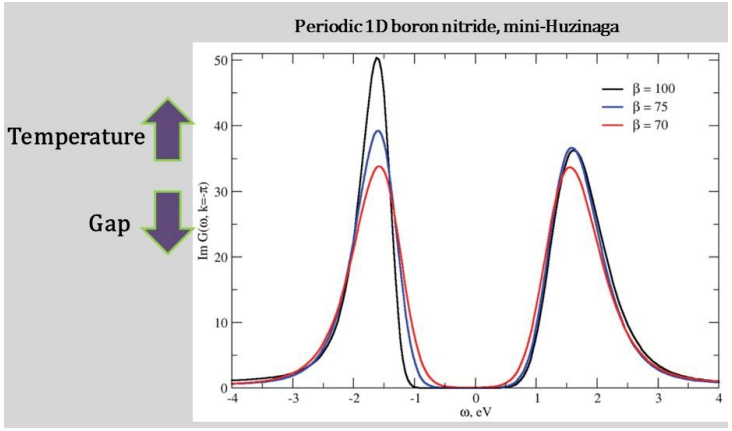
Second-Order perturbative Green's function



Electronic Thermodynamics



Spectra



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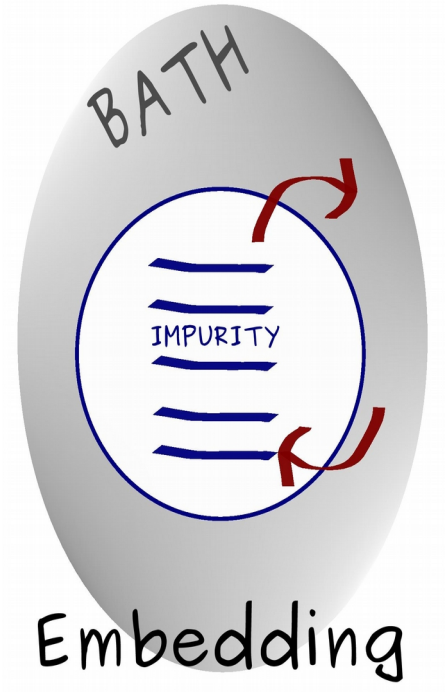
Quantum embedding partitions the system into two parts.

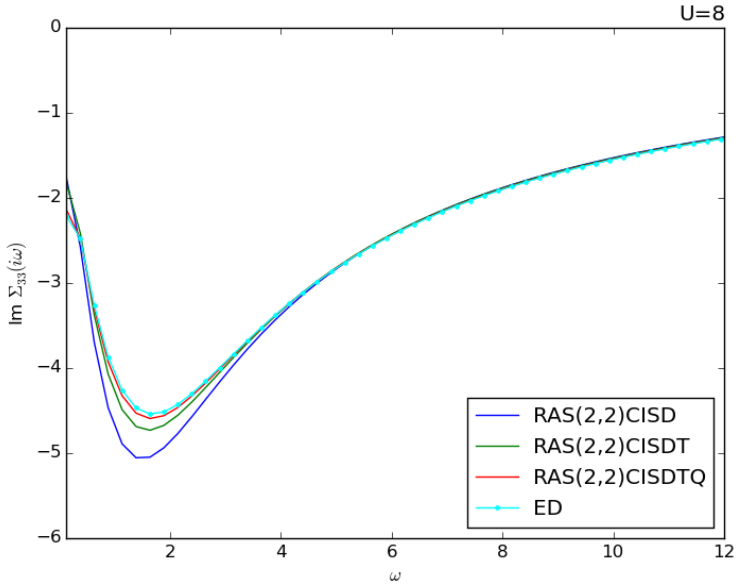
System

"Important" part
High-level method
Strong correlations

Environment

"less important" part
Low-level method
Weak correlations





Hubbard model
2D