Hartree-Fock

$$\mathcal{E}^{HF}(\gamma) = \mathrm{Tr}\left(-\Delta\gamma - \frac{Z}{|x|}\gamma\right) + D[\rho_\gamma] - X(\gamma)$$

$$D[\rho_\gamma] = \frac{1}{2}\iint \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|}\,dx\,dy, \quad \rho_\gamma(x) = \gamma(x,x)$$

$$X(\gamma) = \frac{1}{2}\iint \frac{|\gamma(x,y)|^2}{|x-y|}\,dx\,dy$$

$$E^{HF}(N) = \inf_\gamma \{ \mathcal{E}^{HF}(\gamma) \mid 0 \le \gamma \le 1, \mathrm{Tr}\,\gamma = N \}$$

$$E^M \underset{\substack{\text{conjectured} \\ (N \ge 3)}}{\le} E^S \underset{\text{Lieb's variational principle}}{\le} E^{HF}$$

Müller

$$\mathcal{E}^M(\gamma) = \cdots + X(\gamma^{1/2})$$

Frank ~~et. al.~~ Lieb, Seiringer, Siedentop (2007)

$N \le Z \implies \exists$ minimizers

Ionization conjecture

Frank, Nam, van den Bosch (2016)

Kehle (2017)

$\exists$ minimizer $\implies N \le Z + C$

Ionization conjecture

$$\mathcal{E}(\gamma) = \mathrm{tr}\left(-\Delta\gamma - \frac{Z}{|x|}\gamma\right) + D[\rho_\gamma] \cancel{+} - X(\gamma^{p})$$

$$D[\rho_\gamma] = \frac{1}{2}\iint$$

$$\rho_\gamma(x) = \gamma(x,x)$$

$p \in \left[\frac{1}{2}, 1\right]$

$\cancel{p =}$ Müller $\left(p = \frac{1}{2}\right)$

Hartree-Fock $(p = 1)$

Kehle (2017)

$$N \leq Z + C$$

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Frank, Nam, van den Bosch (20~~17~~)

$$\mathcal{E}^{M} \leq E_S \leq \mathcal{E}^{HF}$$

conjectured ($N \geq 3$)