

# 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  $V_{eN}(r, R)$

Kinetic energy of electrons  $T_e(r)$

Repulsion of electrons  $V_{ee}(r)$

Recall,

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

$V_{eN}(r, R)$

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

$V_N(R)$

external potential on nuclei

$V_e(r)$

external potential on electrons

# Many Body Problems

**Ilya Prigogine, Stuart A. Rice**



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## **Table of Contents Many Body Problems**

1. Understanding the eBook Many Body Problems
  - The Rise of Digital Reading Many Body Problems
  - Advantages of eBooks Over Traditional Books
2. Identifying Many Body Problems
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Many Body Problems
  - User-Friendly Interface
4. Exploring eBook Recommendations from Many Body Problems
  - Personalized Recommendations
  - Many Body Problems User Reviews and Ratings
  - Many Body Problems and Bestseller Lists
5. Accessing Many Body Problems Free and Paid eBooks
  - Many Body Problems Public Domain eBooks
  - Many Body Problems eBook Subscription Services

- Many Body Problems Budget-Friendly Options
- 6. Navigating Many Body Problems eBook Formats
  - ePub, PDF, MOBI, and More
  - Many Body Problems Compatibility with Devices
  - Many Body Problems Enhanced eBook Features
- 7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Many Body Problems
  - Highlighting and Note-Taking Many Body Problems
  - Interactive Elements Many Body Problems
- 8. Staying Engaged with Many Body Problems
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Many Body Problems
- 9. Balancing eBooks and Physical Books Many Body Problems
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Many Body Problems
- 10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
- 11. Cultivating a Reading Routine Many Body Problems
  - Setting Reading Goals Many Body Problems
  - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Many Body Problems
  - Fact-Checking eBook Content of Many Body Problems
  - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
  - Utilizing eBooks for Skill Development
  - Exploring Educational eBooks
- 14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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