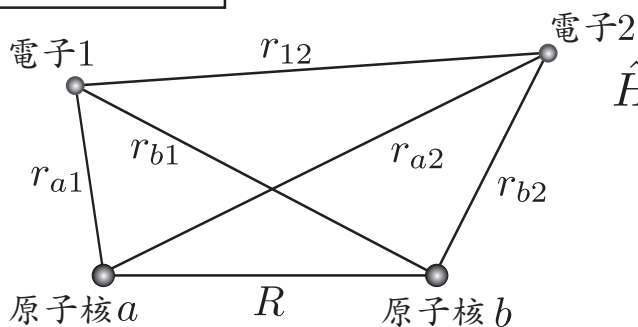


水素分子



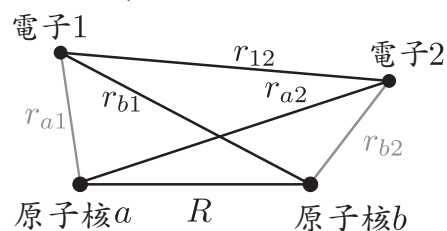
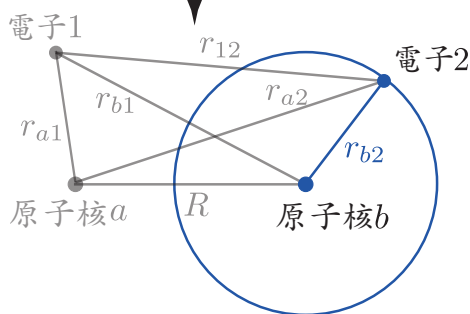
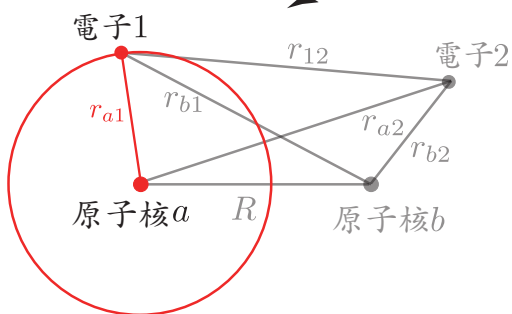
$$\hat{H} = -\frac{1}{2}\Delta_1 - \frac{1}{r_{a1}} - \frac{1}{2}\Delta_2 - \frac{1}{r_{b2}} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{r_{12}} + \frac{1}{R}$$

Valence Bond method

$$\hat{H} = \underbrace{-\frac{1}{2}\Delta_1 - \frac{1}{r_{a1}}}_{\hat{H}_a(1)} - \underbrace{\frac{1}{2}\Delta_2 - \frac{1}{r_{b2}}}_{\hat{H}_b(2)} - \underbrace{\frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{r_{12}} + \frac{1}{R}}_{\hat{H}'(1,2)}$$

$$= \hat{H}_a(1) + \hat{H}_b(2) + \hat{H}'(1,2)$$

摂動項



Molecular Orbital method

$$\hat{H} = \underbrace{-\frac{1}{2}\Delta_1 - \frac{1}{r_{a1}} - \frac{1}{r_{b1}} + \frac{1}{R}}_{\hat{H}_c(1)} - \underbrace{\frac{1}{2}\Delta_2 - \frac{1}{r_{a2}} - \frac{1}{r_{b2}} + \frac{1}{R}}_{\hat{H}_c(2)} + \underbrace{\frac{1}{r_{12}} - \frac{1}{R}}_{\hat{H}'(1,2)}$$

$$= \hat{H}_c(1) + \hat{H}_c(2) + \hat{H}'(1,2)$$

摂動項

