GROUND STATE ENERGY SIMULATIONS USING MONTE CARLO RANDOM WALK

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Abstract. This paper explores the calculation of quantum ground state energies using Monte Carlo random walk simulations derived from the imaginary-time Schrödinger equation, mapping the problem onto a classical diffusion process where the potential energy determines the absorption rate for diffusing walkers. Over long imaginary time, the walker distribution converges to the ground state wavefunction. We implement and compare two algorithms for two different potentials: (1) a Simple Absorption (SA) method applied to a particle in an infinite square well, and (2) a Diffusion Monte Carlo with branching (DMC) method applied to the harmonic oscillator where walkers are removed or duplicated based on their relative potential energy. The SA method yielded an energy estimate of $\overline{\lambda(L/2)^2} = 1.2289 \pm 0.0151(95\%CI : [1.1999, 1.2592])$, consistent with the theoretical value $\pi^2/8 \approx 1.2337$. The DMC method proved more precise estimate for the harmonic oscillator ground state, yielding $\langle V \rangle = 0.5078 \pm 0.0057(95\%CI : [0.4966, 0.5190])$ compared to a theoretical value of 0.5. These results demonstrate the ability for Monte Carlo random walks to do ground state calculations at reasonable accuracies.

Contents

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1. Introduction

Finding the ground state energy is a task done very often in the analysis of quantum mechanical systems but for complex potentials analytical solution to the Schrödinger equation are often extremely difficult. Consequently, numerical methods such as simulations are a powerful, but computationally costly way to solve any given potential. Through transforming the time-dependent Schrödinger equation into imaginary time we can recast the Schrödinger equation into a classical diffusion equation.

This paper explores the application of Monte Carlo random walk for simulating these diffusion equation to receive the ground state energy. We implement and analyse two algorithms:

- Simple Absorption Method: This method uses the case of a free particle in an infinite square well potential where walkers are removed upon reaching the boundary.
- Diffusion Monte Carlo with Branching: This method uses the case of a harmonic oscillator potential, where walkers survive, are duplicated or are killed based on their local potential energy.

For each algorithm we then describe the details of implementation, present example results for both methods, discuss the techniques employed, the accuracy achieved.

2. Method

2.1. Theoretical Foundation.

While the usage of Monte Carlo methods to simulate quantum mechanics may seem strange at first, looking at the time-dependent Schrödinger equation as a diffusion equation in imaginary time reveals the connection that makes it possible. Here is the time-dependent Schrödinger equation for a particle of mass m in a potential $V(x)$:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = \hat{H}\psi(x,t) \tag{2.1}$$

By using $\tau = it$, it becomes:

$$\frac{\partial}{\partial \tau}\psi(x,\tau) = \frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi(x,\tau) - \frac{V(x)}{\hbar}\psi(x,\tau) = -\frac{\hat{H}}{\hbar}\psi(x,\tau) \tag{2.2}$$

This is a diffusion equation with a growth/decay term with a diffusion constant $D = \hbar/2m$ where the growth/decay term determines whether the population density of walkers at a given position increases or decreases.

The general solution to equation 2.2 can be written using the eigenstates and eigenvalues of the Hamiltonian:

$$\psi(x,\tau) = \sum_n c_n\phi_n(x)e^{-E_n\tau/\hbar} \tag{2.3}$$

where $\phi_n(x)$ are the eigenfunctions of the Hamiltonian with corresponding energies E_n, and c_n represents the projection of the initial wavefunction onto each eigenstate. If we consider the case where $\tau \to \infty$, all terms decay exponentially, but the ground state decays the slowest:

$$\lim_{\tau\to\infty}\psi(x,\tau) = c_0\phi_0(x)e^{-E_0\tau/\hbar} \tag{2.4}$$

If we then were able to simulate the diffusion process for a sufficiently long time, then the distribution of our random walkers would approach the ground state wavefunction $\phi_0(x)$, so the decay rate of the walker population would be the ground state energy E_0.

2.2. Implementation Details. In order to not have infinite computation time, we must discretize space and time. To do this we can use a lattice with spatial sites j and temporal sites n. The probability $p(j,n)$ for a walker to be at lattice site j after n time steps satisfies:

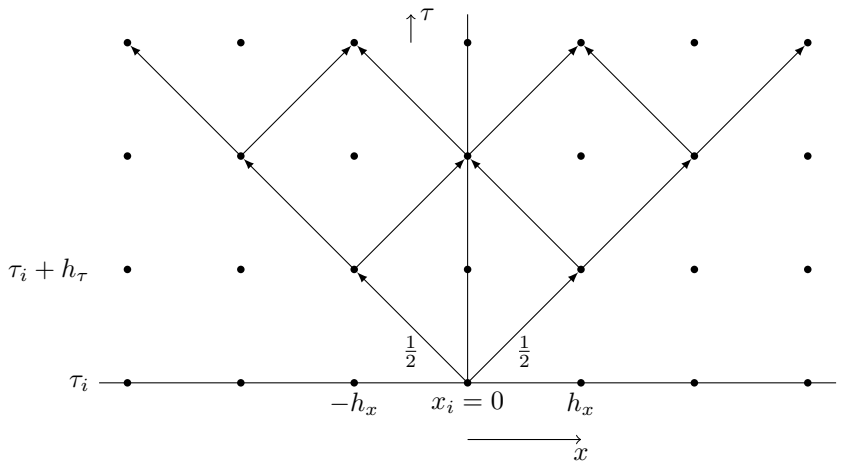

Figure 2.1. A lattice showing the possible moves of a walker at position x_i and time τ_i. The walker can move to any of the neighbouring sites with equal probability.

$$p(j,n+1) = \frac{1}{2}[1-a(j)][p(j-1,n)+p(j+1,n)] \tag{2.5}$$

and converting the lattice to continuous space and time with intervals h_x and h_τ shown in figure 2.1 we get:

$$p(x,\tau+h_\tau) = \frac{1}{2}\left[1-a(x)\right]\left[p(x-h_x,\tau)+p(x+h_x,\tau)\right] \tag{2.6}$$

Here, $a(x) = h_\tau V(x)$ and represents the probability of a walker being absorbed at position x.

So for $\tau\to\infty$, swapping $\psi(x,\tau)$ for $p(x,\tau)$ and defining $h_\tau = h_x^2$ we get the final form of the diffusion equation:

$$\frac{\partial p}{\partial\tau} = \frac{1}{2}\frac{\partial^2 p}{\partial x^2} - V(x)p \tag{2.7}$$

2.3. Algorithm Variants. Using the diffusion equation 2.7 we can derive a couple different ways to simulate the ground state energy of a quantum system.

The simplest method is the simple absorption method, where walkers are absorbed at the boundaries of the lattice. This method is simple to implement but can be computationally expensive for large systems.

A more efficient method is the diffusion Monte Carlo method, which uses branching to kill and birth new walkers. This method is much more efficient but can be more difficult to implement due to the branching process.

2.3.1. *Simple Absorption Method.* In the case for the simple absorption method, our potential is implemented as a infinite square well potential. The probability of a walker being absorbed at a given position is given by:

$$a(x) = \begin{cases} 0 & \text{if } x \in [-L/2, L/2] \\ 1 & \text{otherwise} \end{cases} \tag{2.8}$$

where L is the width of the well.

Using this potential, we can implement the diffusion equation as a random walk on a lattice yielding the following equation for the survival probability of a walker:

$$P_{survival}(\tau) = \int_{-L/2}^{L/2} p(x,\tau)^2 dx \approx e^{-\lambda\tau} \tag{2.9}$$

where λ is the decay rate of the population.

The algorithm is then as follows:

Simple Absorption Method

(1) Initialize N_0 walkers at the centre of the lattice.
(2) For each walker, move it to a neighbouring lattice site with equal probability to move to any of the neighbouring sites.
(3) If the walker is at the boundary of the lattice ($x \geq L/2$), kill it and record the number of steps it took to reach the boundary.
(4) Repeat steps 2-3 for a maximum number of steps. If any of the walkers survive, mark them as surviving.
(5) Find the number of walkers that survive at each step and using a linear regression calculate the decay rate of the population λ.
(6) The ground state energy can then be approximated as $E_0 = \lambda(L/2)^2$.

2.3.2. *Diffusion Monte Carlo with Branching.* The diffusion Monte Carlo with branching method is more complex than the simple absorption method and requires some additional theory. My implementation is based off of both Nakano **??** and Barnes **??**

One of the problems with the simple absorption method is that to get reasonable accuracy, a very large number of initial walkers is required. This can be a problem for large systems since the run time will be $O(N)$ where N is the number of walkers since every walker must be simulated individually.

While we cannot lower the run time, we can lower the number of initial walkers and also greater our chances of finding the ground state. If we were to kill walkers that have a high probability of being absorbed and birth new walkers at positions with a low probability of being absorbed, we can attempt to maintain a more constant number of walkers throughout the simulation.

Since this approach requires us to find the probability of a walker being absorbed at some position, it is reasonable to use a potential that is continuous rather than the infinite square well potential. I have chosen to use the harmonic oscillator potential with $m = \omega = 1$:

$$V(x) = \frac{1}{2}x^2 \tag{2.10}$$

The probability of a walker being absorbed at a given position is then:

$$a(x) = h_\tau V(x) = \frac{1}{2}h_\tau x^2 \tag{2.11}$$

The algorithm is then as follows:

Diffusion Monte Carlo with Branching

(1) (a) Initialize N_0 walkers in a Gaussian distribution around the centre of the lattice and record their positions x_i.
    (b) Compute initial reference potential energy $V_{ref} = \sum_i V(x_i)/N_0$.
(2) For each walker:
    (a) Move it to a neighbouring lattice site with equal probability to move to any of the neighbouring sites.
    (b) Compute the potential energy at the new position $V(x)$ and compute the change in potential energy $\Delta V = V(x) - V_{ref}$.
    (c) If $\Delta V > 0$, kill the walker with probability $|\Delta V \times h_\tau|$. Otherwise, birth a new walker at the new position with the same probability.
(3) Re-calculate $V_{ref} \leftarrow \sum_i \frac{V(x_i)}{N_a} - k\left(\frac{N_a - N_b}{N_b \cdot h_\tau}\right)$ where N_a is the number of walkers after step 2 and N_b is the number of walkers before step 2 and k is a constant to tune.
(4) Repeat steps 2-3 for a maximum number of steps or until the number of walkers reaches zero.
(5) The ground state energy can then be approximated as $E_0 = V_{ref}$.

3. Results

N_0	Max Steps	L	Figure
500	10000	20	3.1; 3.2

Table 1. Parameters used for the Simple Absorption Method.

3.1. Simple Absorption Method.

Running the Simple Absorption Method with the parameters in table 1 yields the following results:

The theoretical value we are comparing against is $\pi^2/8 \approx 1.2337$. Figure 3.1 shows a histogram of how often walkers are found at a given energy value and

provides an mean average energy value of $\overline{\lambda(L/2)^2} = 1.2289$ and has a residual of 0.0048. Standard deviation on this data is $\sigma = 0.3374$ and the range is 0.4895 to 3.9414.

Error analysis shows a standard error of the mean (SEM) of $\sigma_{\bar{x}} = 0.0151$ hence the uncertainty in the residual is 0.0048 ± 0.0151. Error of the relative residual is then $0.39\% \pm 1.23$.

Bootstrap analysis yields a 95% confidence interval of [1.1999, 1.2592].

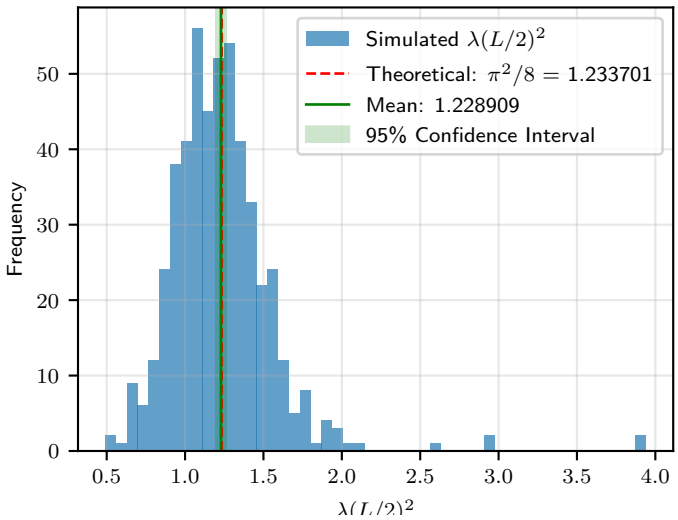

FIGURE 3.1. For the Simple Absorption Method, a histogram showing the distribution of walkers with their energy values compared vs the theoretical value. A 95% confidence interval is shown.

N_0	h_x	Max Steps	Initial Width	Dampening Const k	Equilibration	Figure
50	0.1	50000	1.0	0.5	1000	3.3; 3.4; 3.5; 3.6

TABLE 2. Parameters used for the Diffusion Monte Carlo with Branching method.

3.2. DIFFUSION MONTE CARLO WITH BRANCHING. Running the Diffusion Monte Carlo with Branching method with the parameters in table 2 yields the following results:

The theoretical value we compare to for the ground state energy is 0.5. Figure 3.6 shows a histogram of how often walkers are found at a given energy value and provides an mean average energy value of $\langle V \rangle = 0.5078$ and has a residual of 0.0078.

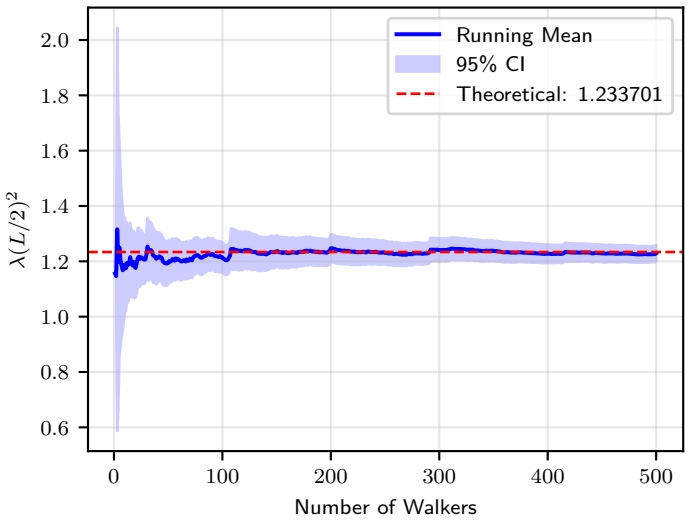

FIGURE 3.2. For the Simple Absorption Method, a running mean of the walkers energy values compared vs the theoretical value as a function of walkers. A 95% confidence interval is shown.

Standard deviation of energy values is $\sigma = 0.0167$ and has an SEM of $\sigma_{\bar{x}} = 0.0001$. Using the SEM to find the uncertainty in the residual is then 0.0078 ± 0.0001 with a error on the relative residual $1.56\% \pm 0.02$.

Autocorrelation analysis revealed an autocorrelation time of 971 steps with an effective number of independent samples of 8.6. Correcting for autocorrelation yields a corrected SEM of $\sigma_{\bar{x}_{corr}} = 0.0057$ and therefore the error on the residual is 0.0078 ± 0.0057 with an error on the relative residual $1.56\% \pm 1.12$.

The corrected 95% confidence interval using $\sigma_{\bar{x}_{corr}}$ is [0.4966, 0.5190].

Finally, the last surviving walkers yield a ground state energy estimate of 0.5005.

4. DISCUSSION

The aim of this paper was to simulate the ground state energy of a quantum system using Monte Carlo methods based on the imaginary-time Schrödinger equation. The two methods used were the simple absorption method and the diffusion Monte Carlo with branching method.

The simple absorption method was based on Barnes and Daniells [1] and was used to simulate the ground state energy of a particle in an infinite square well potential. The method was relatively simple to implement but due to the large number of walkers being simulated at any one time to receive an estimate of the

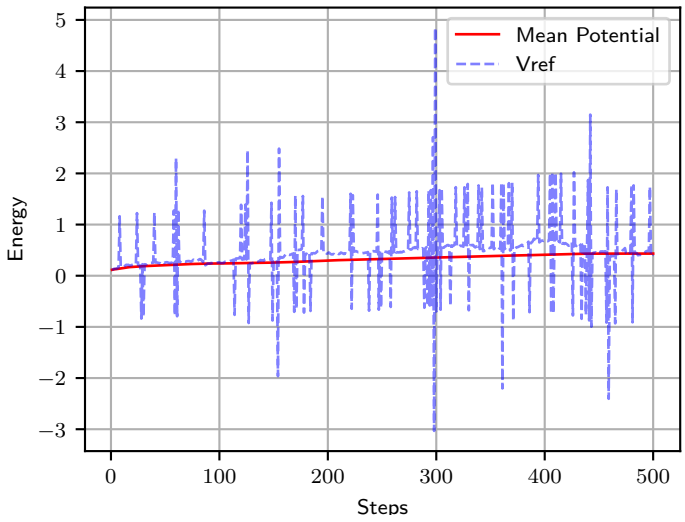

FIGURE 3.3. Time average mean potential energy of all walkers plotted with the estimate of the potential energy, V_{ref} as a function of steps.

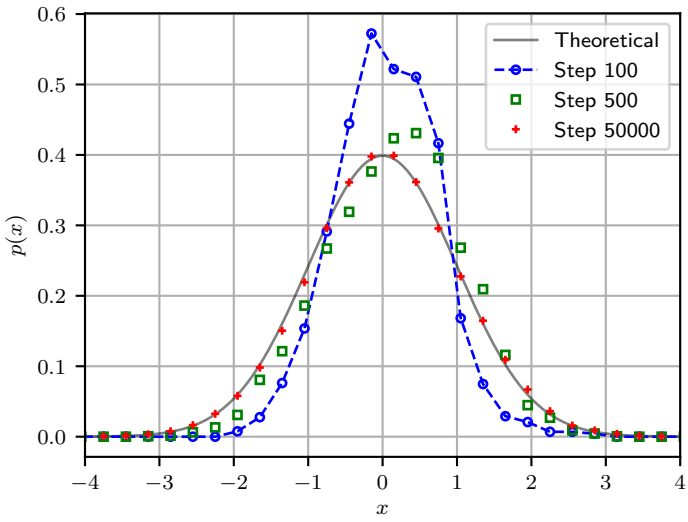

FIGURE 3.4. For the Diffusion Monte Carlo with Branching method, Ground state wavefunction of potential $V(x) = \frac{1}{2}x^2$ at step 100, 500 and 50000 with the theoretical wavefunction as a function of position.

energy to a reasonable accuracy, it was computationally expensive. To mitigate

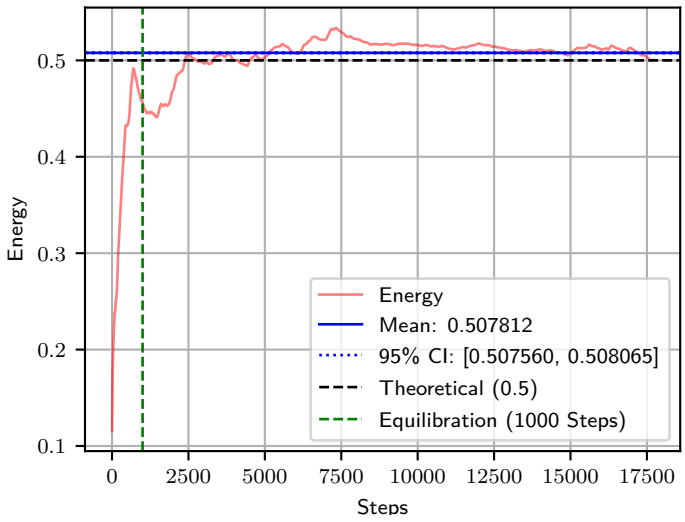

FIGURE 3.5. For the Diffusion Monte Carlo with Branching method, the walkers energy and a mean of the walkers energy compared vs the theoretical value as a function of steps. A 95% confidence interval is shown.

this, I made the simulation multithreaded but on a system with a low thread count this doesn't provide any significant speed-up.

4.1. SIMPLE ABSORPTION METHOD TECHNIQUES. The techniques used for the simple absorption method are, Random Sampling, Linear Regression and Bootstrapping.

Random sampling uses pseudo-random numbers to select a sample from a population with pre-known probabilities of selection. In this case, random sampling was used to select whether a walker moves to the left or right in the lattice with probability 0.5. To ensure the random numbers are random enough, either ChaCha12 [2] or Lcg128Xsl64 [3] (for a seeded generator) were used. ChaCha12 passes the next bit test which requires that the next bit of a random number is negligibly better than equal but Lcg128Xsl64 does not. Perhaps an improvement would be to use ChaCha20 or a seeded pseudo-random number generator that passes the next bit test.

Linear regression models the relationship between a dependant variable and n independent variables by fitting a linear equation to the data. In this case linear regression was used to find the decay rate of the population of walkers. I used the least-squares approach which chooses a line that minimizes the sum of squared residuals. Linear regression however assumes that the relationship between the variables is linear in the first place and is sensitive to outliers which can result in

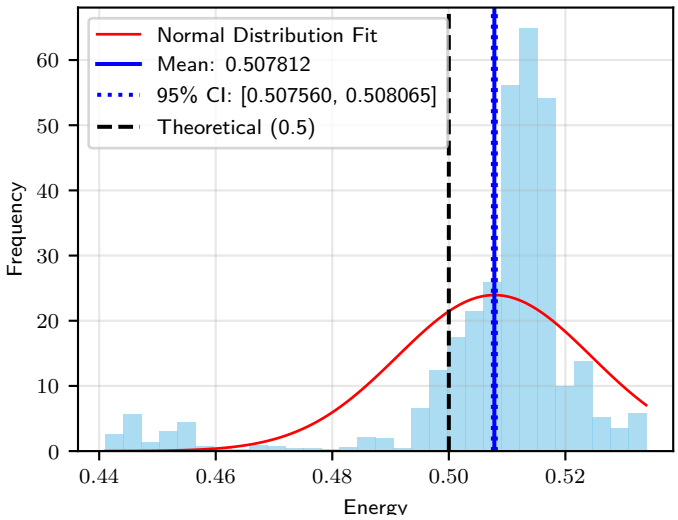

FIGURE 3.6. For the Diffusion Monte Carlo with Branching method, a histogram showing the distribution of walkers with their energy values compared vs the theoretical value. A Normal distribution is fitted to the data and a 95% confidence interval to the mean is shown.

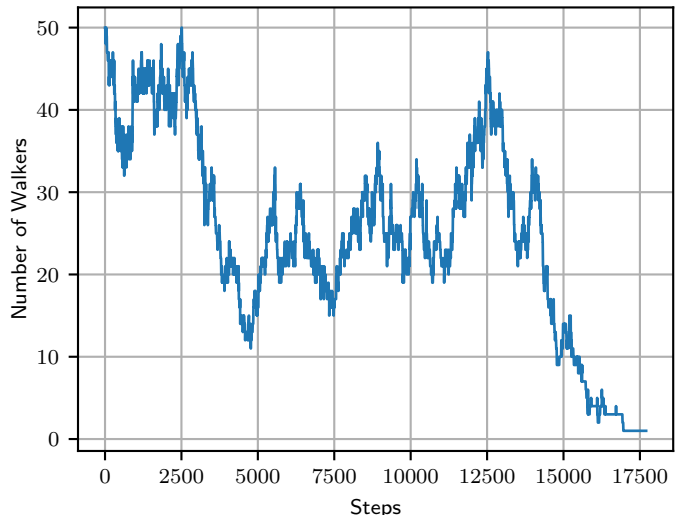

FIGURE 3.7. For the Diffusion Monte Carlo with Branching method, the number of walkers as a function of steps.

some of the anomalies seen in figure 3.1.

Bootstrapping, introduced by Efron in 1979 [4] re-samples the data with replacement, that is to say, when a sample is taken from the dataset it is put back before the next draw. This allows for the estimation of the sampling distribution of a statistic and can be used to find the confidence interval of the mean. In this case, bootstrapping was used to find the 95% confidence interval of the mean energy value. Bootstrapping is less effective when the sample size is small or has high dimensionality. Using bootstrapping on the simple absorption method allows the estimation of a confidence interval without the need to estimate the energy distribution as a normal distribution.

4.2. Diffusion Monte Carlo with Branching Techniques. The techniques used for the diffusion Monte Carlo with branching method are, Random Sampling and Autocorrelation Analysis.

For Random sampling see section 4.1.

Autocorrelation analysis quantifies the correlation between measurements close together in the simulation time series. In this case, a sequence of states or energies (eg. V_{ref}) are not often statistically independent, it may be the case that each step depends on the next one. Ignoring this correlation leads to an underestimation of the actual statistical error when calculating averages. By estimating the autocorrelation time (τ_{corr}), we measure how many steps are required to get an independent sample and hence we can determine the number of truly independent samples as ($N_{eff} \approx N/(2\tau_{corr})$) where N is the number of samples. In this case, the autocorrelation time was found to be 971 steps and the effective number of independent samples was 8.6 and recalculating the SEM with this information yielded a corrected SEM of 0.0057, larger than the original SEM of 0.0001.

4.3. Comments on Results.

4.3.1. *Simple Absorption Method.* The results for the simple absorption method were quite promising. Looking at the residual and its error, we received 0.0048 ± 0.0151. Since the error on the residual is larger than the residual itself, we can confidently say that the simulation achieved an accurate results within error.

Additionally, bootstrap analysis yielded a 95% confidence interval of 1.1999 to 1.2592, which contains the theoretical value of 1.2337. This means that, even with the large standard deviation of the data (which can be seen qualitatively in figure 3.1), the simulation was able to accurately estimate the ground state energy.

Looking at figure 3.2, we can clearly see that as you increase the number of walkers in the simulation the mean slowly converges to the theoretical value. Despite the theoretical value being reached even at around 100 walkers, beyond that point the 95% confidence interval continues to narrow. Theoretically, if the number of walkers was increased to infinity, the mean would converge to the

theoretical value and the confidence interval would be zero.

4.3.2. *Diffusion Monte Carlo with Branching.* The results for the diffusion Monte Carlo with branching method were, in comparison, much more accurate. This is likely due to the branching process where walkers that are less useful to find the ground state are killed and new walkers are born in more useful positions. This does remove some of the complete randomness that the simple absorption method has, but crucially it does not use any information about the theoretical wavefunction, only the potential.

Since the complete randomness is removed, the standard deviations and confidence intervals calculated before the autocorrelation are not useful. As seen in figure 3.5 and figure 3.6, the 95% confidence interval is very tight and the standard deviation is very small. Since the walkers are all converging to the same energy value and the branching process is removing the walkers that are not converging this is expected so to get a more accurate estimate of the error, the autocorrelation is required.

After performing the autocorrelation, the corrected SEM was found to be 0.0057 which is much larger than the original SEM of 0.0001. Although this doesn't allow the error on the mean energy to encompass the theoretical value, calculating a new 95% confidence interval, [0.4966, 0.5190], reveals that the theoretical value does now fall within it (95% confidence interval for the un-corrected SEM was [0.507560, 0.508065]).

This method additionally allows us to plot the wave function as a function of position itself as in figure 3.4. It is clearly shown that a greater number of steps allows the walkers to approach the theoretical wave function. 50000 max steps was chosen as a reasonable upper limit since the wave function approached the theoretical quite closely while not being too costly to run the program. However, we can see that the simulation wasn't actually run for 50000 steps but around 17500 as seem in figure 3.7. As the program approaches the ground state wavefunction, walkers will become much more likely to die leading to the drop off seen at around 12500 steps.

4.4. Parameter Optimization. Each method and program has various parameters seen in tables 1 and 2.

For the simple absorption method, it was key to balance the lattice size L with the max steps, too large a lattice and walkers would never be arrested, to few steps and walkers wouldn't reach the edge of the lattice. Additionally the number of walkers N_0 must be an amount that is reasonably simulate-able with the specification of the computer, too large and process memory and run time would be to large, to small and you would receive a poor estimate of the ground state energy with large error.

For the diffusion Monte Carlo with branching method, parameter tuning is less required, since the walkers active at any one time is relatively stable, a low number of initial walkers N_0 is viable and preferred keeping memory usage and

step simulation time to a minimum. Initial width dampening constant tuning allow for quicker or slower approaches to the ground state wavefunction, but do not change, the end result (assuming you keep the dampening const between 0 and 1). The parameters that have more impact on the result is the equilibration and the step size h_x. In the case of the equilibration, it simply discards the results when calculating the statistics for step numbers below it. Since the values below 1000 for my chosen parameters where clearly not useful, this is the number I chose. Ideally h_x should be as small as possible, but decreasing h_x requires a much greater number of max steps for the walkers to be able to explore the available space. Additionally, we know the theoretical wavefunction approaches 0 at roughly $x = \pm 3$ so having an $h_x > 3$ at maximum will yield results that are not at all useful.

5. Conclusion

This paper successfully demonstrated the simulation of quantum ground state energies using Monte Carlo random walk methods. Two primary algorithms were implemented based on different potentials and evaluated: the Simple Absorption method for the infinite square well and the Diffusion Monte Carlo with Branching method for the harmonic oscillator.

The Simple Absorption method yielded good results for the infinite square well. The simulation produced a mean energy estimate of $\overline{\lambda(L/2)^2} = 1.2289$ corresponding to a residual to the theoretical value ($E_0 = \pi^2/8 \approx 1.2337$) of 0.0048. Although the standard error of the mean was relatively large ($\sigma_{\bar{x}} = 0.0151$), it resulted in an uncertainty that comfortably encompassed the theoretical value. Bootstrap analysis, removing the reliance on the results being normally distributed provided a 95% confidence interval of [1.1999, 1.2592] which too contains the theoretical ground state energy. This indicated that the method can estimate the energy within reasonable error bounds but reducing the error requires substantial computational effort.

In contrast the Diffusion Monte Carlo with Branching method applied to the harmonic oscillator proved significantly more accurate. The simulation converged to a mean energy value of $\langle V \rangle = 0.5078$ with a residual to the theoretical ($E_0 = 0.5$) of 0.0078. Using autocorrelation analysis revealed a long correlation time ($\tau_{corr} = 971$) steps, and as such the standard error mean was calculated to $\sigma_{\bar{x}_{corr}} = 0.0057$. Using a 95% confidence interval with $\sigma_{\bar{x}_{corr}}$ yields [0.4966, 0.5190] which successfully includes the theoritical value.

Diffusion Monte Carlo with branching offers superior accuracy (has smaller residuals and tighter confidence intervals relative to the theoretical value) thoughts its implementation and analysis are more involved and dependant on the potential used.

Future work could involve using these same methods and applying them to more complex potentials, higher dimensional cases and incorporating Monte Carlo importance sampling to explorer wider use cases.

Appendix A. Additional Citations

A.1. Brownian Motion. Einstein's paper in 1905 [**?**] modelled Brownian motion as a random walk, showing that particle movements result from molecular collisions. Since displacements can be treated as independent random variables, Einstein's work to model diffusion in this way is directly tied to this paper. The random walk model managed to predict diffusion coefficients later verified experimentally.

18 Examples

6 for each: random walk, Monte Carlo, random numbers

3 in academia, 3 outside academia

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