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

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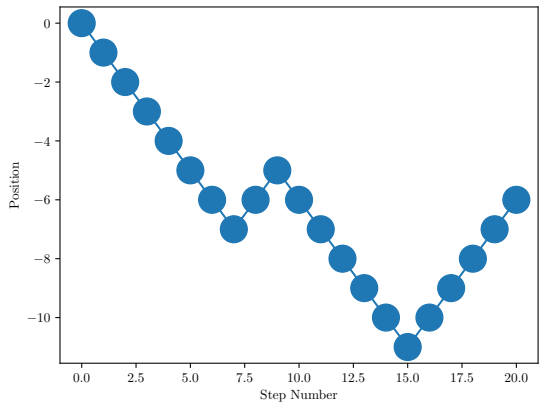

Fig. 1. Illustrations, graphs, and photographs may fit across both columns, if necessary. Your artwork must be in place in the article.

***Abstract*—**

***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 cite 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 more quantum systems.

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.

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:

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

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

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

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

Notice that Equation 2 is in the form of a wave equation, specifically the Schrödinger equation:

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

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. Thus, by running the simulation for a particular 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. Method

The Random Walk is implemented computationally and cite

is extensible to multiple dimensions. For a N-dimensional lattice, at each point there are $2N$ possible directions for the walker to move. So a direction is selected randomly using a Mersenne Twister pseudorandom number generator (pRNG). This algorithm was chosen as it is a very fast implementation of a pRNG and it passes many statistical randomness tests [cite], having a very large period of $2^{19937-1}$.

The random walk ends when a walker dies, with a specifically chosen $a(j)$. Initially, the $a(j)$ is chosen to be that of an infinite square well, that is:

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

where J is a well-defined boundary. So the walker has no chance of dying whilst within the well, but will die immediately once reaching the boundary. As explained in Section II, we expect that given sufficient time, all the walkers will reach the boundary and die. But in order to save computational resources, a maximum number of steps may also be defined, such that a walker will also die should they move that number of steps without reaching a boundary. This was not initially implemented, as it can introduce systemic errors, since there would be a disproportionate number of walkers dying on the maximum number of steps.

Thus, the Schrödinger equation inside a one-dimensional infinite square well 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 $x = J \times j/R$, such that $j = R$ corresponds to the walker being at the boundary, we obtain:

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

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

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

So, by calculating the death rate λ, we can find the ground state energy of a particle in an infinite square well.

But the known ground state of a particle in an infinite square well is $\frac{\pi^2}{8}\frac{\hbar^2}{mJ^2}$. This implies that we expect $\lambda R^2 = \frac{\pi^2}{8}$ where R is the boundary of the well. Thus, we expect to find a λ that is close to this theoretical value.

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

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

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.

Varying the boundary J of the square well will affect the accuracy of the final answer, and this is investigated here.

IV. Results and Discussion

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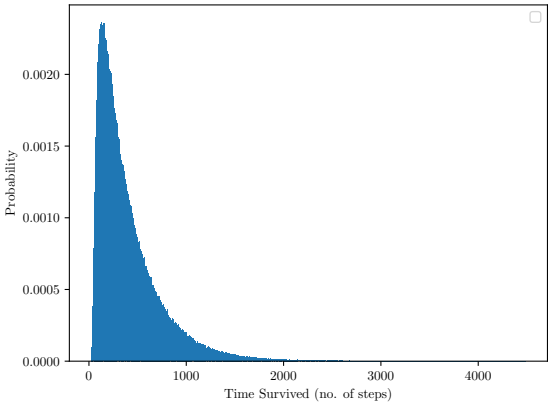

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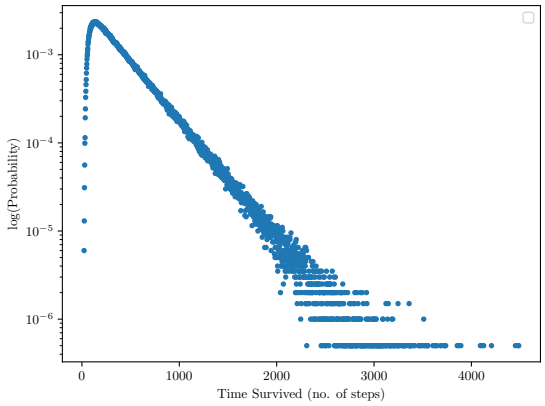

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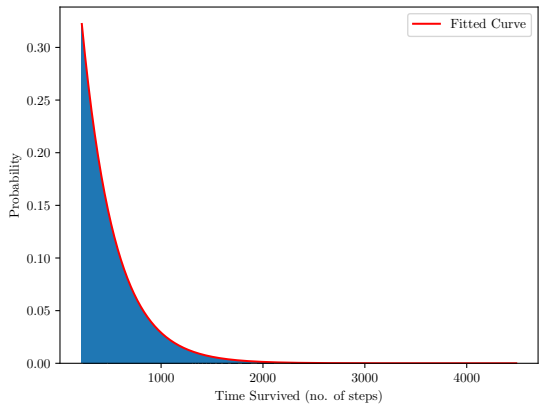

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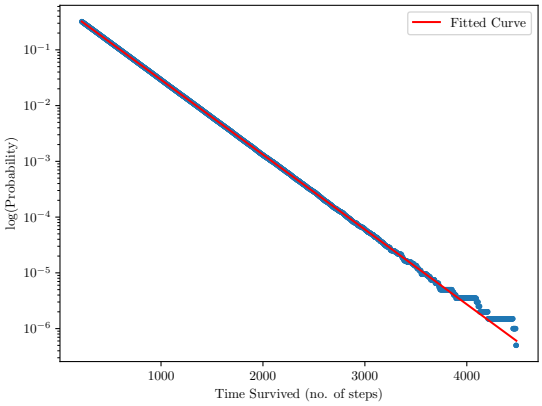

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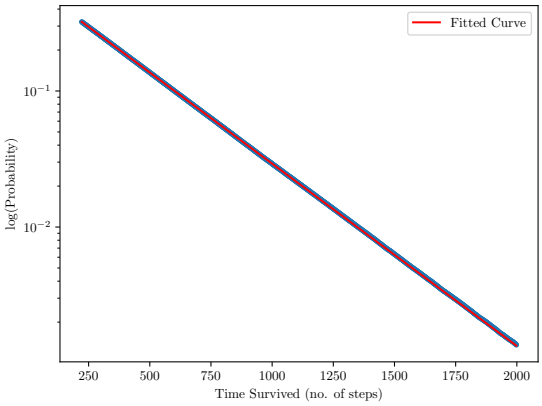

Fig. 6. Illustrations, graphs, and photographs may fit across both columns, if necessary. Your artwork must be in place in the article.

V. 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:

$$p(j,n+1) = \frac{1}{2}(1-a(j))(p(j-1,n)+p(j+1,n)) \quad (4)$$

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 4, 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:

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