

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

$$\hat{H} = \sum_{a=1}^M \frac{-\hbar^2}{2M_a} \nabla_a^2 + \sum_{a=1}^{M-1} \sum_{b=a+1}^M \frac{Z_a Z_b e^2}{R_{ab}} - \sum_{a=1}^M \sum_{i=1}^N \frac{Z_a e^2}{r_{ai}} + \sum_{i=1}^N \frac{-\hbar^2}{2M_e} \nabla_i^2 + \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{e^2}{r_{ij}}$$

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

LL Leslie



Many Body Problems:

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