Using Random Walk Simulations to Calculate Ground State Energies in Quantum Physics

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***Abstract*—**

I. Introduction

THE developments in computer power in recent years has opened up the possibility for novel computational solutions to many problems that were otherwise limited. We now have access to computers that can numerically solve problems and run simulations that were previously too computationally intensive to do.

One such problem is the calculation of the ground state energies of different quantum systems. Many methods exist for solving these problems, using both classical and quantum computational approaches. Whilst generally it may be true that Quantum computating approahes are more suited to solving such problems [1], these approaches are still in infancy and are not readily accessible. Thus, there exist an abundance of classical computing approaches, such as the Variational-Relaxiation algorithm [2]. This is a particularly useful algorithm for two-dimensional systems with non-separable potentials but quickly becomes difficult to implement for more complex systems.

In this investigation, I explore an alternative Monte Carlo method using Random Walk simulations, and demonstrate its efficacy with simple systems.

II. Theoretical Background

A. Random Walk Simulations

Random walks descibe motion as a series of steps in some vector space, with the direction of each step being random, i.e. with there being an equal likelihood of a step in each possible direction. Consider a simple 1-dimensional line and a walker standing at a point labelled the origin. The walker takes 20 steps, the direction of each step (forwards or backwards on the line) is random. The position of the walker at each step is shown in Figure 1.

As we can see from the figure, it is not uncommon for the average position of the walker to be away from the origin once the walk has concluded. This is because the position of the walker at any step is dependent only on the position at the previous step. If the walker happens to take a number of steps in the same direction, it is highly unlikely for the walker to take an equal number of steps in the opposite direction, in order to return to the origin. Thus, in such a case, it is likely that the walker will conclude the walk in a position away from the origin.

In this example, the walker had an equal likelihood of stepping forward or backwards, but we can bias in one way if we want to model a particular phenomenon. The walk is also easily extensible to multiple dimensions, as for each extra dimension, one extra random number must be drawn. This gives a linear increase in time-complexity, which is convenient for more complex systems.

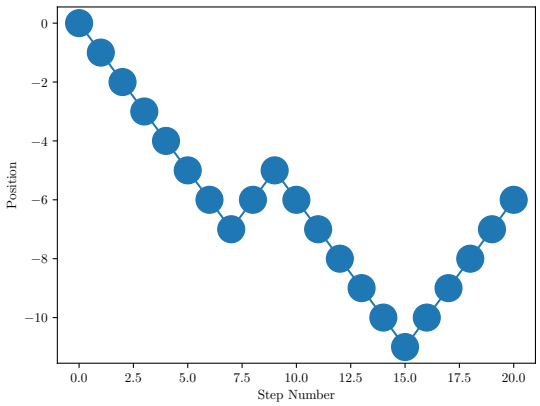


Fig. 1. The position of a walker at each step in a 20-step random walk simulation. The average position of the walker does not necessarily remain at the origin as one might naively expect. Instead it is normal for the walker to finish the walk at some distance from the origin, as shown here.

B. Application to Quantum Systems

This investigation applied Random walk simulations to calculate the ground state energies of Quantum Systems by solving the Schrödinger equation, as shown in . cite

We can extend the simple one-dimensional line model from Figure 1 to a quantum system by imagining it as a one-dimensional simple lattice system. A walker can start at a position labelled the origin, and then proceed in a random walk. The random walk concludes if the walker "dies" on a particular step. The probability that the walker will die is dependent on a defined potential at that point. For example, in an infinite square well system, the potential is 0 within a well, and infinite outside the well. So the walker will have no chance of dying whilst inside the well, but will die if they step outside.

Let us define $p(j, n)$ as the probability that the walker will be at position j after n steps and $a(j)$ as the probability that the walker will die at position j. Thus, for this to be the case, the walker would have had position $j \pm 1$ after $n - 1$ steps. Thus, we can say:

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

If $a(j)$ is small and n is large, we can use Taylor's expansion to expand each term in this expression and obtain a differential equation. If we then make the ansatz substitution:

$$p(j,n) = q(j)\exp(-\lambda n) \tag{1}$$

where $q(j)$ is an arbitrary function and λ is the rate of death, then we find:

$$-\frac{1}{2}\frac{d^2q(j)}{dj^2} + a(j)q(j) = \lambda q(j) \tag{2}$$

The full derivation is taken from [3] and is shown in Appendix A. Notice that Equation 2 is in the form of the Schrödinger equation:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dr^2} + V(r)\psi(r) = E\psi(r) \tag{3}$$

Comparing Equation 2 and Equation 3, we can see that the probability of death $a(j)$ is related to the potential $V(r)$, and the rate of death λ is related to the Energy E.

We can extend this to an infinite square well by choosing our probability of death such that:

$$a(j) = \begin{cases} 0, & \text{if } j < J \\ \infty, & \text{if } j \geq J \end{cases}$$

where J is a well-defined boundary. So the walker cannot die inside the well but wil immediately die when they step outside, which we expect will definitely happen given sufficient time. cite Inside the well, the potential is simply that of a free particle :

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x)$$

where x is the position of the walker. By making the substitution $x = J\frac{j}{R}$, such that $j = R$ corresponds to the walker being at the boundary, we find:

$$-\frac{\hbar^2}{2m}\frac{R^2}{J^2}\frac{d^2\psi}{dj^2} = E\psi(x)$$
$$-\frac{1}{2}\frac{d^2\psi}{dj^2} = \frac{mJ^2E}{\hbar^2R^2}\psi(x)$$

If we compare this to Equation 2, allowing $a(j) = 0$ inside the well, we see that:

$$E = \lambda R^2\frac{\hbar^2}{mJ^2}$$

where only λ is an unknown quantity. Thus, by calculating rate of death λ, we can calculate the ground state energy of the infinite square well. The known ground state energy of an cite infnite square well is $\frac{\pi^2}{8}\frac{\hbar^2}{mJ^2}$, so we expect to find λR^2 close to $\frac{\pi}{8}$.

To find the rate of death λ, we consider Equation 1. With some simple manipulation:

$$p(j,n) = q(j)\exp(-\lambda n)$$
$$\log(p) = \log(q\exp(-\lambda n))$$

$$\log(p) = -\lambda n + log(q) \tag{4}$$

Thus, by plotting the logarithm of the probability of surviving n steps against the number of steps n, we can obtain the death rate λ from the gradient of the line.

III. Method

We implemented the Random Walk simulation computationally in C++ in order to optimise the performance of the simulation, and thereby allow for a larger number of iterations and larger potential wells. The source code is available [4]. The simulation is easily extensible to multiple dimensions with a linear increase in time-complexity as the number of dimensions increases, but this investigation focused on a one-dimensional system.

The random direction is selected using a pseudorandom number generator (pRNG) known as the Mersenne Twister. This algorithm was chosen as it is a very fast implementation of a pRNG [5], passes many statistical randomness tests [6], and has a very large period of $2^{19937} - 1$.

We initially ran the simulation for a boundary of $J = 20$, with 1000000 walkers. The step on which each walker died was recorded so that a probability distribution showing the likelihood of dying on a particular step could be constructed.

We then consider the probability that a walker will survive n steps, and use the relationship between the number of walkers surviving n steps and n to determine the rate of death λ, as shown in Equation 4.

One method of reducing the computing time of the simulation is to introduce a maximum number of steps. The walker will die if they reach the boundary of the well, or if they reach this maximum number of steps, whichever happens first. However, this will introduce some systematic error into the simulation, as there will be a disproportionately high number of walkers dying on the maximum number of steps. We also investigated these effects here.

We expect to see an effect on the accuracy of our final ground state depending on the size of the infinite well. We investigate these effects by comparing the calculated ground state energy to the theoretical energy for different sized wells.

IV. Results and Discussion

The simulation was first run for an infinite square well with boundary $J = 20$, with 1000000 walkers. The step on which each walker died was recorded and then the normalised histogram in Figure 2a was constructed. The histogram has been normalised, and is hence a probability distribution showing the probability that a walker will die on a particular step. As we expect, the peak is far from the origin, since for a walker to die in an inifinite square well with $J = 20$, they would have to walk at least 20 steps. It is also highly unlikely that a walker would walk 20 steps in the same direction consecutively. Thus, the peak is also at a number of steps greater than J. We expect the shape of the decay after the peak to be exponential. We can see this by plotting the histogram on a logarithmic scale.

Figure 2b presents the same histogram data with a logarithmic y scale. In this figure, a straight line is evident in the data, showing the decay was indeed exponential after the peak. The peak probability being away fro the origin is also clearer

in this figure. Figure 2b shows a "widening" of the straight line at higher step numbers. This is because there is a greater variance in the number of walkers surviving to this number as it is highly unlikely.

By taking the cumulative sum of the histograms in Figure 2, we can ensure the peak probability begins at the origin. Figure 3 present the cumulative sums of the histograms. They represent the probability of surviving at least a particular number of steps. Hence, the peak probability of 1 is at the origin, since there is a probability of 1 that a walker will survive the first step.

Figure 3a presents the cumulative summed histogram, with a fitted exponential curve of the form of Equation 1. The fit is very good, with $R^2 = 0.9999998$, very close to 1. There is also negligible numerical error in the fit, i.e. an error smaller than the quoted precision of the fit parameters. This is because the simulation was run for 1000000 walkers, providing a large sample size. Figure 3b presents the same histogram with a logarithmic y-scale and a fitted straight line of the form of Equation 4. This fit has the same R^2 value, as it is simply the same fit on a different y-scale, and is thus equally good.

We observe some fluctuation in the data in the higher steps. This is because there are so few walkers surviving to this many steps that there is more significant variance in their relative numbers. It is possible to remove this variance by introducing a cutoff number of steps, i.e. a maximum number of steps at which the walker will automatically die, regardless of whether they reached a boundary or not. Thus, there will not be such high variance in the number of walkers surviving to high number of steps. This is presented in Figure 4. While this fit is observed to be better, with a higher R^2 value, some systematic error has been introduced since there will now be a disproportionately high number of walkers dying at the cutoff step. Thus, the final λJ^2 value will be less accurate. On a faster computer, with more efficient code, it is possible to forgo the step cutoff and allow the simulation to run until all the walkers die. This may take much longer but will ensure there will not be such a systematic error introduced.

We can use the gradient of the fitted line in Figure 3b as the λ value, and compare λJ^2 with the theoretical value. However, to determine the reliability of the calculated value, it is necessary to repeat the procedure many times and take the average λ and the standard deviation as the error.

It is also necessary to investigate how varying the boundary J affects the accuracy of the final answer. Figure 5 presents the cumulative summed histograms with their fitted lines for many different boundary J values. No step cutoff was introduced. The calculated λJ^2 value is shown in the legend. As shown, the gradient changes, but this is to be expected since the expected highest number of steps would increase as the boundary is larger, since there is more "space" for the walker to move before reaching a boundary. As shown in the legend, the calculated λJ^2 values get closer and closer to the theoretical value as J increases. This is due to the fact that as J increases, there are more walkers surviving to larger number of steps. . Thus, we can say that using a larger value of J will result in a more accurate answer but will also be more computationally intensive and take longer. Thus, we make a tradeoff between speed and accuracy and choose $J = 20$ for the final investigation.

truncate numbers

make plot of lambda J against J

Running the simulation 10 times and taking the average λJ^2 with error being standard deviation, we find: $\lambda J^2 = 1.2339 \pm 0.0008$. We quote the precision to the decimal place at which there is variation from the theoretical result of 1.2337. We notice also that the error in the calculated answer is small (since there is not much variation between repeated simulations) and the theoretical result is within the range of the calculated answer.

circular well

fix centering of cum plot

cite

V. Conclusions

In this investigation we demonstrated a method of calculating ground state energies of a quantum system using Random walk computational simulations. The investigation focussed on an Infinite Square Well, but is easily extended to a Symmetric potential. The simualation was written in C++ to maximise performance and is available at .

The investigation explored the effects of varying the size of the well in determining the ground state energy of a quantum system, and showed that this method is more effective for larger wells, i.e. wells with larger boundaries. This is because for wells with larger boundaries, the walker can take a larger number of steps on average before dying, and thus can populate larger step bins. Thus, this method produces data that is close to the theoretical result for larger infinite square wells.

The general theoretical result for the ground state energy of an infinite square well is $\frac{\pi^2}{8}\frac{\hbar^2}{mJ^2}$ where J is the boundary of the well, and this method allows for the calculation of $\lambda R^2 \frac{\hbar^2}{mJ^2}$, where R also corresponds to the boundary of the well. Thus, we expect our calculated result to be $\lambda R^2 = \lambda J^2 = \frac{\pi^2}{8}$.

This method provided $\lambda J^2 = 1.2339 \pm 0.0008$, which lies within the range of the theoretical result.

This method can be easily extended to multiple dimensions with only a linear increase in time complexity for each added dimension. Thus, while this method may not be very efficient for low number of dimensions, it quickly becomes effective at a higher number of dimensions.

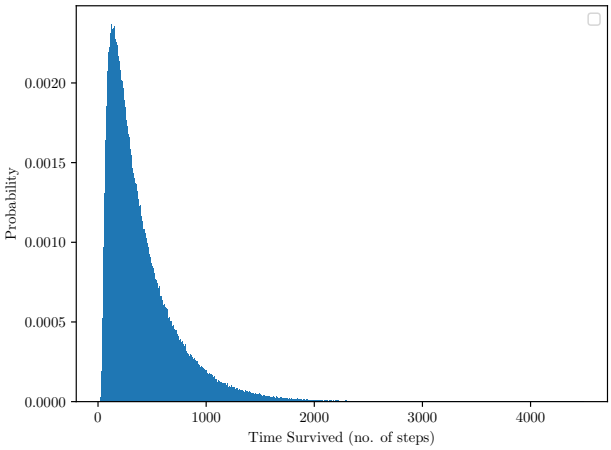
Appendix A
Random walk Schrödinger Equation Derivation

Let us denote the probability that the walker is at position j after n steps as $p(j, n)$ and the probabilty that the walker will die at position j as $a(j)$. We will denote the position-step number coordinates as $[j, n]$. Thus, for a walker to have coordinates $[j, n+1]$, in the previous step, they must have had coordinates $[j \pm 1, n]$. So we can say:

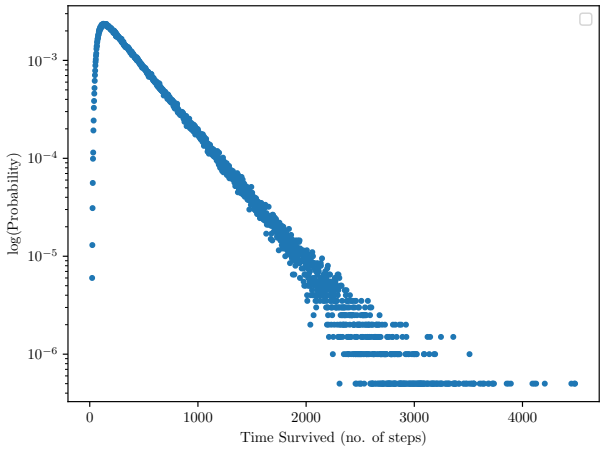
$$p(j, n+1) = \frac{1}{2}(1 - a(j))(p(j-1, n) + p(j+1, n)) \quad (5)$$

If $a(j)$ is small and n is large, then we can say $p(j, n)$ is a continuous function and we can use Taylor expansion to expand each of $p(j+1, n)$, $p(j-1, n)$, and $p(j, n+1)$:

$$p(j+1, n) = p(j, n) + \frac{\partial p}{\partial j} + \frac{1}{2}\frac{\partial^2 p}{\partial j^2} + ...$$

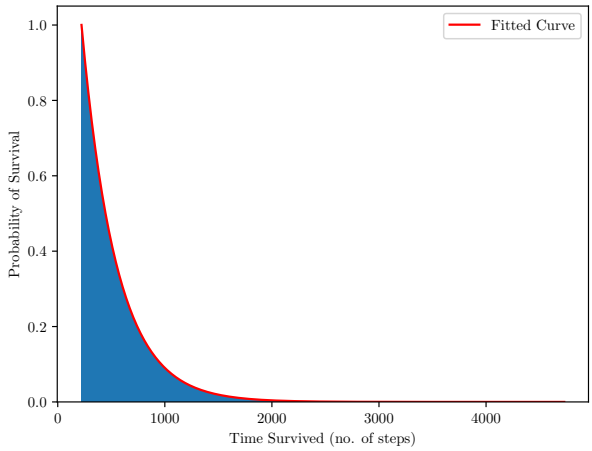


(a) Histogram of probability of dying on particlar step

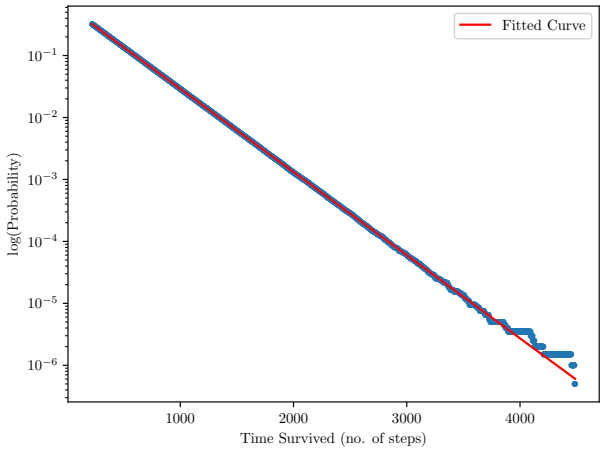


(b) Histogram of probability of dying on particular step in a logarithmic scale

Fig. 2. Histograms showing the Probability of dying on a particular step in an infinite square well with $J = 20$. As can be seen, the peak is away from the origin, as is expected since it is not likely for a walker to die on a step n where $n < J$. The exponential decay after the peak is evident, implying a straight line shape if plotted on a logarithmic scale, which can be seen on the right hand side plot. In this logarithmic scale plot, the peak being away from the origin is clearer.



(a) Histogram of probability of surviving to at least a particlar step



(b) Histogram of probability of surviving to at least a particular step in a logarithmic scale

Fig. 3. Histogram showing the Probability of surviving to at least a particular step in an infinite square well with $J = 20$. This is a cumulative sum of the bins in Figure 2a. As can be seen, the peak is at the origin, since it is certain that no walker will die on the first step. An exponential decay curve provides a good fit, with an R^2 value of 0.9999998, very close to 1. Plotting on a logarithmic scale shows the straight line fit, the gradient of which is λ, giving $\lambda J^2 = 1.2334$, with a negligible error.

$$p(j-1,n) = p(j,n) - \frac{\partial p}{\partial j} + \frac{1}{2}\frac{\partial^2 p}{+\partial j^2} + ...$$

$$p(j,n+1) = p(j,n) + \frac{\partial p}{\partial n} + ...$$

We can now substitute these expansions into Equation 5, we find:

$$p(j,n) + \frac{\partial p}{\partial n} = (1 - a(j))\Big(p + \frac{1}{2}\frac{\partial^2 p}{\partial j^2}\Big)$$

But the probability of death $a(j)$ and the second derivative are so small, that their product is neglected. We also let $p(j,n) = q(j)\exp(-\lambda n)$ so that:

$$-\frac{1}{2}\frac{d^2 q(j)}{dj^2} + a(j)q(j) = \lambda q(j)$$

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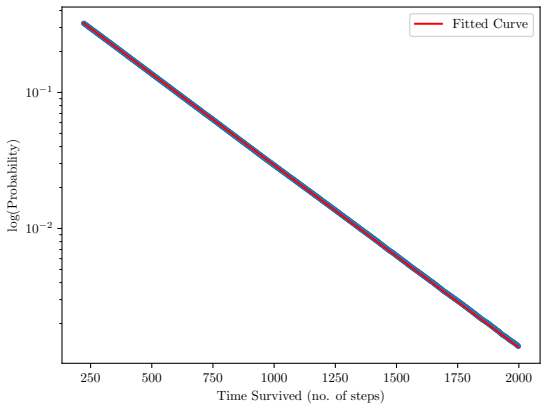

Fig. 4. Histogram plotted on a logarithmic scale showing the Probability of surviving to at least a particular step in an infinite square well with $J = 20$, and also introducing a maximum number of steps at 2000, after which all walkers will die. This saves computational resources but introduces some systematic error, as there will now be a disproportionately high number of walkers in the 2000 steps bin.

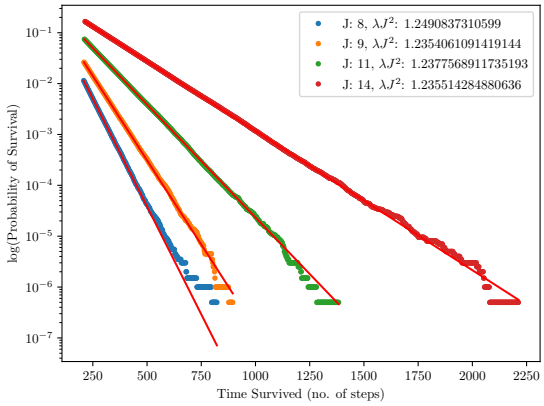

Fig. 5. Histogram plotted on a logarithmic scale showing the Probability of surviving to at least a particualr step in different infinite square wells with different boundaries J. The λJ^2 values for each are shown. The values get closer to the theoretical value of $\frac{\pi^2}{8}$ as we increase the size of the well. This is likely due to more walkers surviving to a higher number of steps, as the well size is increased.

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