PHYS6017 Project B2

COMPUTER TECHNIQUES IN PHYSICS

Random walks for quantum mechanics

Consider an N dimensional simple lattice. A drunkard starts at the origin and makes a step to any of the $2N$ adjacent lattice points. He then makes similar steps to adjacent points. This random walk described in projects "Recurrent random walks on lattices" and "Theoretical results on recurrent random walks" can be used to get the ground state energy of quantum systems.

The extra feature necessary is that there is a probability of the drunkard being arrested that depends on the potential at that point. The ground state energy depends on the average time he survives before being arrested. For the moment we consider the one dimensional problem. Let $p(j,n)$ be the probability that the drunkard is at site j after n steps. If he is at site j after $n+1$ steps then two things must have happened: he must not have just been arrested and he was either at site $j-1$ or at site $j+1$ after n steps. The probabilities are therefore related by:

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

where $a(j)$ is the probability of being arrested at site j. If the probability of being arrested is very small and the drunkard has been walking for a long time $p(j,n)$ will vary smoothly with j and with n. We can therefore regard p as a function of continuous variables j and n and use Taylor's theorem to write

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

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

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

Putting these into the above equation we get

$$p + \frac{\partial p}{\partial n} = [1-a(j)]\left[p + \frac{1}{2}\frac{\partial^2 p}{\partial j^2}\right].$$

The term a(j) is small and so is the second derivative, so their product can be neglected. This gives

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

Finally if we let $p(j,n) = q(j)\exp(-\lambda n)$ we get

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

which looks similar to the Schrödinger equation. The fact that $p(j,n)$ decays exponentially reflects the fact that drunkards are being arrested, and then their walks are

terminated. We can estimate the rate of arrest λ by counting noting the number of drunkards k that survive n steps and plotting $\log k$ against n to get the slope .

It is implicit in the assumption that $p(j,n)$ can be written as the product of a spatial distribution and a time decay that n is large so that the drunkard has covered a reasonable fraction of the possible sites; some experimenting will be required to find how small it can be made without introducing significant errors. If it is too small the graph of $\log k$ against n will show significant curvature and there is no point in continuing until all the walkers have been arrested because the small numbers surviving at the end show such large fluctuations that no useful information is gained.

To show how the random walk is used to obtain energies I will go over the details for one particular potential, and I suggest that you reproduce the known results numerically before attempting a new problem.

Consider the case of a particle confined in an infinite square well potential. The potential V can be taken as zero for $-a < x < +a$ and infinite outside this range. The Schrödinger equation is

$$\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi.$$

Let $x = aj/J$, so that $j = J$ corresponds to the edge of the well. Making this change of variable gives

$$-\frac{1}{2}\frac{\mathrm{d}^2\psi}{\mathrm{d}j^2} = \frac{ma^2E}{\hbar^2J^2}\psi.$$

To compare with the drunkard's walk we note the energy E is related to the rate of arrest λ by $\lambda = Ema^2/\hbar^2J^2$ so $E = (\hbar^2/ma^2)(\lambda J^2)$. The quantity λJ^2 is conveniently determined by the computer program, the remaining constants can be inserted if the energy is required in joules. The energy of the ground state of a particle in a potential well is $E = \pi^2\hbar^2/8ma^2$, so the value for λJ^2 should be $\pi^2/8$.

The walk is started at $j = 0$ and continues, incrementing or decrementing j, until the drunkard reaches $j = +J$or$-J$ when he is instantly arrested, or the walk has gone on so long that he is very lucky to have survived so far.

A reasonable starting value for J is 8 and initially you should continue walks for up to 100 steps. Several hundred walks surviving to 50 steps will be needed to get anything like a reliable estimate of the energy. You should repeat your measurements several times to get some idea of the reliability. Confirm the theoretical result for the energy and determine the range of n that contributes usefully to the answer.

Try varying J to see the effect. A smaller value of J will produce systematic errors because the continuum of space has been replaced by a lattice of $2J$ points. On a fast computer there is scope for increasing J and increasing the duration of the walks to reduce systematic errors.

The Schrödinger equation for a particle in a two dimensional well is

$$\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}\right] = E\psi$$

where the potential is $V(x,y) = 0$ for $x^2 + y^2 < b^2$, $V(x,y) = \infty$ for $x^2 + y^2 > b^2$.

The algorithm for the two dimensional case is similar to the one dimensional but you will need to work through the derivation from the beginning. The probability $p(j,n)$

will become a function of two integers j_1 and j_2 corresponding to the x and y coordinates and there is a probability of $\frac{1}{4}$ of the drunkard moving to one of the four adjacent lattice points, $j_1 \pm 1, j_2 \pm 1$. Otherwise the coding is similar to the previous case. Obtain the ground state energy and an estimate of its reliability.

The method described gives the ground state energy. In the case of a symmetric potential one of the excited states will have a nodal line in the wavefunction along the x or y axis and will be two-fold degenerate. Another will have nodal lines along both axes. The energy of these states can be found by starting the walk away from the origin and immediately arresting the drunkard if he (or she) ever gets to the appropriate axis as well as to the circular boundary. You will probably run out of computer power before finding these energies at all accurately, but try.

You will rapidly discover that as a method of solution of the one or two dimensional Schrödinger equation this is incredibly inefficient. Its importance lies in the fact that it works almost as well in many dimensions whereas other methods deteriorate badly.

Further details can be found in Barnes and Daniell, Nuclear Physics B257, [FS14], 173, 1985.

So that you can check your results the energies for the circular well are in the ratio 1.44 : 3.61 : 6.50, but pretend you don't know this.