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**University of Johannesburg**  
**PHY8X08: Computational Physics**  
**Exam 2022, Paper B**

**Examiner: Dr. R. Warmbier**  
**Moderator: Prof. Michael Chapwanya (UP)**  
**Time: 150 minutes**  
**Total Marks: 70**



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Please note:

- This is an individual assessment. University examination rules must be obeyed.
- Read all questions carefully.
- The paper has 3 pages including this cover page.
- In addition you are provided with a formula sheet.
- Check for completeness of the material.
- Hint: The marks for each question scale roughly with the effort required to answer. Avoid overly long answers.

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1. Answer the following short questions. [XX]

- (a) Define underflow and overflow in the context of number representation on the computer. Give an example when these can occur.

Devise an algorithm (list of steps or flowchart) to test for the under- and overflow of a computer. Present it in such a way, that it can be programmed unambiguously. (4)

- (b) Explain the following python snippet and its output. (3)

```
>>> xt = 1.e20; yt = -1.e20; zt = 1.
>>> (xt + yt) + zt
1.0
>>> xt + (yt + zt)
0.0
```

- (c) Explain the concept of compensated summation. Give an algorithm on how use it. (3)

- (d) Describe the idea of finite representation of a function  $f(x)$  on a regular grid in an interval  $[a, b]$ . How can we use finite differences to compute derivatives, and why would we use this approach? (3)

- (e) How is the particle number  $N(t)$  modelled for decay processes in the limit of small and large  $N$ ? Connect the two expressions mathematically. (3)

- (f) Explain the variance reduction method, defined as  $\int_a^b f(x)dx = \int_a^b [f(x) - g(x)]dx - \int_a^b g(x)dx$ . What is  $g(x)$ ? (2)

2. Assume that numbers  $x_c$  stored on a computer are related to the exact numbers  $x$  by  $x_c \simeq x(1 + \varepsilon_x)$ . [8]

- (a) Define and explain subtractive cancellation in words. (2)

- (b) Derive an expression for the error in  $c_c$  for  $c = b - a$ . (2)

- (c) For  $y = \sqrt{x^2 - \ell^2} - x$ , when is the error in  $y$  largest and why? (2)

- (d) Derive an expression for the error in  $c = \frac{a}{b}$  and discuss. (2)

3. For the first derivative central difference equation  $f'(x) = \frac{f(x+h)-f(x-h)}{h}$  do the following: [11]

- (a) Derive the above equation. (5)

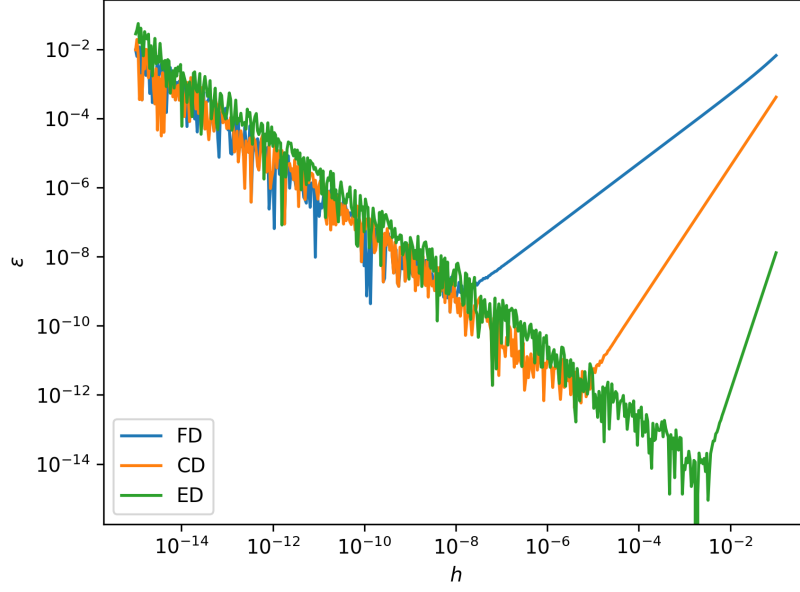
- (b) Give the expression for the total error  $\mathcal{E}$ . Justify or directly derive. (2)

- (c) Determine the optimal step size  $h_{opt}$  and the corresponding error  $\mathcal{E}(h_{opt})$ . (4)

4. The attached programme `numerical_derivatives.py` produces the figure below. [10]

- (a) Briefly describe the functionality of the code, including which quantities are plotted. Use the line numbers printed on the left to refer to specific lines of code. (4)

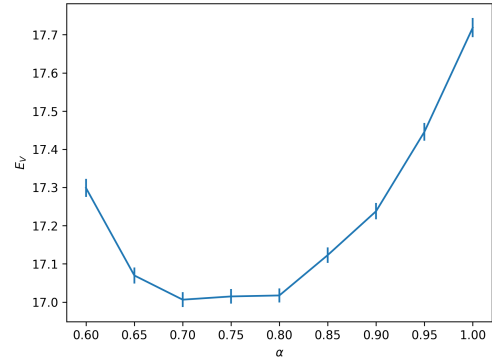
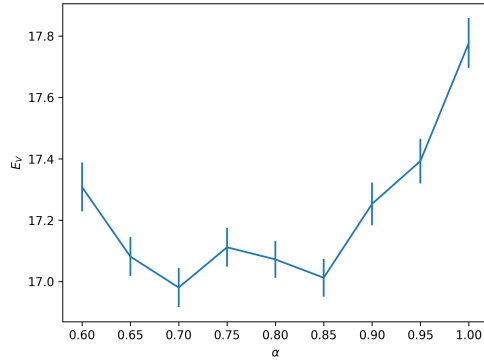
- (b) Give a detailed analysis and interpretation of the figure, including theoretical justifications of why we see what we see. (6)



5. Derive the condition number for a matrix problem  $\mathbf{A}\vec{x} = \vec{b}$  under the assumption that a perturbed matrix  $\mathbf{A} + \Delta\mathbf{A}$  will yield a perturbed solution vector  $\vec{x} + \Delta\vec{x}$ . [6]
6. Derive the approximation error of the mid-point version of rectangle rule  $\int_{x_i}^{x_{i+1}} f(x)dx \approx hf(x_i + \frac{h}{2})$ . Give expressions for both a single panel and the whole interval  $[a, b]$ . [6]
7. The Variational Monte-Carlo method can be used to solve high-dimensional eigenvalue problems, like an interacting  $n$  electron system with the Hamiltonian [11]

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{j=0}^{n-1} \nabla_j^2 + \frac{1}{2}m \sum_{j=0}^{n-1} \{\omega_x^2[(\vec{r}_j)_x]^2 + \omega_y^2[(\vec{r}_j)_y]^2 + \omega_z^2[(\vec{r}_j)_z]^2\} + g \sum_{\substack{j,k=0 \\ j < k}}^{n-1} \exp[-(\vec{r}_j - \vec{r}_k)^2].$$

- (a) Shortly describe how to use random numbers to evaluate the integral of a function. (2)
- (b) Make use of arguments, equations, and the python codes in `eloc.py` and `vmc.py` to explain how Variational Monto Carlo works and how we can use it to find an approximation for the ground-state solution of  $\hat{H}$ . 6
- (c) The below figures show the results of `vmc.py` for  $N_{\text{calc}} = 1000$  on the left and  $N_{\text{calc}} = 10000$  on the right. Discuss the results. [3]



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