Random Walks for Determining Energies of Quantum Systems

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Abstract

A computer simulation is used to estimate the energy of the ground state of different quantum systems. The ground state energy of an infinite 2-Dimensional circular well was estimated with the second quantum number m = 0, 1, 2. The ratio of these was found to be 1.39 : 3.64 : 6.66. The usefulness of this method and when it's use could be appropriate is also discussed.

1 Introduction

Consider an N-dimensional simple lattice. A drunkard starts at the origin of the lattice and takes a random step towards one of the 2N adjacent lattice points. He then continues to do this towards the concurrent adjacent lattice points. The probability that he ever returns to his starting point is required to get the ground state energy of quantum systems.

An extra feature necessary for this simulation is that the drunkard has a probability of being arrested, and his walk stopped at each lattice point, depending on the potential at that point. The ground state energy depends on the average time before the drunkard gets arrested.

In this report the ground state energy for the infinite 2-Dimensional circular well is estimated. After this has been obtained the simulation is then altered to find the ground state energies for the same system with the second quantum number at m=1 and m=2.

When these results have been found, and their accuracy estimated, the usefulness and accuracy of this simulation is assessed and when it might be appropriate to use is discussed.

2 Theory

For the 2-Dimensional problem we consider the coordinates j_1 and j_2 as the coordinates of the drunkard in the lattice and n as the number of steps he has taken. The probability $p(j_1, j_2, n)$ is the probability that the drunkard is at site (j_1, j_2) after n steps. If he is at site (j_1, j_2) after $n+1$ steps then two things must be true: he has not been arrested and he was at either site (j_1-1, j_2), (j_1+1, j_2), (j_1, j_2-1) or (j_1, j_2+1) after n steps. The probabilities are therefore related by:

$$p(j_1, j_2, n+1)=\frac{1}{2}[1-a(j_1, j_2)][p(j_1+1, j_2, n)+p(j_1-1, j_2, n)+p(j_1, j_2+1, n)+p(j_1, j_2-1, n)]$$

where $a(j_1, j_2)$ is the probability of the drunkard being arrested at site (j_1, j_2).If the probability of being arrested is small and the walk continues for a long time then we can assume $p(j_1, j_2, n)$ will vary smoothly with j_1, j_2 and n. We can then use Taylor's theorem to write:

$$p(j_1+1, j_2, n)=p(j_1, j_2, n)+\frac{\partial p}{\partial j_1}+\frac{1}{2}\frac{\partial^2 p}{\partial j_1^2}+...$$

$$p(j_1-1, j_2, n)=p(j_1, j_2, n)-\frac{\partial p}{\partial j_1}+\frac{1}{2}\frac{\partial^2 p}{\partial j_1^2}+...$$

$$p(j_1, j_2+1, n) = p(j_1, j_2, n) + \frac{\partial p}{\partial j_2} + \frac{1}{2}\frac{\partial^2 p}{\partial j_2^2} + \ldots$$

$$p(j_1, j_2-1, n) = p(j_1, j_2, n) - \frac{\partial p}{\partial j_2} + \frac{1}{2}\frac{\partial^2 p}{\partial j_2^2} + \ldots$$

$$p(j_1, j_2, n+1) = p(j_1, j_2, n) + \frac{\partial p}{\partial n} + \ldots$$

Substituting these values into the original formula gives:

$$p + \frac{\partial p}{\partial n} = [1 - a(j_1, j_2)][4\mathrm{p} + \frac{\partial^2 p}{\partial j_1^2} + \frac{\partial^2 p}{\partial j_2^2}]$$

Since *a* is small its product with the second derivatives can be neglected giving:

$$\frac{\partial p}{\partial n} = \frac{1}{4}[\frac{\partial^2 p}{\partial j_1^2} + \frac{\partial^2 p}{\partial j_2^2}] - a(j_1, j_2)\, p$$

If we let $p(j_1, j_2, n) = q(j_1, j_2)\exp(-\lambda n)$ then:

$$-\frac{1}{4}[\frac{\partial^2 q}{\partial j_1^2} + \frac{\partial^2 q}{\partial j_2^2}] + a(j_1, j_2)q = \lambda q$$

This is similar in appearance to the Schrödinger equation. To estimate the rate of arrest λ we can record the number of drunkards *k* that survive *n* steps, plot a graph of log*k* against *n* and measure the slope.

The Schrödinger equation for a particle in a 2-Dimensional well is:

$$\frac{\hbar^2}{2\mathrm{m}}[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2}] = E\Psi$$

For an infinite circular well the potential is $V(x, y) = 0$ for $x^2 + y^2 < b^2$ and $V(x, y) = \infty$ for $x^2 + y^2 > b^2$

If we let $x^2 + y^2 = b^2\frac{(j_1^2 + j_2^2)}{J^2}$ so that $x^2 + y^2 = b^2$ when $j_1^2 + j_2^2 = J^2$, this gives:

$$-\frac{1}{4}[\frac{\partial^2 \Psi}{\partial j_1^2} + \frac{\partial^2 \Psi}{\partial j_2^2}] = \frac{Emb^2}{2\hbar^2 J^2}\Psi$$

Comparing this to the drunkards walk we find that the energy *E* is related to the rate of arrest λ by:

$$\frac{Emb^2}{2\hbar^2 J^2} = \lambda \quad \text{so that,} \quad E = \frac{2\hbar^2}{mb^2}(\lambda J^2)$$

(λJ^2) can be estimated by the simulation meaning we only need to work it out and multiply it by the constants given in order to estimate the energy of the ground state of the system.

3 The Computer Simulation

It is a fairly simple process to create a program that will simulate the drunkards walk, however to get reliable and accurate results many walks need to be simulated, and for the more complicated problems (m = 1, 2) this can prove difficult with limited computing power available.

The value of *J* in the program determines how much systematic error there is in the result. Smaller values of *J* produce more systematic error because the continuum in the well needs to be replaced by a lattice of discrete points. In order to achieve the most accurate results possible the value of *J* was increased along with the number of walks done (this needs to be increased alongside *J* to maintain the precision of results) until the program took an unreasonably long time to run (< 60 seconds). The number of walks done was increased prior to this until the graph produced had little error, and the results of each graph were consistent (within ~10% of each other). With a small value of J (J = 8) this was achieved without needing too much processing time, leaving scope for increasing J.

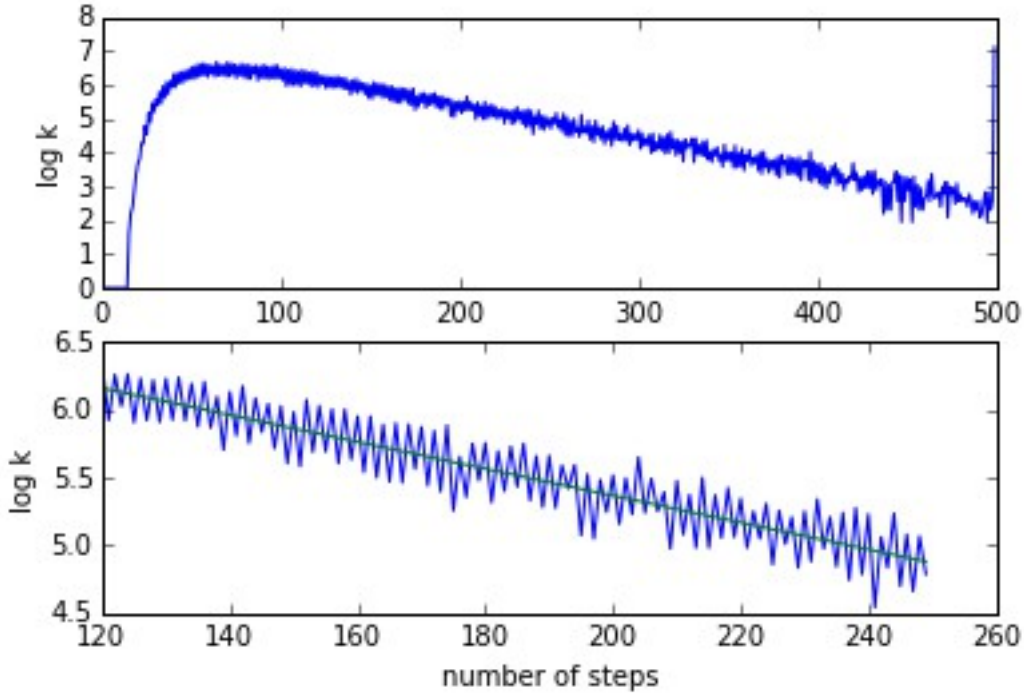
After these values of *J* and number of walks were found the programs were run again, 5 times to make sure the results were still within ~10% of each other and the mean of these values was used for the final results.

In order to find the value of λ, the polyfit() function of numpy was used to get a linear line of best fit for the straight line part of the log graph. The gradient of this line was multiplied by J^2 to find the energy ratios of m = 0, 1, 2.

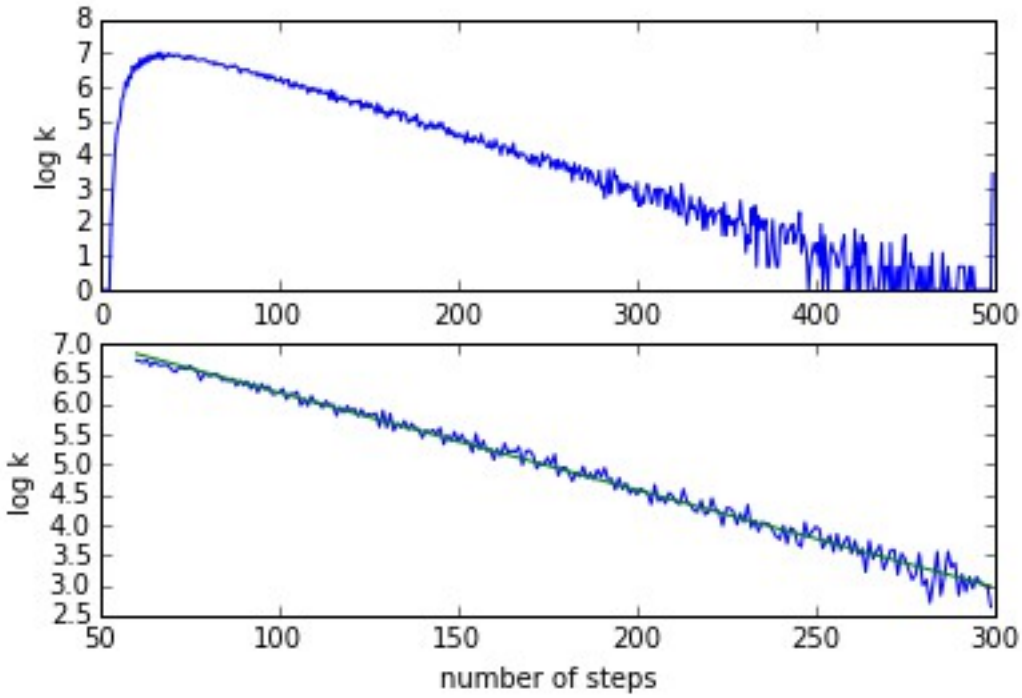
To find the ground state energies of m = 1, 2 only a small change in the simulation was necessary. Since m = 1 has a nodal line along the x or y axis, the program was changed so the drunkard started at either x or y = J/2 and he was arrested if he got to the relevant axis (x or y = 0). Similarly, since m = 2 has two nodal lines on the x and y axis, the program was changed so the drunkard started at x, y = J/2 and he was arrested if he ever crossed the x or y axis.

4 Results

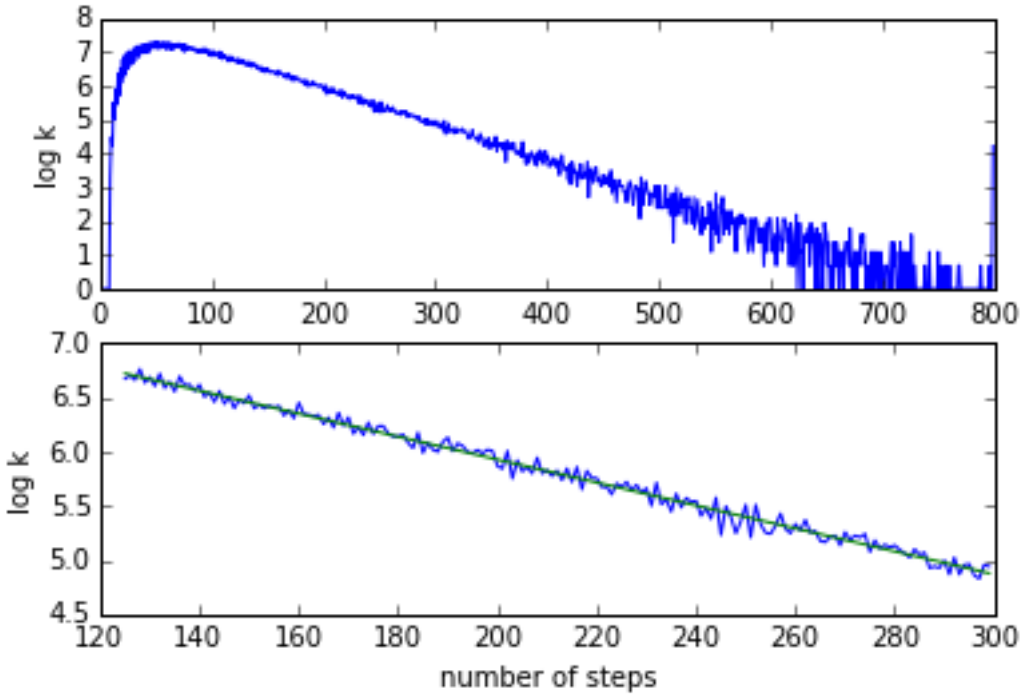
Figures 1 and 2 show the results for m = 0. The second figure is the truncated version of the full figure, showing which part of the graph the gradient was taken from. As expected the graph peaks, then exponentially declines. Figures 3 and 4, and 5 and 6, show the data for m = 1 and m = 2 respectively.



Figures 1 and 2: Drunkards walk graph for m = 0



Figures 3 and 4: Drunkards walk graph for m = 1



Figures 5 and 6: Drunkards walk graph for m = 2

After all these simulations were run the results were tabulated, and the mean and standard deviations of each value of *m* worked out in figure 7, below.

	1st λJ^2 value	2nd λJ^2 value	3rd λJ^2 value	4th λJ^2 value	5th λJ^2 value	Mean λJ^2 value	Standard Deviation
M = 0	1.428	1.410	1.360	1.341	1.433	1.394	0.041 (0.01845)
M = 1	3.645	3.633	3.623	3.688	3.635	3.645	0.012 (0.0054)
M = 2	6.582	6.702	6.674	6.710	6.616	6.657	0.046 (0.0210)

Figure 7: Table showing all results from the simulation

Using this data the ratio of energies in the circular well with m = 0, 1, 2 are:
1.39 +/- 0.02 : 3.64 +/- 0.01 : 6.66 +/- 0.02

However these results, especially for the higher values of *m,* are likely to be out by a small margin due to systematic errors in the simulation.

5 Discussion and Conclusion

From these results we can conclude that using a computer simulation to calculate the ground state energy of quantum systems can be very precise, due to the program's results being very reliable and having low standard deviations, however it is unclear just how accurate they are.

When changing the value of J in the computer program, the average results didn't vary by more than a margin of ~10% though, so I think we can be confident the energies we have obtained are accurate to at least this margin.

In performing these simulations, I have found that this method of computing energies is very inefficient. Even to get these values a lot of computing time was needed. To get energies at a more accurate level (e.g. 1%) the values of J and the number of walks performed would need to be increased a huge amount and could easily take hours, or even days, to produce good results.

However, the program was extremely easy to alter to calculate the energies for m = 1, 2, and changing the number of dimensions in the lattice was also very easy. Therefore I think this method of calculating the energies of quantum systems, could be useful for calculating the energies of higher dimensional systems, and values of *m*.

Bibliography

Barnes and Daniell, Nuclear Physics B257, [FS14], 173, 1985.