B.Sc.(Hons.) Physics PHC401-32221401 Teacher: Mamta

# S.G.T.B. Khalsa College Mathematical Physics III (2021-22) Lab Assignment # 4 Gauss Hermite

Due Date and Time: 10.03.2022, 11:59PM Max. Marks : 25

## Note:

- Perform this assignment in groups of two. Please partner with a student in the same practical group (A1 or A2).
- Use the template for the cover page as first page in your assignment.
- Submit one pdf file that contains theory and discussion (either typed in Latex and converted to pdf or handwritten neatly on A4 size sheets and scanned), the source code and the output (containing the terminal output shoeing the input you have given, any table or graphs). Besides this pdf you are also required to submit any data file and the source code (.py file). Name all files as 2020PHYXXXX\_A5.pdf, 2020PHYXXXX\_A5.py, 2020PHYXXXX\_A5\_graphs.jpeg, etc. Here 'XXXX' are the last four digits of your class roll number.
- Also submit the modified integration module.
- The first line in your code should contain the following information as comment:
  - 1. Your Name and Roll No
  - 2. Your partner's name and Roll No
- Print your roll no as the first line in your output.

#### 1. Theory

[8]

- (a) Explain Hermite Gauss Quadrature method for integration. What kind of integrals are evaluated by this method?
- (b) Write down the Hermite differential equation and first five Hermite polynomials.
- (c) Write down the recursion formulae and orthogonality conditions for Hermite polynomials.
- (d) Explicitly derive the 2-point quadrature formula for this method.

### 2. Algorithm or Pseudocode

[2]

(a) Write the pseudocode/algorithm for a python function MyHermiteQuad(f, n) that approximates the integral  $\int_{-\infty}^{\infty} e^{-x^2} f(x) dx$  using n-point Gauss Hermite quadrature method.

### 3. Programming

[12]

- (a) Make the python functions MyHermiteQuad(f, n) to approximate the integral  $\int_{-\infty}^{\infty} e^{-x^2} f(x) dx$  using n-point Gauss Hermite quadrature method. You may use the inbuilt function numpy.polynomial.hermite.hermgauss or  $scipy.special.roots\_hermite$  for computing the points and weights. Add this function MyHermiteQuad to your integration module.
- (b) Write a python program named MyHermiteQuad to test above function and use it to
  - i. verify that n-point quadrature formula gives exact result when f(x) is a polynomial of order 2n-1 taking n=2 and n=4. Take these polynomial functions as input (do not define in your program).
  - ii. evaluate the following integrals:

$$(i) \quad I_1 \quad = \quad \int_{-\infty}^{\infty} \frac{e^{-x^2}}{1+x^2} \mathrm{d}x$$

$$(ii) \quad I_2 \quad = \quad \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{1+x^2}$$

Table 1: Values of  $I_1$  and  $I_2$  approximated by Gauss Hermite Quadrature with n-point formula.

n	$I_1$	$I_2$
2		
:	:	:
128	•	•

with n-point quadrature formula. Show your results for n=2, n=4, n=8, n=16, ..., n=128 and store the result in a tabulated format as shown below in a text file named quad-herm-xxxx.out where xxxx are the last four digits of your class roll no.

- (c) Explicitly show the computation using two-point quadrature on paper.
- (d) Now extend your code to compute the above integrals by Simpson method. Use the appropriate function from your module.
- (e) Show the output comparing the two methods. (Think of the ways to compare )

# 4. Discussion

Interpret and discuss your results and graphs.

[3]