Overview

Some important features of electronic structure methods:

- what is the Ansatz for the wavefunction?
- how are exchange and correlation treated?
- can static correlation/multireference problems be treated?
- is the method variational (i.e. is E always ≥ E_{true})?
- is the method size consistent (i.e. is the energy of two noninteracting systems the sum of the single systems?)
- can excited states be treated with the same method?
- what is the scaling of the method (i.e. how does the computational cost grow if I double the system size?)

Method	wavefunction	exchange	correlation	variational?	Size-consistentt?	multi-ref?	Excited states?	Scaling
HF	1 determinant	exact	none	yes	yes	no	no	N^2-N^4
MPn	contributions from excited determinants through perturbation	exact	some	no	yes	CAS-PT2	CAS-PT2	MP2 N^5 MP3 N^6 MP4 N^7
Truncated CI	selected determinants	exact	some	yes	no	no	yes	e.g. CISD N^6
CASSCF	selected dets determinants	exact	little	yes	no	yes	yes	exp, N_{act}*N_{det}^4
CC	contribution of selected excitations through infinite order	exact	some	no	yes	no	EOM-CC CC2	CCSD N^6 CCSD(T) N^7 CCSDT N^8 CCSDTQ N^{10}
Full CI	exact wf within basis set, linear combination of all possible excited determinants	exact	all	yes	yes	yes	yes	$N!/N_{el}!(N-N_{el})!$
Exact DFT	electron density	exact	exact	yes	yes	no	TDDFT	N
Orbital-free DFT	electron density	some	some	no	yes	no	TDDFT	N
KS-DFT	electron density	some	some	no	yes	no	TDDFT	N^2-N^3