$$H_{\text{tot}}\Psi_{\text{tot}} = E_{\text{tot}}\Psi_{\text{tot}}$$

$$\Psi(\text{nuclei, electrons}) = \Psi(\text{nuclei})\Psi(\text{electrons})$$

Born-Oppenheimer approx.

Electrons at a fixed set of nuclei

$$E_{\text{tot}} = E(\text{nuclei}) + E(\text{electrons})$$

$$H_{\text{ele}}\Psi_{\text{ele}} = E_{\text{ele}}\Psi_{\text{ele}}$$

Separation of variables

Many-electron Hamiltonian

$$H_{\text{ele}} = H_1 + H_2 + \ldots + H_N$$

noninteracting electrons

Many-electron wave function

$$\Psi_{\text{ele}} = \chi_1(1)\chi_2(2)\ldots\chi_N(N)$$

does not satisfy antisymmetry and Pauli principles of electrons

Slater determinant

satisfies antisymmetry and Pauli principles

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