CHEM302
Introduction to Computational Chemistry

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“ψ … is an oracle” – C. J. Cramer

$$\hat{\mathcal{H}}\psi = E\psi$$

Molecular Hamiltonian

$$\hat{\mathcal{H}} = -\sum_i \frac{1}{2}\nabla_i^2 - \sum_k \frac{1}{2}\nabla_k^2 - \sum_i \sum_k \frac{Z_k}{r_{ik}} + \sum_{i<j} \frac{1}{r_{ij}} + \sum_{k<l} \frac{Z_k Z_l}{r_{kl}}$$

Variational Principle

Born-Oppenheimer Approximation

$$\Psi = \psi_1(1)\psi_2(2)...\psi_N(N)$$

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$$-\Psi = \mathrm{P}(\Psi)$$

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_1(1) & \chi_2(1) & \dots & \chi_N(1) \\ \chi_1(2) & \chi_2(2) & \dots & \chi_N(2) \\ \vdots & & \ddots & \vdots \\ \chi_1(N) & \chi_2(N) & \dots & \chi_N(N) \end{vmatrix}$$

Self-consistent field (SCF)