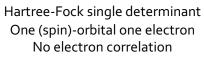
Electron Correlation Summary



$$\Psi_{\rm HF} = |\psi_1(1) \cdots \psi_n(n)|$$

$$\Psi_{\mathrm{MB}} = t_0 \Psi_{\mathrm{HF}} + \sum_{ia} t_i^a \Psi_i^a + \cdots$$

Introduce correlation with many-body wavefunction
Add excited state determinants to H-F ground state

Add a handful of excited configurations

Add all configurations of a given excitation

Add configurations of a given perturbation

MCSCF CASSCF

Variational
Not size-consistent
Good for describing static
correlation—bond breaking
Not so good for quantitative
energies

CISD
Full CI
Variational
Not size-consistent
Good for describing excited
states and spectroscopy
Not so good for quantitative
energies

CIS

MPn/MBPTn Coupled-cluster (CC..) Quadratic CI (QCI..) Size consistent Not variational

Good general purpose methods Excellent structures/energies for "normal" things