Assignment 2 Marking Scheme (Content/104*80 + Presentation/40*10 + Formality/10*10)

Problem: Compute the first order correction to energy of the state, for three different perturbed potential.

Objective:
- Compare Trapezoidal, Simpson and Guass-Legendre methods, and understand their limits
- Investigate relative efficiency between different methods, in terms of fractional error
- Investigate the effect of scaling x, such as step size choice and integration range
- Implement Romberg's Method, and explore it for different tolerance value

Part A) Comparing Trapezoidal, Simpson and Guass-Legendre (*total 116pt: 80 for content & 36 for presentation)*

A1) Data: *81pt (45 for content & 36pt for presentation)*

1. Tables *9pt*

OptionA

delta E1 vs N	**lambda=L**	**lambda=10^-2 L**	**lambda=10^-4 L**
deltaV1	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*
deltaV2	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*
deltaV3	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*

delta E13 vs N	**lambda=L**	**lambda=10^-2 L**	**lambda=10^-4 L**
deltaV1	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*
deltaV2	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*
deltaV3	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*	- Trapezoidal, Simpson, GL *0.5pt*

OptionB

delta E1 vs N	Trapezoidal	Simpson	G-L
deltaV1	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*
deltaV2	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*
deltaV3	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*

delta E13 vs N	Trapezoidal	Simpson	G-L
deltaV1	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*
deltaV2	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*
deltaV3	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*	- L, 10^-2 L, 10^-4 L *0.5pt*

2. Plots *72pt*
OptionA

delta E1 vs N	lambda=L	lambda=10^-2 L	lambda=10^-4 L
deltaV1	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*
deltaV2	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*
deltaV3	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*

delta E13 vs N	lambda=L	lambda=10^-2 L	lambda=10^-4 L
deltaV1	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*
deltaV2	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*
deltaV3	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*	- Trapezoidal, Simpson, GL *4pt*

OptionB

delta E1 vs N	Trapezoidal	Simpson	G-L
deltaV1	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*
deltaV2	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*
deltaV3	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*

delta E13 vs N	Trapezoidal	Simpson	G-L
deltaV1	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*
deltaV2	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*
deltaV3	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*	- L, 10^-2 L, 10^-4 L *4pt*

Note: 2 out of 4 for content(-1 if N is not large enough to show convergence); 2 out of 4 for presentation

A2) Discussion: *35pt*
1) Compare the performance of the three methods, *5pt*
2) and explain in terms of the feature of the three methods 3**5pt*
3) Compare the performance in the case of the three lambda values, *5pt*
4) explain in terms of the function shape, *5pt*
5) Identify the shape of different perturbation, and how it affects the computation *5pt*

(Bonus: 5*pt*)
1) Investigating the fractional error of the three approximation methods, and relating the order of fractional error to the slope of fractional error vs number of points *5pt*

B) Romberg's Method (*total* 28*pt : 24pt for content & 4pt for presentation*)

B1) Data: *8pt (4pt for content & 4pt for presentation)*

1. Table/Plots *8pt*

OptionA

tolerance vs iteration#	E1	E13
	deltaV1 & delta V2 *4pt*	deltaV1 & delta V2 *4pt*

OptionB

tolerance vs iteration#	deltaV1	deltaV2
	E1 & E13 *4pt*	E1 & E13 *4pt*

Note:
1) 2 out of 4 for content (-1pt if only one value of lambda is used) ; 2 out of 4 for presentation

B2) Discussion: *20pt*
1) Identify the relation between tolerance and number of iteration *5pt*
2) and explain the relation *5pt*
3) Compare the number of iterations needed for different perturbation function, *5pt*
4) and explain the relation *5pt*

Formality

Mark (Max 10)	Description
0	Problem not stated, content and graphs unorganized, hard to follow the flow of content
2.5	Problem poorly stated with many missing details, content not organized, graphs shown in messy order
5	Problem stated with some missing details, content roughly organized, graphs shown in order but far from the related content
7.5	Problem briefly stated, content moderately organized, graphs shown around the discussion/comment
10	Problem clealy stated, content well organized, graphs presented in an organized and reader-friendly form

Remark:
Content
- Please read the question carefully, and ask if anything is unclear. (Only one student in the class tabulate the result for part A)
- Please comment and explain as much as you can, regarding the content of the assignment, on the observations you have made
- Visualizing the shape of function is important. The step size needed should be foreseeable from the scaling factor lambda.

Presentation
- Please have the plots clearly labelled, including the scale of it. If you need to correct something, you can always do it by hand.

Formality
- Stating your methods would help showing your understanding or help us identifying the problem if any of the plots does not look right.
- Grouping the related graphs together and putting them side by side would make it easier to compare.