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

Sai Pandian, ID: 29899923

***Abstract*—Provide a summary of the session. What was done, what measurements were taken, brief methods, what calculations, brief conclusion. The Abstract should be approximately 250 words or fewer, italicized, in 10-point Times (or Times Roman.) Please leave two spaces between the Abstract and the heading of your first section. It should briefly summarize the essence of the paper and address the following areas without using specific subsection titles. Objective: Briefly state the problem or issue addressed, in language accessible to a general scientific audience. Technology or Method: Briefly summarize the technological innovation or method used to address the problem. Results: Provide a brief summary of the results and findings. Conclusions: Give brief concluding remarks on your outcomes. Detailed discussion of these aspects should be provided in the main body of the paper.**

***Index Terms*—keywords, temperature, xxxx equation, etc.**

I. Introduction

RANDOM walks are a simple model of motion in which a path is described as a succession of steps with each step being in a random direction on some vector space. Random walks are useful in modelling many physical processes that are perceived as having a pseudo-random mechanism . Their applications range from Biology to the Stock Market. This paper aims to explore how Random Walk Simulations can be implemented to calculate the ground state energies of different quantum systems.

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II. Theoretical Background

Random walks work descibe motion as a series of steps, with the direction of each step being random. Figure 1 demonstrates this concept by considering a one-dimensional line. On this line, the "walker" starts at the origin, and walks a total of 20 steps. The walker at each step has a equal chance of stepping forwards, or stepping backwards.

As can be seen 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 long computations.

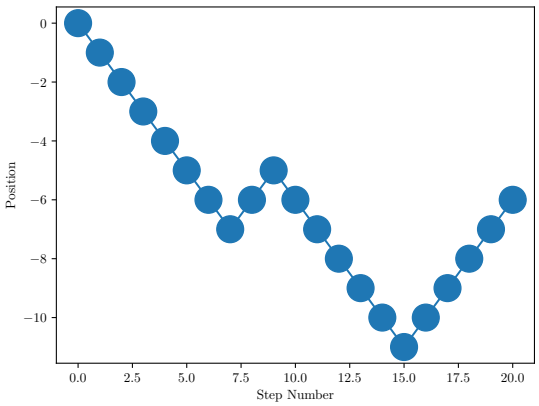

Fig. 1. Illustrations, graphs, and photographs may fit across both columns, if necessary. Your artwork must be in place in the article.

Random Walk simulations can be applied to calculate the ground state energies of Quantum Systems by solving the Schrödinger equation. Consider 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 after a certain number of steps or 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. If we say:

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

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

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

The full derivation is taken from and is shown in Appendix A.

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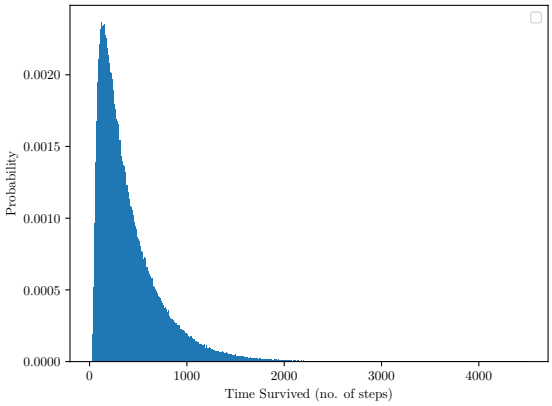
Notice that Equation 1 is in the form of a wave equation, specifically the Schrödinger equation:

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

Comparing Equation 1 and Equation 2, we can see that the probability of death $a(j)$ is analogous to the potential $V(r)$, and the rate of death λ is analogous to the Energy E. Thus, by running the simulation for a particulat potential (i.e. rate of death), one can determine the ground state energy of a system by calculating the rate of death. This is the technique employed in this paper.

III. Results and Discussion

Sample Text



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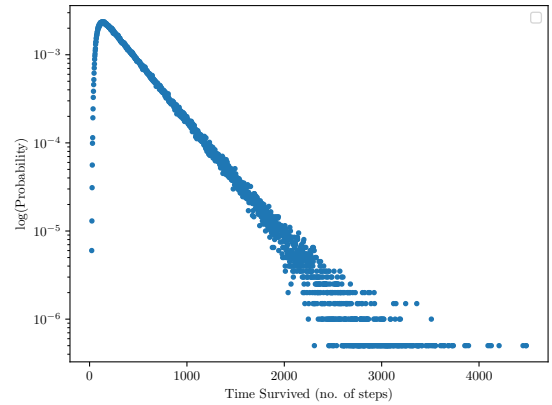

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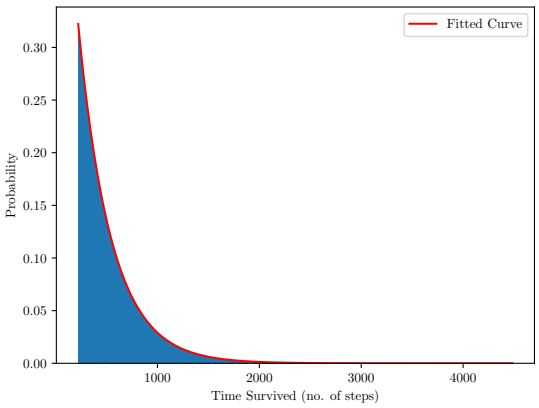

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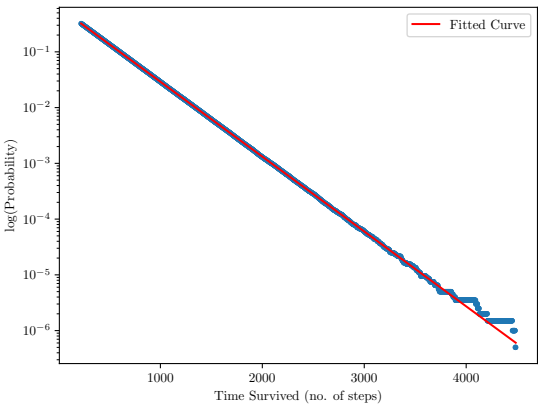

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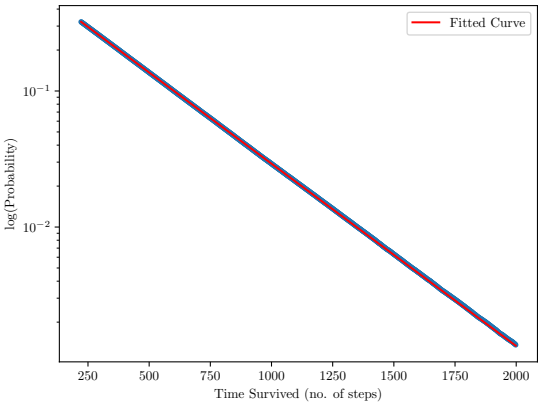

Fig. 6. Illustrations, graphs, and photographs may fit across both columns, if necessary. Your artwork must be in place in the article.

IV. Conclusions

Sample Text

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 $[j\pm1,n]$. So we can say:

$$p(j,n+1)=\frac{1}{2}(1-a(j))(p(j-1,n)+p(j+1,n)) \quad (3)$$

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 $p(j,n+1)$:

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

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

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

We can now substitute these expansions into Equation 3, 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:

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

Acknowledgment

The authors would like to thank...