ONE DIMENSIONAL RANDOM WALK WITH A PARTIALLY REFLECTING BARRIER

By G. Lehner

Laboratorio Gas Ionizzati (EURATOM—C.N.E.N.)

0. Summary. In the present paper we consider the one dimensional random walk of a particle restricted by a partially reflecting barrier. The reflecting barrier is described by a coefficient of reflection r. The probability of finding a particle at a lattice point m after N steps is calculated and expressed in terms of hypergeometric functions of the ${}_{2}F_{1}$ -type.

Other theorems are deduced concerning the one dimensional random walk. For instance the number of paths leading from one lattice point to another lattice point in N steps and showing a given number of reflections at the barrier is calculated.

1. Introduction. We consider a particle moving on the lattice points of a straight line. The distances between these points are constant and equal L. In equally spaced intervals of time the particle moves one step to the right or one step to the left in a purely statistical manner with probabilities $\frac{1}{2}$. One calls this a random walk in one dimension [1], [3]. It is a discrete model of diffusion or Brownian motion, which one can derive from it by certain limiting processes [1], [4].

In the simplest case the motion of the particle is not restricted by any boundary conditions and it is easy to calculate the probability P(m, N) of finding the particle at the lattice point mL after N steps assuming that it was at the origin at the beginning (see for instance [3]). The result is

(1)
$$P(m, N) = \left(\frac{1}{2}\right)^{N} {N \choose (N-m)/2} \quad \text{if } N-m \text{ even,}$$

$$= 0 \quad \text{if } N-m \text{ odd.}$$

If there is a reflecting or absorbing barrier at the lattice point m_1L , one can reduce the problem to Equation (1). One makes use of a reflection principle, that is the use of the image point of m at the mirror m_1 ,

$$(2) m_2 = 2m_1 - m.$$

Omitting the unit of length one derives the equation

(3)
$$P(m, N; m_1)$$

$$= \left(\frac{1}{2}\right)^N \cdot \left[\binom{N}{(N-m)/2} \pm \binom{N}{(N-m_2)/2} \right] \quad \text{if } N-m \text{ even}$$

$$= 0 \quad \text{if } N-m \text{ odd}$$

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where the upper sign holds for a reflecting barrier and the lower sign for an absorbing barrier.

These are two special cases of the general problem of a partially absorbing and partially reflecting barrier. This is a problem of practical interest, because plasmas and gases are often confined by such barriers. This generalized problem will be considered in the present paper.

The barrier is described by a coefficient of reflection r, which is the probability that a particle hitting the barrier will be reflected. Then (1-r) is the probability of absorption. Usually one considers that $0 \le r \le 1$, but one can also consider that r > 1, thinking for example of the production of secondary particles. In this case one cannot speak of probabilities. One could rather call r a coefficient of secondary emission and P a particle density. The equations derived below are not changed by this difference.

We denote by $P(m, N; m_1, r)$ the probability of a particle going from 0 to m in N steps in the presence of a partially reflecting barrier (r) at m_1 . The next three subsections will be devoted to the calculation of this quantity.

2. Procedure for the calculation of P. We start by considering the number of paths leading from 0 to m in N steps with n reflections at m_1 . This number we denote by $Z_n(m, N; m_1)$. The maximum number of reflections is

$$(N+m)/2 - m_1 + 1 = (N-m_2)/2 + 1.$$

Abbreviating

$$(4) \qquad (N-m_2)/2 = y$$

we have

(5)
$$P(m, N; m_1, r) = \sum_{n=0}^{y+1} \left(\frac{1}{2}\right)^{N-n} Z_n(N, m; m_1) r^n$$
$$= \left(\frac{1}{2}\right)^N \sum_{n=0}^{y+1} Z_n \cdot (2r)^n.$$

It is useful to apply again the above mentioned reflection principle (see Equation (2)). Defining a new function $Y_n(m_2, N; m_1)$ which is the number of paths leading from 0 to m_2 in N steps touching or crossing m_1 n times. For $n \ge 1$, Z_n may be related to Y_n :

(6)
$$2^{n-1}Z_n(m, N; m_1) = Y_n(m_2, N; m_1), \quad m_2 = 2m_1 - m$$

while for n = 0

(7)
$$Z_0(m, N; m_1) = {N \choose (N-m)/2} - {N \choose y}$$

so that from (5)

(8)
$$P(m, N; m_1, r) = \left(\frac{1}{2}\right)^N \left[\binom{N}{(N-m)/2} - \binom{N}{y} + 2 \sum_{n=1}^{y+1} Y_n(m_2, N; m_1) r^n \right].$$

In the two following sections we will calculate the numbers Z_n and Y_n and evaluate the sum in Equation (8).

- 3. Calculation of Z_n and Y_n . We start from two theorems concerning the one-dimensional random walk, which are derived in reference [3] (Theorems 2 and 3, pages 76, 77). Here notations will be slightly changed.
- (a) The number of paths leading from 0 to m such that m is reached for the first time at the Nth step is

(9)
$$f_N^m = (m/N) \binom{N}{(N+m)/2} \quad \text{if } N+m \text{ even } and \ N \ge m$$
$$= 0 \quad \text{if either } N+m \text{ odd } or \ N < m.$$

(b) The number of paths starting from 0, which after N steps return to 0 for the nth time is

(10)
$$g_N^n = 2^n [n/(N-n)] \binom{N-n}{N/2} = 2^n f_{N-n}^n \quad \text{if } N \text{ even}$$
$$= 0 \quad \text{if } N \text{ odd.}$$

As f_N^m for m = 0 and N = 0, and g_N^n for n = 0, N = 0 are not yet defined by Equations (9) and (10) we complete these equations by setting

(11)
$$f_N^0 = \delta_{0N}, \quad g_N^0 \doteq \delta_{0N}.$$

With the help of Equations (9) and (10) we can write

$$(12) Y_n(m_2, N; m_1) = \sum_{l>k}^{N-m_2+m_1} \sum_{k=m_1}^{N-m_2+m_1} f_k^{m_1} f_{N-l}^{m_2-m_1} g_{l-k}^{n-1}, 1 \le n \le y+1.$$

The contributions do not vanish only if N + m, $m_1 + k$ and $m_1 - l$ all are even. We can fulfill the last two conditions by the introduction of new indices of summation, $2k' = k - m_1$, $2l' = l - m_1$. Writing again k, l instead of k', l' and using Equations (4) and (10) we derive from Equation (12)

$$(13) Y_n(m_2, N; m_1) = \sum_{l \ge k}^{y} \sum_{k=0}^{m_1} f_{m_1+2k}^{m_1-m} f_{N-m_1-2l}^{n-1} f_{2(l-k)-n+1}^{n-1} 2^{n-1}$$

Let us consider Y_1 first. From Equation (11) it follows that

(14)
$$Y_1(m_2, N; m_1) = \sum_{k=0}^{y} f_{m_1+2k}^{m_1} f_{m_2-m_1+2y-2k}^{m_2-m_1}.$$

It is possible to show that Y_1 is independent of m_1 if m_2 is fixed. So we can sum (14) using any m_1 we like, for instance $m_1 = 0$. Using Equation (11) we thus get

$$(15) Y_1 = f_{m_2 + 2y}^{m_2}.$$

We may reach the same result by using the relation

(16)
$$\sum_{k=0}^{y} f_{a+2k}^{a} f_{b+2y-2k}^{b} = f_{a+b+2y}^{a+b}$$

which can be verified by induction with respect to b.

By applying Equation (16) twice one can evaluate the double sum (13) to get

(17)
$$Y_n = 2^{n-1} f_{m_2+2\nu-n+1}^{m_2+n-1} Z_n = f_{m_2+2\nu-n+1}^{m_2+n-1}$$

Before proceeding we shall discuss some relations between these numbers. The number of all paths from 0 to m_2 is according to Equation (1)

$$\binom{n}{(N-m_2)/2}=\binom{2y+m_2}{y+m_2}.$$

Therefore,

(18)
$$\sum_{n=1}^{y+1} Y_n = \sum_{n=1}^{y+1} 2^{n-1} f_{m_2+2y-n+1}^{m_2+n-1} = \begin{pmatrix} 2y + m_2 \\ y + m_2 \end{pmatrix}$$

which can also be proved by induction again. Writing (18) in a different way we have the interesting relation

(19)
$$\sum_{k=0}^{(b-a)/2} f_{b-k}^{a+k} \cdot 2^k = \binom{b}{(b+a)/2}.$$

Furthermore it is interesting to observe that the \mathbb{Z}_n fulfill the difference equation

$$(20) Z_n(y, m_2) - Z_{n+1}(y, m_2) = Z_{n-1}(y-1, m_2).$$

This gives a scheme for a step-by-step calculation of $Z_n(y, m_2)$ in terms of $Z_1(y, m_2)$. $Z_n = 0$ for n > y + 1 and $Z_{y+1} = 1$, so that we have the following table:

			y		
n	0	1	2	3	• • •
1	1	m_2	$(m_2^2 + 3m_2)/2$		
2	0	1	$1 + m_2$	$(m_2^2 + 5m_2 + 4)/2$	
3	0	0	1	$2 + m_2$	
4	0	0	0	1	
:		,			

Another consequence of Equation (20) is

(21)
$$Z_n(y, m_2) = \sum_{k=n-1}^{y} Z_k(y-1, m_2).$$

We can rewrite this equation in a form similar to Equation (19), namely,

(22)
$$\sum_{k=0}^{(b-a)/2} f_{b-k}^{a+k} = f_{b+1}^{a+1}.$$

This again can be directly provided by induction.

To conclude this section we can formulate the following theorems:

(a) The number of paths from 0 to m in N steps showing n reflections at m_1 ($m_1 \ge m, n \ge 1$) is given by

(23)
$$Z_n(m, N; m_1) = f_{N-n+1}^{2m_1-m+n-1}$$

(b) The number of paths from 0 to m_2 in N steps crossing or touching n times m_1 ($0 \le m_1 \le m_2$, $n \ge 1$) is given by

$$(24) Y_n(m_2, N) = f_{N-n+1}^{m_2+n-1}$$

(c) The number of paths from 0 to m in N steps never crossing m_1 but showing at least one reflection at m_1 is given by

(25)
$$\sum_{n=1}^{y+1} Z_n(m, N; m_1) = f_{n+1}^{2m_1 - m + 1}.$$

This is proved with the help of Equation (22). Equations (16), (19) and (22) are important relations between the f's completing these theorems.

Many well-known theorems are special cases of Equations (23), (24), (25) (see for instance [3]).

4. The summation of all the contributions. With k = n - 1 we find that corresponding to Equations (8) and (17)

(26)
$$P(m, N; m_1, r) = {\left(\frac{1}{2}\right)}^N \left[{N \choose (N-m)/2} - {N \choose (N-m_2)/2} + 2r \sum_{k=0}^y f_{m_2+2y-k}^{m_2+k} (2r)^k \right]$$

where from Equation (9)

(27)
$$f_{m_2+2y-k}^{m_2+k} = \frac{m_2+k}{m_2+2y-k} \cdot \frac{(m_2+2y-k)!}{(m_2+y)!(y-k)!}$$

Three special cases can be treated immediately. For r=0 and r=1 we get the result mentioned in Equation (3), where in the case r=1 we have to apply Equation (19). Applying Equation (22) we can treat the case $r=\frac{1}{2}$ and find

(28)
$$P(m, N; m, \frac{1}{2}) = (\frac{1}{2})^N \left[\binom{N}{(N-m)/2} - \binom{N}{[N-(m_2+2)]/2} \right].$$

We see that a barrier with $r = \frac{1}{2}$ at m_1 has the same effect as a barrier with r = 0 at $m_1 + 1$, which is easy to understand.

In general one gets hypergeometric functions of the type ${}_{2}F_{1}$. For the relations among the ${}_{2}F_{1}$ we refer to [2]. Applying the definition of ${}_{2}F_{1}$ by a series we find for the sum in Equation (26)

$$\sum_{k=0}^{y} \frac{m_2 + k}{m_2 + 2y - k} \cdot \frac{(m_2 + 2y - k)!}{(m_2 + y)!(y - k)!} (2r)^k$$

$$= \frac{m_2}{(m_2 + y)!} \sum_{k=0}^{y} \frac{(m_2 + 2y - k - 1)! \ k!}{(y - k)!} \frac{(2r)^k}{k!}$$

$$+ \frac{2r}{(m_2 + y)!} \frac{d}{d(2r)} \left(\sum_{k=0}^{y} \frac{(m_2 + 2y - k - 1)! \ k!}{(y - k)!} \frac{(2r)^k}{k!} \right)$$

$$= \frac{(m_2 + 2y - 1)!}{(m_2 + y)! \ y!} \left[m_2 \cdot {}_2F_1(1, -y; -m_2 - 2y + 1; 2r) \right]$$

$$+ 2r \frac{d}{d(2r)} {}_2F_1(1, -y; -m_2 - 2y + 1; 2r) \right]$$

where for the derivative

(30)
$$\frac{d}{dz}[{}_{2}F_{1}(1,b;c;z)] = \frac{b}{c} {}_{2}F_{1}(2,b+1;c+1;z).$$

By virtue of the relations among the so called "contiguous hypergeometric functions" and since

$${}_{2}F_{1}(0,b;c;z) = 1$$

one can express ${}_{2}F_{1}(2, b+1; c+1; z)$ in terms of ${}_{2}F_{1}(1, b; c; z)$ finding

(32)
$$\frac{d}{dz}[{}_{2}F_{1}(1,b;c;z)] = \frac{(1+bz-c){}_{2}F_{1}(1,b;c;z)+c-1}{z(1-z)}.$$

We see that our hypergeometric function fulfills a differential equation of the first order, while in general the hypergeometric functions fulfill a second order equation only,

(33)
$$z(1-z)\frac{d^2u}{dz^2} + [c - (a+b+1)z]\frac{du}{dz} - abu = 0$$

which has two linearly independent solutions,

(34)
$$u_1 = {}_2F_1(a, b; c; z)$$

(35)
$$u_2 = z^{1-c} {}_{2}F_{1}(a-c+1,b-c+1;2-c;z).$$

Now, if one of the two parameters a or b equals 1, for instance if a = 1, we can integrate (33), directly

(36)
$$z(1-z)(du/dz) + (c-1-bz)u = K$$

where K is a constant of integration. Putting K = 0 Equation (36) yields u_2 . Putting K = c - 1 it yields u_1 , which brings us back to Equation (32) again.

Equations (26), (27), (29) and (32) after again applying the relations among contiguous hypergeometric functions may be shown to give

(37)
$$P(m, N; m_1, r) = \left(\frac{1}{2}\right)^N \left\{ \binom{N}{(N-m)/2} + \binom{N}{(N+m-2m_1)/2} \cdot \left[2(r-1)_2 F_1(1, -(N+m-2m_1)/2; -N; 2r) + 1\right] \right\}.$$

This only holds if $m < m_1$. We will come back to the case $m = m_1$ in the next section. Again r = 0 and r = 1 are trivial. To find the previous result for $r = \frac{1}{2}$ anew, one makes use of the relation

$$_{2}F_{1}(1, -b; -c; 1) = 1 + \frac{b}{c} + \frac{b(b-1)}{c(c-1)} + \dots + \frac{b!}{c(c-1)\cdots(c-b+1)} = \frac{1+c}{1+c-b}$$

which holds if b < c and which can be proved by induction.

If r is very small we have to the first order, that is if we consider only paths showing not more than one reflection,

(38)
$$P(m, N; m_1, r) = \left(\frac{1}{2}\right)^N \left[\binom{N}{(N-m)/2} - \binom{N}{(N+m-2m_1)/2} \left[1 - (2m_1-m)2r/N \right] \right].$$

If on the other hand r is very large we use only the highest order term in r, that is the last term of the finite series for ${}_{2}F_{1}$,

$$(39) P(m, N; m_1, r) = \left(\frac{1}{2}\right)^{(N+2m_1-m-2)/2} r^{(N-2m_1+m+2)/2} = \left(\frac{1}{2}\right)^{N-y-1} r^{y+1}$$

which is obvious because the maximum number of reflections is y + 1.

5. Absorption. We now calculate the probability that a particle reaches the barrier at m_1 at its Nth step and is absorbed. First let us consider the probability that the particle reaches the barrier at the Nth step,

$$Q(m_1, N; m_1, r) = \frac{1}{2} P(m_1 - 1, N - 1; m_1, r)$$

$$= \left(\frac{1}{2}\right)^N \binom{N}{(N - m_1)/2}$$

$$\cdot [1 + (r - 1) {}_2F_1(1, -(N - m_1)/2; -N; 2r)]/r$$

which differs from the value $P(m_1, N; m_1, r)$ according to Equation (37) by a factor (1/2r). The probability for absorption consequently is

(41)
$$A(m_1, N; r) = (1 - r) \left(\frac{1}{2}\right)^N \binom{N}{(N - m_1)/2} \cdot \left[1 + (r - 1) {}_2F_1(1, -(N - m_1)/2; -N; 2r)\right]/r.$$

If r is very small this yields

(42)
$$A(m_1, N; r) = \left(\frac{1}{2}\right)^N {N \choose (N - m_1)/2} m_1/N$$

because

$$_{2}F_{1}(1,-(N-m_{1})/2;-N;2r)=1+(N-m_{1})r/N+\cdots$$

- 6. Conclusion. In this paper it has been shown that one can calculate the random walk of a particle restricted by one partially reflecting barrier using combinatorial methods. An attempt has been made to solve the problem of a particle between two partially reflecting barriers using the methods of the present paper and the methods developed by Kac [4] based on the diagonalization of the stochastic matrix of the Markov chain equivalent to the random walk. To date these have not produced any positive results.
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