

# Nonrelativistic Schrödinger equation

$$\hat{H}\Psi(\{\underset{\text{e}}{r_i}\}, \{\underset{\text{+}}{R_I}\}) = E\Psi(\{\underset{\text{e}}{r_i}\}, \{\underset{\text{+}}{R_I}\})$$

Function of 3N coordinates of Nucleus and Electrons



nuclear Hamiltonian      electron-nuclear Hamiltonian

electronic Hamiltonian

$$\hat{H} = \underbrace{\sum_{a=1}^M \frac{-\hbar^2}{2M_a} \nabla_a^2}_{\text{Kinetic energy of nuclei } T_N(R)} + \underbrace{\sum_{a=1}^{M-1} \sum_{b=a+1}^M \frac{Z_a Z_b e^2}{R_{ab}}}_{\text{Repulsion of nuclei } V_{NN}(R)} - \underbrace{\sum_{a=1}^M \sum_{i=1}^N \frac{Z_a e^2}{r_{ai}}}_{\text{Attraction between nuclei and electrons } V_{eN}(r, R)} + \underbrace{\sum_{i=1}^N \frac{-\hbar^2}{2M_e} \nabla_i^2}_{\text{Kinetic energy of electrons } T_e(r)} + \underbrace{\sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{e^2}{r_{ij}}}_{\text{Repulsion of electrons } V_{ee}(r)}$$

Kinetic energy of nuclei  $T_N(R)$       Repulsion of nuclei  $V_{NN}(R)$

Attraction between nuclei and electrons  $V_{eN}(r, R)$

$$r_{ai} = |\mathbf{R}_a - \mathbf{r}_i|$$

Kinetic energy of electrons  $T_e(r)$       Repulsion of electrons  $V_{ee}(r)$

Recall,

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$$

$$V_N(R)$$

external potential on nuclei

$$V_e(r)$$

external potential on electrons

# Many Body Problems

**Yicheng Fang**



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