



# TwoBody.jl

Search docs (Ctrl + /)

## Home

- Install
- Usage
- API reference

## Hamiltonian

### Rayleigh-Ritz Method

### Finite Difference Method

### API reference

Run the following code before each use.

```
using TwoBody
```

Define the [Hamiltonian](#). This is an example for the non-relativistic Hamiltonian of hydrogen atom in atomic units:

$$\hat{H} = -\frac{1}{2}\nabla^2 - \frac{1}{r}$$

```
H = Hamiltonian(  
  NonRelativisticKinetic(ħ = 1, m = 1),  
  CoulombPotential(coefficient = -1),  
)
```

The usage depends on the method. Define the basis set for the [Rayleigh-Ritz Method](#):

$$\phi_1(r) = \exp(-13.00773 r^2),$$

$$\phi_2(r) = \exp(-1.962079 r^2),$$

$$\phi_3(r) = \exp(-0.444529 r^2),$$

$$\phi_4(r) = \exp(-0.1219492 r^2).$$

```
BS = BasisSet(  
  SimpleGaussianBasis(13.00773),  
  SimpleGaussianBasis(1.962079),  
  SimpleGaussianBasis(0.444529),  
  SimpleGaussianBasis(0.1219492),  
)
```

You should find

$$E_{b,1} = -0.499278 E_h,$$

which is amazingly good for only four basis functions according to [Thijssen\(2007\)](#). The exact ground-state energy is  $-0.5 E_h$ .

# Fewbody Problems

**Marcel A. Müller**



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## **Table of Contents Fewbody Problems**

1. Understanding the eBook Fewbody Problems
  - The Rise of Digital Reading Fewbody Problems
  - Advantages of eBooks Over Traditional Books
2. Identifying Fewbody 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 Fewbody Problems
  - User-Friendly Interface
4. Exploring eBook Recommendations from Fewbody Problems
  - Personalized Recommendations
  - Fewbody Problems User Reviews and Ratings
  - Fewbody Problems and Bestseller Lists
5. Accessing Fewbody Problems Free and Paid eBooks
  - Fewbody Problems Public Domain eBooks
  - Fewbody Problems eBook Subscription Services

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