# Solving Quantum Systems Using Numerical Methods

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***Abstract* — This report presents an investigation of the use of numerical methods to solve quantum systems. The extended trapezoidal and extended Simpson's rules, as well as Monte Carlo methods were used to estimate the probability of finding a particle within some space, in a 1 or 3-dimensional simple harmonic oscillator (SHO) potential. The probability of finding a particle in the ground state of a 1D SHO potential in the range $x \in [0,\ 2\sqrt{\hbar/m\omega}\ ]$ was estimated at 0.49766108 and 0.49766113 with the extended Trapezoidal and Simpson's rules respectively, at a relative accuracy of $\varepsilon = 10^{-6}$, as well as at 0.49676611359 and 0.4976611343 using Monte Carlo integration with uniform and importance sampling respectively, at a relative standard error of $\varepsilon = 10^{-4}$. For the 3D ground state of a SHO potential, the probability of a particle within the same range in each dimension was estimated at 0.123214 and 0.123247 using the Trapezoidal and Simpson's rules, and at 0.1232546 and 0.123258 with uniform and importance sampling Monte Carlo methods respectively, at $\varepsilon = 10^{-3}$. Moreover, for a state with one unit of orbital angular momentum in 3D, the probability of the particle being in the same volume was estimated at 0.118089, 0.118129, 0.118144 and 0.118108 with the methods in the order above, at $\varepsilon = 10^{-3}$. Finally, the methods and the code written for them were validated to ensure they work correctly, handle edge cases, and that errors and sampling follow expected trends.**

## I. Introduction

In quantum mechanics, as well as in other areas of physics, various quantities cannot be calculated through analytical methods. Hence, oftentimes, numerical methods can be used instead, enabling to estimate values without requiring a closed-form expression. This is one of the great advantages of numerical methods, enabling us to obtain solutions regardless of the mathematical form of the problem at hand.

Since numerical methods can only approximate a solution, they are usually stated at a specific tolerance – until a given criterion of relative error or accuracy is satisfied. This level of tolerance informs us about the ability of a method to converge to some value, but does not necessarily indicate its accuracy, which needs to be taken into consideration. Since various numerical methods exist, each with different advantages of error, time and space complexity, they can be compared to obtain a better indication of an estimated quantity.

As a result, three different numerical methods were coded and used for this investigation, estimating the probability of finding a particle in some space, described by a wavefunction that cannot be integrated analytically. These are: the extended trapezoidal rule, the extended Simpson's rule, and Monte Carlo integration with uniform and importance sampling. The first two belong in the 'Newton-Cotes' group of numerical methods, named after Isaac Newton and Roger Cotes, while Monte Carlo integration is based on a non-deterministic approach that uses random numbers and the Law of large numbers to obtain an estimate of a definite integral with an associated error. All three methods used were compared and validated to ensure they work correctly.

## II. Theory

### A. Quantum System in 1D

In the first part of this investigation, a particle was considered in the 1D ground state of a simple harmonic oscillator (SHO) potential. The 1D ground state wavefunction is given by:

$$\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-m\omega x^2/2\hbar}, \qquad (1)[1]$$

where m: mass of the particle, ω: natural angular frequency of the oscillator. As for any wavefunction, the probability of the particle being found within $x \in [x_1, x_2]$ is given by the integral of the magnitude squared of the wavefunction, as follows:

$$P = \int_{x_1}^{x_2} |\psi(x)|^2\, dx, \qquad (2)$$

which for Eqn. (1) can be re-written as:

$$P = \int_0^{2\sqrt{\hbar/m\omega}} \left| \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-m\omega x^2/2\hbar} \right|^2 dx. \qquad (3)$$

By inspection, it is evident that the following substitution of a scaled, dimensionless position variable:

$$u = \frac{m\omega}{2\hbar}x, \qquad (4)$$

followed by a substitution with a dummy variable $x = u$, enables to transform Eqn. (3) into Eqn. (5):

$$P_{ground\ state,1D} = \frac{1}{\sqrt{\pi}} \int_0^2 e^{-x^2}\, dx, \qquad (5)$$

executing nondimensionalisation of the integral, and utilising units which are more sensible – avoiding very small numbers for which computer rounding errors have a larger effect.

### B. Quantum System in 3D

In the last part of the investigation, the 3D ground-state and 3D state with one unit of orbital angular momentum were considered. In 3D, the ground state wavefunction of a particle in a SHO potential is given by:

$$\Psi_0(x, y, z) = \psi_0(x)\psi_0(y)\psi_0(z), \qquad (6)[1]$$

where $\psi_0$ is described by Eqn. (1). As a result, the probability of finding a particle bounded by $[0,\ 2\sqrt{\hbar/m\omega}\ ]$ in each dimension, and expressing it in scaled, dimensionless units as shown above, is given by:

$$P_{ground\ state,3D} = \left(\frac{1}{\sqrt{\pi}}\right)^3 \int_0^2 \int_0^2 \int_0^2 e^{-(x^2+y^2+z^2)}\, dxdydz\,. \qquad (7)$$

Finally, the 3D state with one unit of orbital angular momentum can be expressed as a combination of 1D ground states and first excited states as such:

$$\Psi_1(x) = \frac{1}{\sqrt{2}}[\psi_1(x)\psi_0(y) + i\psi_0(x)\psi_1(y)]\psi_0(z), \quad (8)[1]$$

where $\psi_1(x)$ is the 1D first excited state, given by:

$$\psi_1(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}}\, x\, e^{-m\omega x^2/2\hbar}. \quad (9)[1]$$

Combining the states together, and taking the magnitude squared of Eqn. (8) while using scaled, dimensionless variables, results in the probability below:

$$P_{1,3D} = \left(\frac{1}{\pi}\right)^{3/2} \int_0^2 \int_0^2 \int_0^2 (x^2 + y^2) e^{-(x^2+y^2+z^2)}\, dxdydz, \quad (10)$$

for the same boundaries in each dimension as used before.

## III. Numerical Methods

For this investigation, 3 main numerical methods were used, that can be placed into two categories: Newton-Cotes and Monte Carlo methods.

### A. Newton-Cotes Methods

Newton-Cotes is a family of numerical methods that use equally spaced points to estimate an integral. Two such methods that were used are the extended trapezoidal rule and the extended Simpson's rule.

#### 1. 1-Dimension:

##### a) Extended Trapezoidal Rule

The extended trapezoidal rule estimates a definite integral between $a$ and $b$, by splitting it into $N$ samples with a step size of $h = \frac{b-a}{N}$, and evaluates the area of $N-1$ trapeziums all of base $h$ and heights given by $f(x_i)$ and $f(x_{i+1})$, where $i$ goes from $0$ *to* $N-1$. This assumes linear interpolation between samples, introducing an error to an estimate of order $O\left(h^3 \frac{d^2 f}{dx^2}\right)$ [2].

This method was implemented by following the steps outlined in the '*Computational Physics Course Notes Week 3*', page 36 [2], to estimate an integral to a specified relative accuracy:

$$\varepsilon = \left|\frac{int_{i+1} - int_i}{int_i}\right|, \quad (11)$$

where $int_i$ represents the i[th] estimate of the integral. Detailed explanations of the method can be found in main.py, lines: 37 to 104. The sampling strategy of this algorithm avoids re-generating the same samples, by only introducing midpoint values in each next iteration, allowing to obtain the next estimate using the iterative relation below:

$$T_{j+1} = \frac{1}{2}T_j + \frac{1}{2}h_j \sum_{i=1}^{2^{j-1}} f\left(x_0 + \frac{2i-1}{2}h_j\right), \quad (12)[2]$$

where $h$ is decreased, by a factor of 2, in each iteration.

##### b) Extended Simpson's Rule

Simpson's rule is similar to the trapezoidal rule, however, it is a 3-point rule, performing quadratic interpolation between points, and designed in such a way that error terms of order $h^3$ and $h^4$ from the trapezoidal rule cancel out. As a result, it can be implemented by combining and weighing accordingly iterations of the trapezoidal rule as such:

$$S_j = \frac{4}{3}T_{j+1} - \frac{1}{3}T_j, \quad (13)[2]$$

with a much smaller error term of order $O\left(h^5 \frac{d^4 f}{dx^4}\right)$ [2].

#### 2. 3-Dimensions

The extended trapezoidal and Simpson's rules were extended to 3D, in the same way that 3D integrals are solved analytically. A 3D integral of the form:

$$\int_a^b \int_c^d \int_e^f f(x,y,z)\, dzdydx,$$

can be broken-down into 3 1D-integrals as such:

$$g(x,y) = \int_e^f f(x,y,z)\, dz$$

$$h(x) = \int_c^d g(x,y)\, dy$$

$$\int_a^b \int_c^d \int_e^f f(x,y,z)\, dzdydx = \int_a^b h(x)\, dx,$$

where each 1D integral is solved with the Newton-Cotes methods as described in section **III.A.1.a**. This was implemented with 3 recursive calls of the 1D method, shown in main.py lines 107 to 138. In effect, the 3D ground state integral was solved by stacking 2D planes for fixed z-values, as shown in Figure 1.

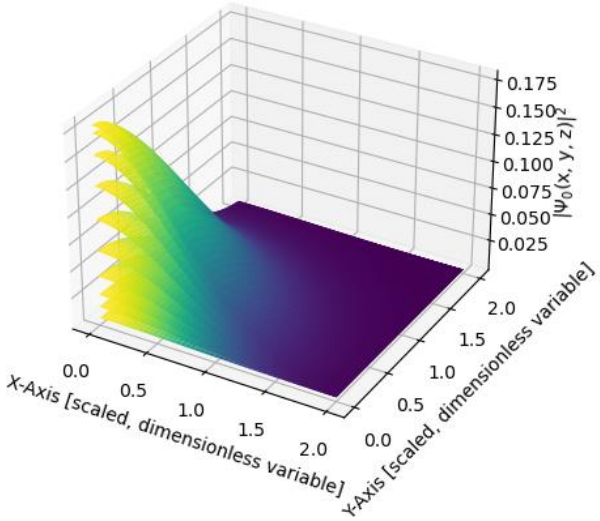


Fig. 1. 3D ground state PDF in SHO potential for fixed z-values, $z \in [0,1,\ldots,10]$. Adding stacked planes in 2D for fixed z-values gives an estimate of the 3D integral – where 2D planes are estimated in the same manner by adding 1D functions.

### B. *Monte Carlo Integration*

Monte Carlo integration follows the Law of large numbers, to estimate an integral by taking $N$ random points within the integral volume to obtain the mean of the function $f(\vec{x})$:

$$I = \frac{1}{N}\sum_{i=1}^{N} Q(\vec{x}_i) \pm \frac{1}{\sqrt{N}}\sigma_{Q_i}, \qquad (14)[2]$$

where $Q(\vec{x}) = f(\vec{x})/P(\vec{x})$, $P(\vec{x})$ is the sampling PDF, and $\sigma_{Q_i}$ is given by:

$$\sigma_{Q_i}^2 = \frac{1}{N-1}\sum_{i=1}^{N}(Q(\vec{x}_i) - \langle Q\rangle)^2. \qquad (15)[2]$$

A typical option is to use uniform sampling, where:

$$P(x)dx = \begin{cases} dx & 0 \le x < 1 \\ 0 & otherwise \end{cases}. \qquad (16)$$

However, oftentimes functions are much more concentrated in specific areas of the domain, in which case importance sampling can be used, sampling more points from where the function is more concentrated – resulting in a faster convergence, as the variance of sampling, $\sigma_{Q_i}^2$, is reduced.

In this investigation, both uniform and importance sampling were used and compared. For importance sampling, this normalised, linear PDF, obtained with the transformation method, was used:

$$P(\vec{x}) = -\vec{x} + 1.5, \qquad (17)$$

as all the wavefunctions of interest follow the shape shown in Figure 2 in all dimensions.

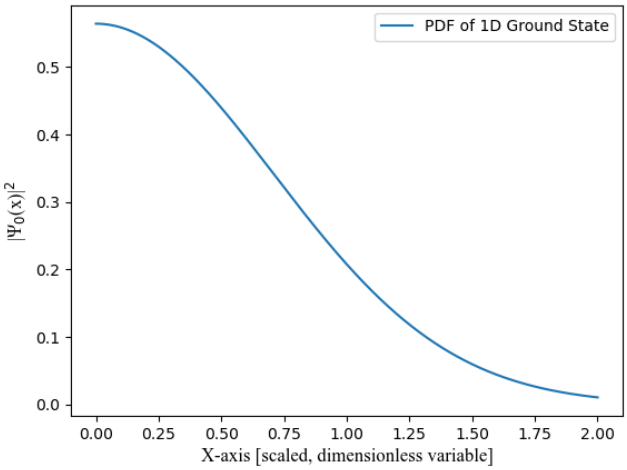


Fig. 2. 1D ground state PDF in SHO potential, demonstrating the reason for choosing a negative-slope linear PDF Eqn. (17), for importance sampling.

## IV. Validations

All methods were individually tested (unit testing) to ensure that they work for any general function, handle edge cases, do not accept invalid or non-sensible parameters, and produce expected results, demonstrating that they work correctly.

Initially, all 4 methods, both Newton-Cotes and MC integration with uniform and importance sampling, were tested for 1D and 3D functions that could potentially cause the algorithms to fail. These included: $f_1(x) = \frac{\sin(x)}{x}$, $f_2 = 0$, $f_3(x) = x$ and $f_4(x,y,z) = \sin(xy)e^{yz}$, all of which can be tested by running 'python testing.py -t 0', where all 4 methods produce the correct results. The first function demonstrated that the methods handle cases with 'DivideByZero' errors, while the second function showed that repeated estimates of 0 do not cause the methods to get stuck in an infinite loop due to a relative error of 0. The third function was used to test the Newton-Cotes methods, which as expected, give the exact numerical answer for linear functions. This occurs due to the linear interpolation between samples for the trapezoidal rule. However, Simpson's rule was tested for quadratic and cubic functions $f(x) = x^2$ and $f(x) = x^3$, integrated between 0 and 1, also giving exact numerical answers of $\frac{1}{3}$ and $\frac{1}{4}$ respectively, as Simpson's rule has an error of order $O\left(h^5\frac{d^4f}{dx^4}\right)$. In fact, for $f(x) = x^3$ the answer returned was 0.24999999999999997, being the nearest smaller representable number to $\frac{1}{4}$, as all methods are limited by the rounding error of the computer. Finally, the fourth function demonstrated that the methods work for any 3D function, which can be non-separable in each dimension.

In addition, to validate that Monte Carlo methods use the intended sampling PDFs, a histogram of the probabilities generated from the PDFs used was plotted, both for uniform and importance sampling shown in Figures 3, 4, by running 'python plots_and_results.py -p 3'.

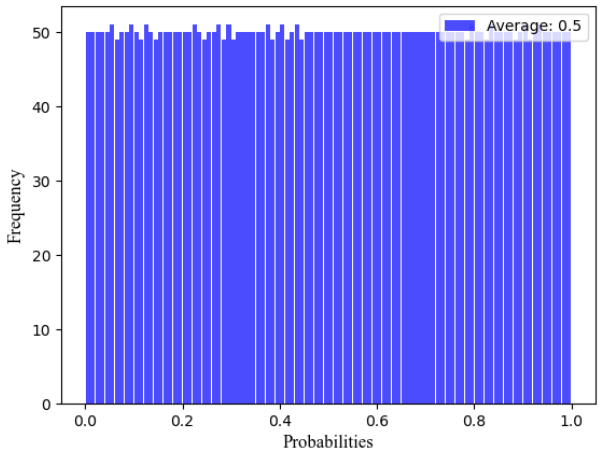


Fig. 3. Histogram of probabilities generated by MC integration with uniform sampling, when integrating $f_1(x) = \frac{\sin(x)}{x}$ from 0 to 1, at $\varepsilon = 10^{-3}$.

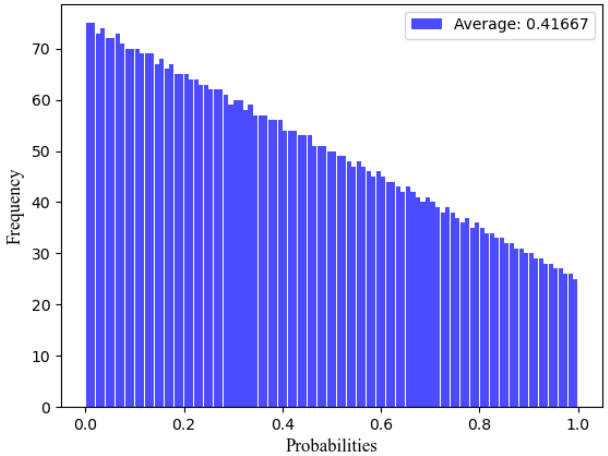


Fig. 4. Histogram of probabilities generated by MC integration, with importance sampling, using $P(\vec{x}) = -\vec{x} + 1.5$, when integrating $f_1(x) = \frac{\sin(x)}{x}$ from 0 to 1, at $\varepsilon = 10^{-3}$.

In addition, to validate that importance sampling with the PDF described by Eqn. (17) was an appropriate choice for the wavefunctions of interest, the number of samples required to achieve a given relative standard error was compared for the two sampling methods. Integrating the 3D ground state from 0 to 2 in all dimensions at $\varepsilon = 10^{-2}$ took 160,000 samples for uniform sampling and 40,000 samples for importance sampling. This demonstrates that fewer samples are needed to meet the convergence criterion with importance sampling, as more points are sampled from the dominant domain of the wavefunction. Furthermore, when a large number of estimates is produced with the same number of samples for uniform and importance sampling, their histograms, shown in Figure 5, demonstrate that importance sampling has a smaller variance, hence, converges faster to an estimate.

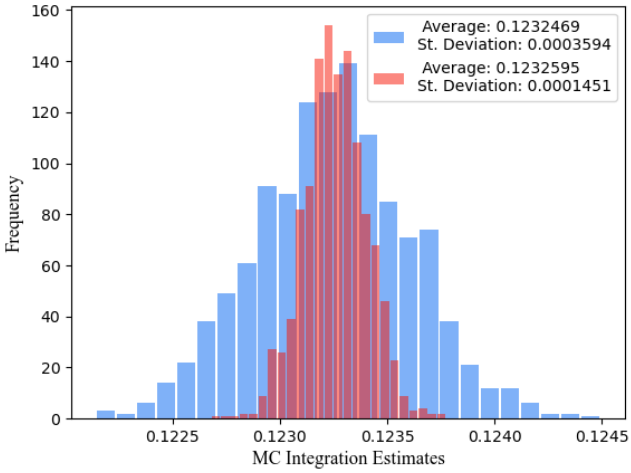


Fig. 5. Histograms of 1,200 MC integration estimates for the 3D ground state, integrated from 0 to 2 in all dimensions, with 160,000 samples for both sampling techniques. Blue: uniform sampling, Red: importance sampling.

Finally, all parts of the code, including individual functions and command-line argument parsers, have various validation checks for: type errors, value errors and exception errors, to make sure that the algorithms will work correctly. For example, the methods validate that the relative accuracy is bounded by 0 and 1, that numerical parameters are always of numeric type, or that the number of function parameters matches the number of dimensions of the integrator methods. All these validations can be checked by running 'python testing.py -t x' where x can take any value from 0 to 7.

## V. Results

Initially, the Newton-Cotes methods were used to estimate the probability of finding a particle in the 1D ground state of a SHO potential bounded by $x \in [0,\ 2\sqrt{\hbar/m\omega}\,]$. For a relative accuracy of $\varepsilon = 10^{-6}$ the results obtained were 0.4976610799507482 and 0.49766113031942405, which required 513 and 65 samples, for the extended trapezoidal and Simpson's rule, respectively. As it can be seen, Simpson's rule required far fewer samples, as it has a smaller error, and its non-linear interpolation approximates the 1D ground state wavefunction better.

The Monte Carlo integration method was also used to estimate the probability with uniform and importance sampling, using Eqn. (17) for the sampling PDF. Table 1 lists the estimates and Table 2 lists the respective number of samples required for 3 different relative standard errors.

TABLE I
MC Estimates for 1D Ground State

| Relative Standard Error | $10^{-3}$ | $10^{-4}$ | $10^{-5}$ |
|---|---|---|---|
| Uniform | 0.4976611705 | 0.497661126 | 0.49766113222 |
| Importance | 0.4976610763 | 0.4976611350 | 0.4976611323 |

Fig. 6. Monte Carlo estimates for the 1D ground state SHO potential integrated between 0 and 2, using both uniform and importance sampling for 3 different relative standard errors.

TABLE II
MC Number of Samples for 1D Ground State

| Relative Standard Error | $10^{-3}$ | $10^{-4}$ | $10^{-5}$ |
|---|---|---|---|
| Uniform | 640,000 | 81,920,000 | 10,485,760,000 |
| Importance | 320,000 | 40,960,000 | 2,621,440,000 |

Fig. 7. Number of samples required for Monte Carlo integration for the 1D ground state SHO potential integrated between 0 and 2, using both uniform and importance sampling for 3 different relative standard errors.

The estimate for a relative standard error of $\varepsilon = 10^{-6}$ was not generated as it would require over 15 hours to be calculated. It was estimated, using $\sin(x)$ as a test function, that the number of samples is related to the error, as expected, by:

$$\varepsilon \sim \frac{1}{\sqrt{N}}, \tag{18}$$

shown in Figure 8, where the observed errors from $\sin(x)$ follow Eqn. (18) with a p-value of 0.9999999993.

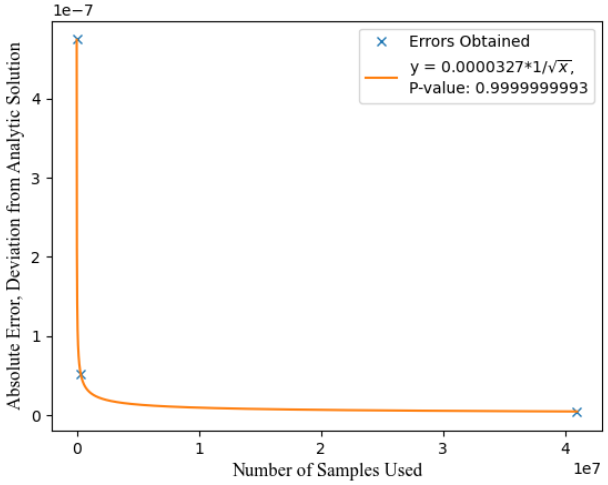


Fig. 8. Error against number of samples for MC integration with uniform sampling, for $\sin(x)$, integrated between 0 and 1 for relative standard errors of $10^{-2}$, $10^{-3}$ and $10^{-4}$.

As a result, the estimate for $\varepsilon = 10^{-6}$ would require approximately 100 times more samples than for $\varepsilon = 10^{-5}$. Given Table 2, it would require ~1,048,576,000,000 samples for uniform sampling, and ~262,144,000,000 samples for importance sampling to achieve a relative standard error of $\varepsilon = 10^{-6}$.

Moreover, an initial trial of adaptive importance sampling demonstrated that it requires even fewer samples to achieve the same relative standard error, requiring 8,192,000 samples to achieve $\varepsilon = 10^{-3}$ for the 3D ground state, compared to 10,240,000 samples without adaptive sampling; seen by running 'python metropolis.py'.

Similar plots were obtained for comparison, from the extended trapezoidal rule, shown in Figures 9 and 10. The error is related to the number of samples by Eqn. (19) for 1D and Eqn. (20) for 3D:

$$\varepsilon \sim N^{-2}, \tag{19}$$

$$\varepsilon \sim N^{-2/3}, \tag{20}$$

where the observed errors from $\sin(x)$ follow Eqn. (19) with a p-value of 0.99999985 and the observed errors from $x^2 + y^2 + z^2$ with a p-value of 0.9995799.

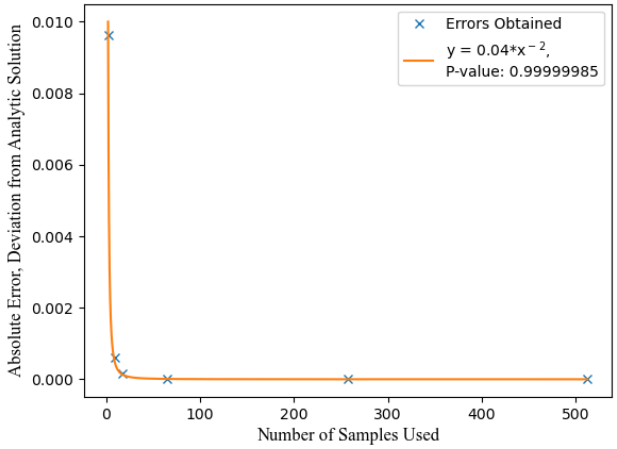


Fig. 9. Error against number of samples for the extended trapezoidal rule, for $\sin(x)$, integrated between 0 and 1 for relative accuracies of $10^{-3}$, $0.5 \times 10^{-4}$, $10^{-4}$, $0.5 \times 10^{-5}$, $10^{-5}$ and $0.5 \times 10^{-6}$.

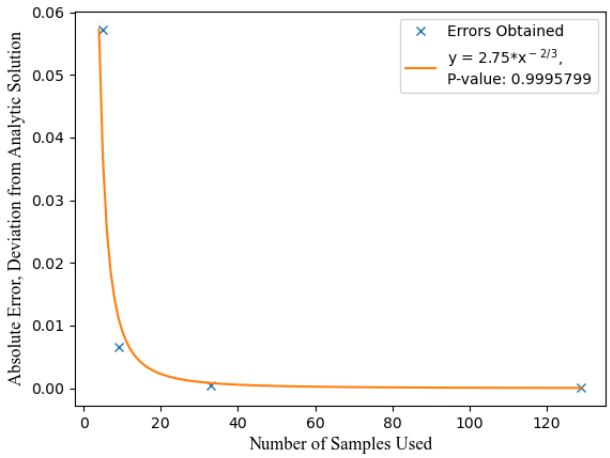


Fig. 10. Error against number of samples for the extended trapezoidal rule, for $x^2 + y^2 + z^2$, integrated between 0 and 1 in each dimension, for relative accuracies of $10^{-1}$, $10^{-2}$, $10^{-3}$and $10^{-4}$.

Finally, all methods were used to estimate the probability of finding a particle at the 3D ground state and the 3D state with one unit of orbital angular momentum, within $[0,\ 2\sqrt{\hbar/m\omega}\,]$ in each dimension. For the 3D ground state, the probability was estimated at 0.123214 and 0.123247 using the Trapezoidal and Simpson's rules, and at 0.1232546 and 0.123258 with uniform and importance sampling Monte Carlo methods respectively at $\varepsilon = 10^{-3}$. It can be seen that the probability of finding the particle in the 3D ground state is the cube root of the probability of finding it in the 1D ground state, as the 3D ground state is the product of the 1D ground states in each dimension. Moreover, for the 3D state with one unit of orbital angular momentum, the probability of the particle being in the same volume was estimated at 0.118089, 0.118129, 0.118144 and 0.118108, with the methods in the order above, at $\varepsilon = 10^{-3}$.

## VI. Conclusion

Three types of numerical methods were used to estimate the probability of a particle to be found in a given space for the 1D ground state, 3D ground state and the 3D state with one unit of orbital angular momentum of a Simple Harmonic Oscillator potential. The extended trapezoidal rule, extended Simpson's rule, and Monte Carlo method, with uniform and importance sampling, were successfully used, giving estimates for these probabilities, and were validated to ensure they work correctly.

The performance of these methods was achieved by ensuring that code was vectorised, and that variables were used instead of lists, avoiding memory issues with large numbers, and taking advantage of the space complexity provided by dynamic programming.

Improvements for this investigation could include trying additional numerical methods, such as Boole's rule, or extending current methods like MC integration, to include the ability to perform adaptive sampling. Finally, libraries that execute Python code using C++ compilers could be used to speed-up computational operations and reduce the time execution of the methods.

## VII. References

[1] Scott M., Dauncey P., (2020), "Computational Physics Projects", pg. 8, Imperial College London

[2] Scott M., Dauncey P., (2020), "Computational Physics Course Notes", Imperial College London

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*excluding tables, figure captions, references, and head titles.