计算物理作业 5

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喜闻徐夫子体恤民情!

1　题目 1：五点公式

1.1　题目描述

Derive the five-point formula for the second-order derivative.

1.2　程序描述

1.3　伪代码

1.4　结果示例

2　题目 2：Romberg 积分

2.1　题目描述

Consider the function $f(x) = e^{-x^2}$ on the interval $[0, 1]$. Use at least four layers of Romberg integration to compute the integral of $f(x)$ over $[0, 1]$ and estimate the result's precision.

2.2　程序描述

2.3　伪代码

2.4　结果示例

3　题目 3：波函数 Gauss 积分

3.1　题目描述

The radial wave function of the 3s orbital is given by:

$$R_{3s}(r) = \frac{1}{9\sqrt{3}} \times \left(6 - 6\rho + \rho^2\right) \times Z^{3/2} \times e^{-\rho/2},$$

where:

- r: radius expressed in atomic units (1 Bohr radius = 52.9 pm),

- $e \approx 2.71828$,
- Z: effective nuclear charge for that atom,
- $\rho = \frac{2Zr}{n}$, where n is the principal quantum number (3 for the 3s orbital).

Compute the integral $\int_0^{40} |R_{3s}|^2 \, r^2 \, dr$ for a Si atom ($Z = 14$) using Simpson's rule with two different radial grids:

(1) **Equal spacing grids**:

$$r[i] = (i-1)h, \quad i = 1, \ldots, N$$

Try different values of N.

(2) **Non-uniform integration grid**: more finely spaced at small r than at large r:

$$r[i] = r_0(e^{t[i]} - 1), \quad t[i] = (i-1)h, \quad i = 1, \ldots, N$$

Typically, choose $r_0 = 0.0005$ a.u. (1 a.u. = 1 Bohr radius).

Discuss the efficiency of each approach and explain the reasons.

3.2 程序描述

3.3 伪代码

3.4 结果示例