Nonrelativistic Schrödinger equation

$$\widehat{H}\Psi(\{r_i,\},\{R_I\}) = E\Psi(\{r_i\},\{R_I\})$$

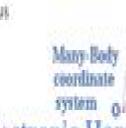
Function of 3N coordinates of Nucleus and Electrons







electron-nuclear Hamiltonian



R_a R_{be}

nuclear Hamiltonian

$$\left(\frac{-\hbar^2}{2M} \nabla_a^2 + \sum_{a=0}^{M-1} \sum_{b=0}^{M} \frac{Z_a Z_b e^2}{D} \right)$$

$$-\sum_{\alpha=1}^{M}\sum_{i=1}^{N}\frac{Z_{\alpha}}{i}$$

$$+ \sum_{i=1}^{N} \frac{-\hbar^{2}}{2M_{e}} \nabla_{i}^{2} + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{e^{2}}{r_{ij}}$$

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

Attraction between nuclei and electrons

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

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

external petential refectrons

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