



TwoBody.jl

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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

TD Snyder



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