计算物理作业7

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在尝试抵御 GPT 的诱惑!

1 题目 1: 单摆运动积分

1.1 题目描述

Write a code to numerically solves the motion of a simple pendulum using **Euler's method**, **midpoint method**, **RK4 method** and **Euler-trapezoidal method** (implement these methods by yourself). Plot the angle and total energy as a function of time. Explain the results.

1.2 程序描述

1.3 伪代码

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1.4 结果示例

2 题目 2: 径向薛定谔方程求解

2.1 题目描述

Write a code to numerically solve the radial Schrödinger equation for

$$\left[-\frac{1}{2}\nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad V(\mathbf{r}) = V(r)$$

- 1. $V(r) = \frac{1}{r}$ (hydrogen atom)
- 2. Considering the following potential:

$$V(r) = -\frac{Z_{\text{ion}}}{r} \operatorname{erf}\left(\frac{r}{\sqrt{2}r_{\text{loc}}}\right) + \exp\left[-\frac{1}{2}\left(\frac{r}{r_{\text{loc}}}\right)^{\frac{1}{2}}\right] \times \left[C_1 + C_2\left(\frac{r}{r_{\text{loc}}}\right)^2 + C_3\left(\frac{r}{r_{\text{loc}}}\right)^4 + C_4\left(\frac{r}{r_{\text{loc}}}\right)^6\right]$$

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where erf is the error function. And for Li, you could set:

•
$$Z_{\text{ion}} = 3$$

•
$$r_{\rm loc} = 0.4$$

- $C_1 = -14.0093922$
- $C_2 = 9.5099073$
- $C_3 = -1.7532723$
- $C_4 = 0.0834586$

Compute and plot the first three eigenstates. You could find more information about 'how to solve radial Schrödinger equation' and 'use of non-uniform grid (optional)' in the PPT.

Special Note: You may call any library functions for diagonalization.

2.2 程序描述

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2.4 结果示例