GROUND STATE ENERGY SIMULATIONS USING MONTE CARLO RANDOM WALK

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Abstract. Placeholder for abstract.

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1. Introduction

Overview of the challenges in solving the Schrödinger equation numerically The connection between the imaginary-time Schrödinger equation and diffusion processes Historical development of Monte Carlo methods in quantum mechanics Brief comparison with alternative numerical approaches (matrix diagonalization, variational methods) Motivation: why random walks are particularly well-suited for ground state energy calculations

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:

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

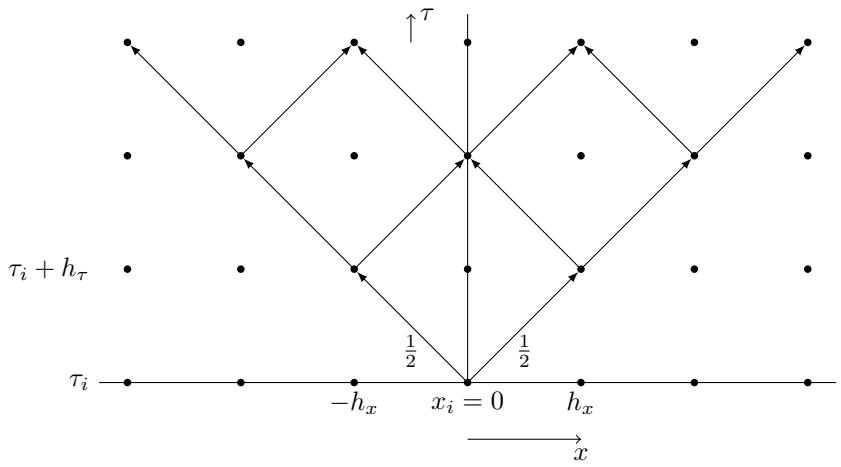

FIGURE 2.1. A lattice showing the possible moves of a walker at position x_i and time τ_i. The walker can move to any of the neighbouring sites with equal probability.

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.

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. Relative error of the simulation is then $0.39\% \pm 1.23$.

Bootstrap analysis yields a 95% confidence interval of 1.1999 to 1.2592.

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:

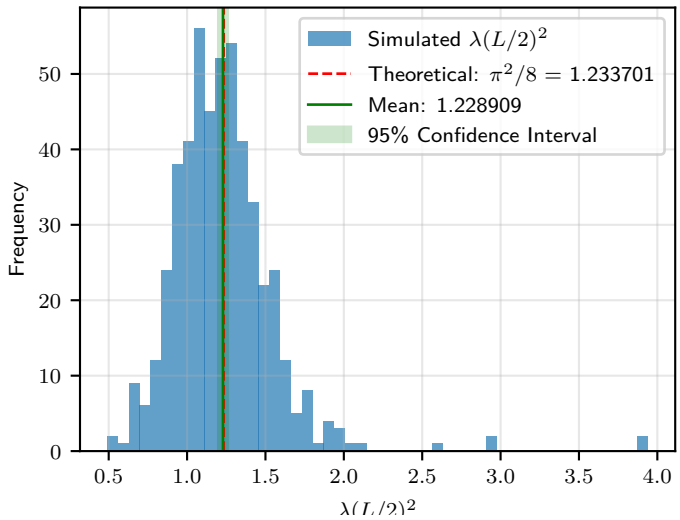

FIGURE 3.1. For the Simple Absorption Method, a histogram showing the distribution of walkers with their energy values compared vs the theoretical value. A 95% confidence interval is shown.

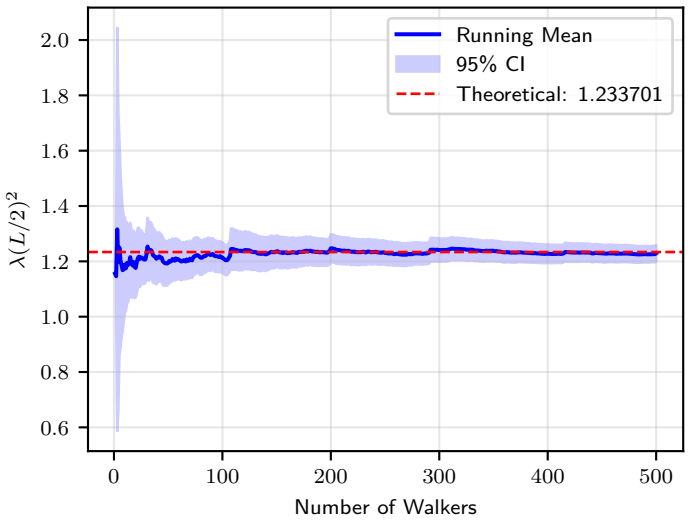

FIGURE 3.2. For the Simple Absorption Method, a running mean of the walkers energy values compared vs the theoretical value as a function of walkers. A 95% confidence interval is shown.

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.

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.

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 relative error of $1.56\% \pm 0.02$.

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 uncertainty in the residual is 0.0078 ± 0.0057 with a relative error of $1.56\% \pm 1.12$.

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

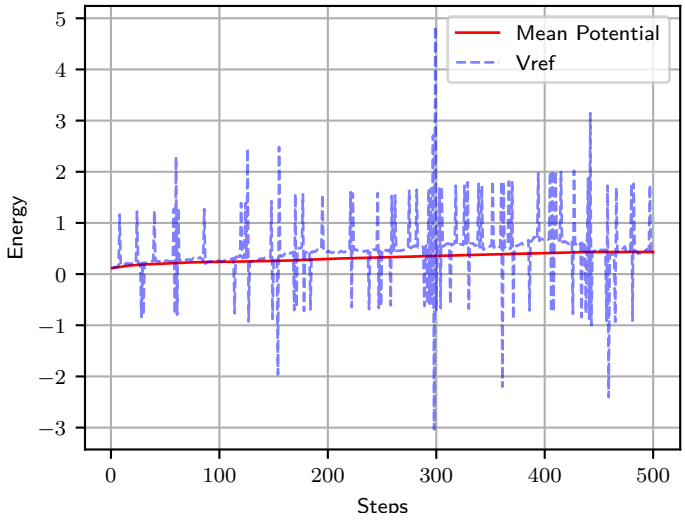

FIGURE 3.3. Time average mean potential energy of all walkers plotted with the estimate of the potential energy, V_{ref} as a function of steps.

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.

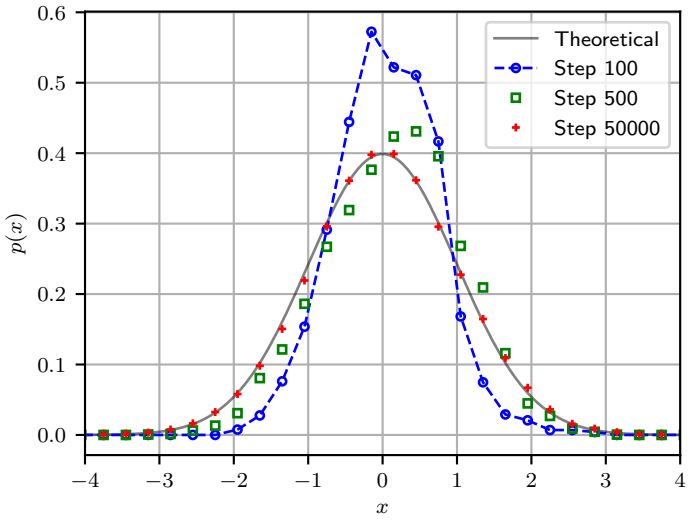

FIGURE 3.4. For the Diffusion Monte Carlo with Branching method, Ground state wavefunction of potential $V(x) = \frac{1}{2}x^2$ at step 100, 500 and 50000 with the theoretical wavefunction as a function of position.

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

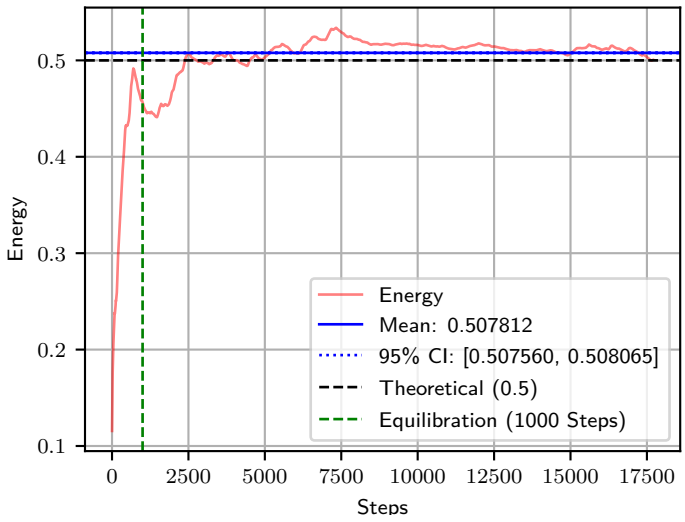

FIGURE 3.5. For the Diffusion Monte Carlo with Branching method, the walkers energy and a mean of the walkers energy compared vs the theoretical value as a function of steps. A 95% confidence interval is shown.

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 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

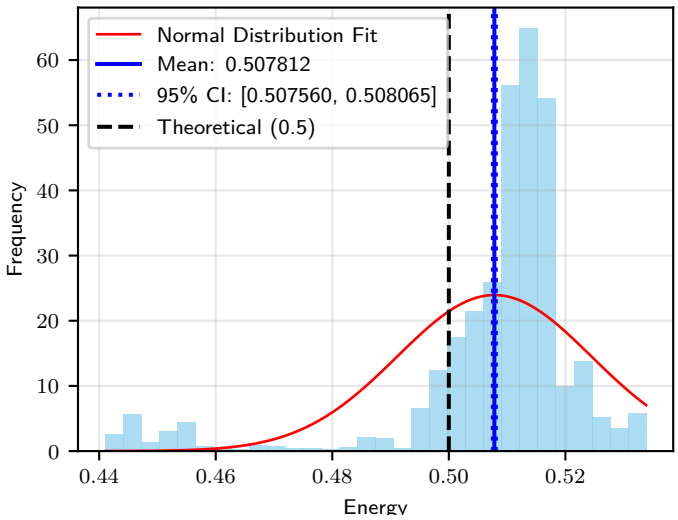

FIGURE 3.6. For the Diffusion Monte Carlo with Branching method, a histogram showing the distribution of walkers with their energy values compared vs the theoretical value. A Normal distribution is fitted to the data and a 95% confidence interval to the mean is shown.

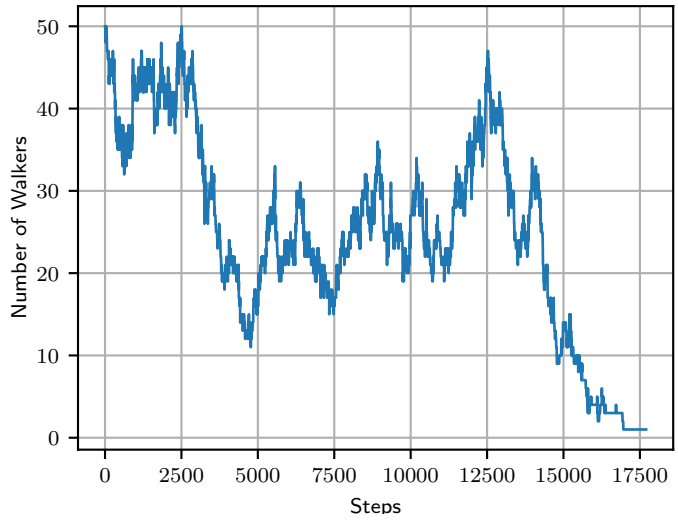

FIGURE 3.7. For the Diffusion Monte Carlo with Branching method, the number of walkers as a function of steps.

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. Parameter Optimization.

4.4. Method Strengths and Limitations.

5. Conclusion

Summary of key findings and method effectiveness Practical recommendations for implementation Future directions for method improvement Potential applications to more complex quantum systems

Appendix A. Additional Citations

18 Examples
6 for each: random walk, Monte Carlo, random numbers
3 in academia, 3 outside academia

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