Nonrelativistic Schrödinger equation

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

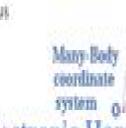
Function of 3N coordinates of Nucleus and Electrons







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

Many Body Problems

LL Leslie



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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
 - o 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
 - o 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

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