Z. Phys. B – Condensed Matter 72, 131–138 (1988)

Condensed
Zeitschrift für Physik B Matter

On multiple visits in lattice random walks

G.L. Bleris and P. Argyrakis
Department of Physics, University of Thessaloniki, Thessaloniki, Greece

Received December 14, 1987; revised version March 1, 1988

In the present work we treat in detail the problem of multiple visits in lattice random walks. We show that this problem is closely related to the well-studied property of the number of distinct sites visited at least one in an n-step walk. With simple algebraic manipulations we provide new analytical solutions for the mean number of sites visited exactly a certain number of times, and the mean number of sites visited at least a certain number of times. We find that the moments of these quantities vary asymptotically with time. The resulting exponents exhibit constant gap scaling. Computer simulations are given that are within excellent agreement with the derived expressions.

1. Introduction

The problem of multiple visits (occupancy) during a random walk with jumps only to nearest-neighbor lattice points is quite old [1–5], but still unsolved in its full context. For a particle that performs a random walk in discrete time-steps (n) the occupancy of a lattice site is defined as the number of visits (r) that the particle has made to that site. The occupancy problem refers to the average value of the number of lattice sites with r such visits. Two distinctly different expectation numbers arise here as these sites may have: *(1) exactly* r visits in an n-step walk, or *(2) at least* r visits in such a walk. A special limiting case of the latter property is the number of sites visited at least once (i.e. $r=1$) during an n-step walk, the famous S_n, a property that has attracted considerably more attention over the years [1–10], probably because of its greater relevance to problems of physical and/or chemical character, such as in excitation transfer in solids [9], in biological systems and in trapping [10], etc. However, as it was pointed out recently [11], S_n is useful only when exploring concepts that refer to the overall range of an area or volume, since this range is related to a trapping probability, a cross-section probability for reaction, etc. It gives no information on such characteristics of the walk as the revisitation probability, the distribution of steps in the visited area, etc. Clearly it is properties 1 and 2 mentioned above that fill in this gap. On the basis of these occupancy properties it was thus found [11] that it is possible to recast the S_n formalism in a scaling-type picture via the newly defined information dimension of a random walk process. This is a more generalized form since in addition to periodic lattices it is valid for disordered ones as well, e.g. fractals (with different numerical exponents).

The systematic formalism and techniques developed for these ideas are certainly due to Montroll [2, 3]. He employed a certain form of Green's function, the so-called random walk generating function, from which he was able to derive the asymptotic properties of S_n using a Tauberian theorem. Then, by casting the generating function in the proper form practically all random walk problems were re-defined and solved for: recurrence and first passage times, the occupancy characteristics, the number of visits to a given lattice point, etc. For all these properties only the leading terms were given, which in some cases sufficed and in some did not. Therefore, several works followed in the literature [6–8] that provided explicit correction terms and somewhat revised expressions for the above properties, but mainly for S_n. In this work we discuss these forms for the problem of multiple occupancies, and we solve it exactly in terms of other well-known random walk parameters. We perform all necessary Monte-Carlo computer simulations as additional verification. In Sect. 2 the theo-

retical formalism is developed, the required expressions are derived together with a discussion of previous achievements in studies of these properties. In Sect. 3 the details of the numerical calculations are explained. In Sect. 4 we discuss the problem of the moments of these quantities, and we derive a recursive formula for the moments of all orders. Finally, in Sect. 5 our results are given in several figures with a discussion and conclusions.

2. Theory

The mean number of distinct sites visited at least r times in an n-step walk is $S(r, n)$, while the mean number of distinct sites visited exactly r times is $V(r, n)$. Both $S(r, n)$ and $V(r, n)$ were firstly given by Montroll and Weiss [3] in approximate forms as follows:

$$S(r, n)=n(1-f)f^{r-1} \tag{1}$$

$$V(r, n)=n(1-f)^2 f^{r-1} \tag{2}$$

where f is a function of n and the lattice geometry only. It is rather obvious from Eqs. (1) and (2) that $V(r, n)$ and $S(r, n)$ are directly related as:

$$V(r, n)=(1-f)S(r, n). \tag{3}$$

It is well known that the order of approximation in these expressions varies with the dimensionality and with n: in 3-dim lattices the expressions are rather satisfactory for small n, while in the 2-dim case this happens for extremely large n. Various improvements have thus appeared recently, especially for the 2-dim case [6, 7], that now provide the full $S(1, n)$ behavior with an agreement of the order of 0.1% when compared to the most sophisticated Monte-Carlo simulation data. Thus, Henyey and Seshadri [6] worked out the 2-dim case: they expanded exactly the $S(1, n)$ function in a series with all logarithmic corrections. The resulting integrals were evaluated using a contour integration and the saddle-point technique. Their result is:

$$S(1, n)=[A\,n/\ln B\,n]\sum_{j=0}^{\infty}[C_j/(\ln B\,n)^j] \tag{4}$$

where A, B and C are given constants that depend on the geometry of the 2-dim lattice. The first 20 terms in the series in Eq. (4) were also given [6], but in practice one needs only the first 6 or 7 terms to achieve satisfactory convergence for $S(1, n)$.

Similarly, for 3-dim lattices Blumen and Zumofen [8] improved the Montroll-Weiss treatment for $S(1, n)$ leading to:

$$S(1, n)=a\,n+b\,n^{\frac{1}{2}}+c \tag{5}$$

where a, b, and c are constants depending on the lattice geometry. For simple cubic lattices $a=0.659463$, $b=0.573921$, and $c=0.5827$. Equations (4) and (5) have provided considerable improvement over the original Montroll-Weiss work. They have been tested by their authors, by us, and several others with extensive computer simulations, and it is generally believed that they provide an accuracy of the order of 0.1%. Still they are limited in that they describe only the first term in (1), i.e. the special case when $r=1$. We extend here this work to include any values of r and n by making the appropriate combination of (1) and (2), and by making use of the improvements given in formulae (4) and (5).

In Fig. 1 we can easily see that (2) is only a very rough approximation. Here $V(r, n)$ is plotted as a function of r for a given n, together with simulation results. We observe in this logarithmic plot that both the theoretical prediction and simulation results produce straight lines, but with considerably different slopes, both for the 2-dim and 3-dim cases. One is tempted then to introduce a correction term that would leave the form of the original equation intact, but would affect only its slope. We thus make the assumption – certainly to be tested later on – that the correction is given by two variables, x and y, inserted in the exponents of (2).

By taking the logarithm of both sides the proper $V(r, n)$ equation would have the following form:

$$\ln V(r, n)=x\ln[n(1-f)^2]+y(r-1)\ln(f) \tag{6}$$

where x and y are the necessary correction parameters. It is also true that:

$$\begin{aligned}\sum_r V(r, n)\,r&=[n(1-f)^2]^x\sum_r r\,c^{r-1}\\&=[n(1-f)^2]^x(1+2c+3c^2+4c^3+\ldots)\\&=n\end{aligned} \tag{7}$$

where $c=f^y$. From the above summation we obtain the equation:

$$[n(1-f)^2]^x=n(1-f^y)^2 \tag{8}$$

which shows a non-linear dependence between x and y and allows us to eliminate one of the two parameters (x or y). We thus write:

$$V(r, n)=n(1-f^y)^2(f^y)^{r-1} \tag{9}$$

where x has been eliminated. Equation (9) is a preferable form since it contains the correction term (y) in variable f only, as opposed to x which appears in both n and f. Following the Montroll-Weiss [3] for-

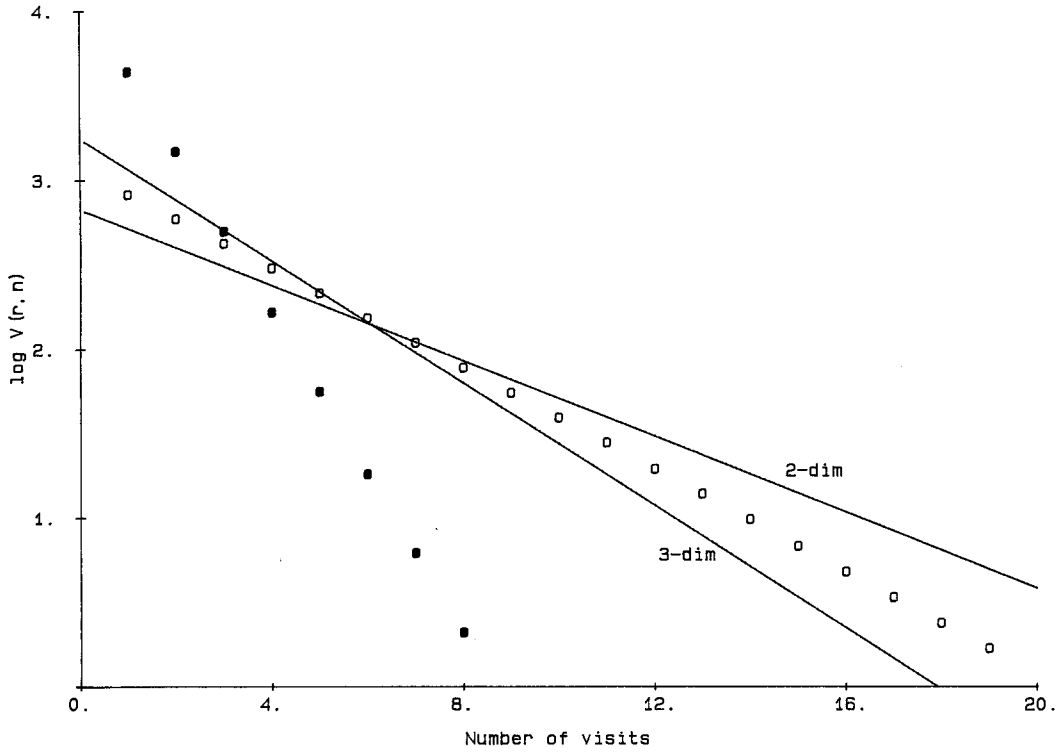

Fig. 1. Logarithmic plot of $V(r, n)$ as a function of r for 2-dim and 3-dim lattices. The solid lines are solutions of (2) (with the f values from (10) and (11)); the circles are simulation results, filled circles: 3-dim, empty circles: 2-dim (see text for details of procedures). Here $n = 10000$ steps

malism f is given by:

$$f = 1 - [\pi/\ln(n)] \quad \text{(2-dim)} \tag{10}$$

$$f = 1 - [2\pi(1/3)^{\frac{3}{2}}/\ln(n)] \quad \text{(3-dim)}. \tag{11}$$

It has also been shown [4] that f is directly connected to the probability for return to the origin, since $f = 1/[1 - P(0, 1)]$, and it is clearly a function of n only. In order to obtain y at this point we could easily make a fitting by using our simulation results. Actually only one numerical result would be required, $V(1, n)$, and we would thus have:

$$y = \ln[1 - (V(1, n)/n)^{\frac{1}{2}}]/\ln(f). \tag{12}$$

However, since $y = y(n)$ this form is not general and therefore not very useful. We avoid this difficulty by noticing that the sum of the number of points that have been occupied exactly r times gives:

$$\begin{aligned} \sum_r V(r, n) &= n(1 - f^y)^2 \sum_r (f^y)^{r-1} \\ &= n(1 - f^y) \\ &= S(1, n). \end{aligned} \tag{13}$$

Thus y can be directly obtained from the relationship:

$$y = \ln[1 - S(1, n)/n]/\ln(f) \tag{14}$$

and we arrive at the desired form by simply eliminating $y(n)$ between (9) and (14). The result is:

$$V(r, n) = [S(1, n)^2/n]\,[1 - S(1, n)/n]^{r-1}. \tag{15}$$

Equation (15) is a function of n and $S(1, n)$ only. From the recent works mentioned earlier we now have exact forms for $S(1, n)$, also tested by numerical simulation.

From this discussion it is rather obvious that (1) may now be written as:

$$S(r, n) = n(1 - f^y)(f^y)^{r-1} \tag{16}$$

$$S(r, n) = S(1, n)\,[1 - S(1, n)/n] \tag{17}$$

$$S(r, n) = S(1, n) - \sum_{i=1}^{r-1} V(i, n). \tag{18}$$

Equation (17) is the desired form for $S(r, n)$.

3. Numerical methods

Monte-carlo random walk simulations are used as independent tests of the formalism presented. Lattices

are generated in 2-dim square lattice geometry (size 300×300), and in 3-dim simple cubic geometry (size $100 \times 100 \times 100$). We monitor a random walk process by using an index on each lattice site, signifying the number of visits for this site at any given instance. This index is initially zero for all sites. A particle is placed at random on the lattice and starts performing a random walk. Every time it steps on a site the occupancy index is incremented by one for this particular site, and the process is repeated. The value of this index at the end of each realization is the $V(r, n)$ value. All other details, such as direction of motion, cyclic boundary conditions, random number generators, etc. are the same as in our past studies of random walks [12]. The average is taken after 1000 realizations, separately for each r value. Five values of n are examined: 2000, 4000, 6000, 8000, and 10000 steps. Checks are made to ensure that there are no artifacts due to finite size (artificial revisitation) etc. by appropriately summing the $V(r, n)$ for all values of r. Obviously this results in $S(1, n)$, whose numerical value is well known, and agrees excellently (within 0.1%) with our calculations. Also the mean-square displacement $R^2(n)$ is calculated and found to be in very good agreement with past studies. All simulation algorithms are implemented in Fortran and Pascal, and executed on a Vax computer.

4. Moments

We shall employ the concept of moments for the quantities we studied as it is customarily used in multifractality [13]. The curious question to investigate is how do these moments scale with time. To do this we must first derive the appropriate formula that expresses the moments directly as a function of time and other random walk parameters. The expression for the moments of the $V(r, n)$ quantity is:

$$M_q = \sum_r r^q V(r, n). \tag{19}$$

Using (15) we get:

$$M_q = n(1-w)^2 \sum_r r^q w^{r-1} \tag{20}$$

where $w = 1 - S(1, n)/n$. Obviously using this formula:

$$M_0 = S(1, n). \tag{21}$$

$$M_1 = n \tag{22}$$

In order to calculate the higher order moments we observe that:

$$\begin{aligned}
\Sigma_{q+1} &= \sum_r r^{q+1} w^{r-1} = \sum_r r^q \frac{\mathrm{d}w^r}{\mathrm{d}w} \\
&= \sum_r \frac{\mathrm{d}}{\mathrm{d}w}(r^q w^r) \\
&= \frac{\mathrm{d}}{\mathrm{d}w}\left[\sum_r r^q w^r\right] \\
&= \frac{\mathrm{d}}{\mathrm{d}w}\left[w \sum_r r^q w^{r-1}\right] \\
&= \frac{\mathrm{d}}{\mathrm{d}w}[w \Sigma_q].
\end{aligned} \tag{23}$$

Using (23) the moments then are given by the recursive formula:

$$\begin{aligned}
M_q &= n(1-w)^2 \Sigma_q \\
&= n(1-w)^2 \frac{\mathrm{d}}{\mathrm{d}w}(w \Sigma_{q-1}) \\
&= (1-w)^2 \frac{\mathrm{d}}{\mathrm{d}w}\left[\frac{w}{(1-w)^2} M_{q-1}\right]
\end{aligned} \tag{24}$$

or similarly:

$$M_q = \frac{\mathrm{d}}{\mathrm{d}w}(w M_{q-1}) + \frac{2w}{1-w} M_{q-1}. \tag{25}$$

Thus, we have derived a recursive formula for all moments, with only the zeroth order moment being necessary to generate the series. This is:

$$M_0 = n(1-w). \tag{26}$$

Table 3 contains in the second column the first few moments as derived using formula (25). Assuming that the moments vary asymptotically with time, i.e.

$$M_q = \sum_r r^q V(r, n) \sim n^{\tau(q)} \tag{27}$$

it is an interesting question to test the dependence of the $\tau(q)$ scaling exponents. A few of these moments are shown in Fig. 6, where $\tau(q)$ is given directly as the slope in a log-log plot of M vs. n. The M_q moments here are calculated using the explicit forms in Table 3. The slopes are given in the last two columns for the 2-dim and 3-dim lattices. From this Table we surmise that within the calculated accuracy of two significant figures the $\tau(q)$ in both cases can be considered to differ by a constant amount, as q varies, and therefore we may argue that this is a case of constant gap scaling.

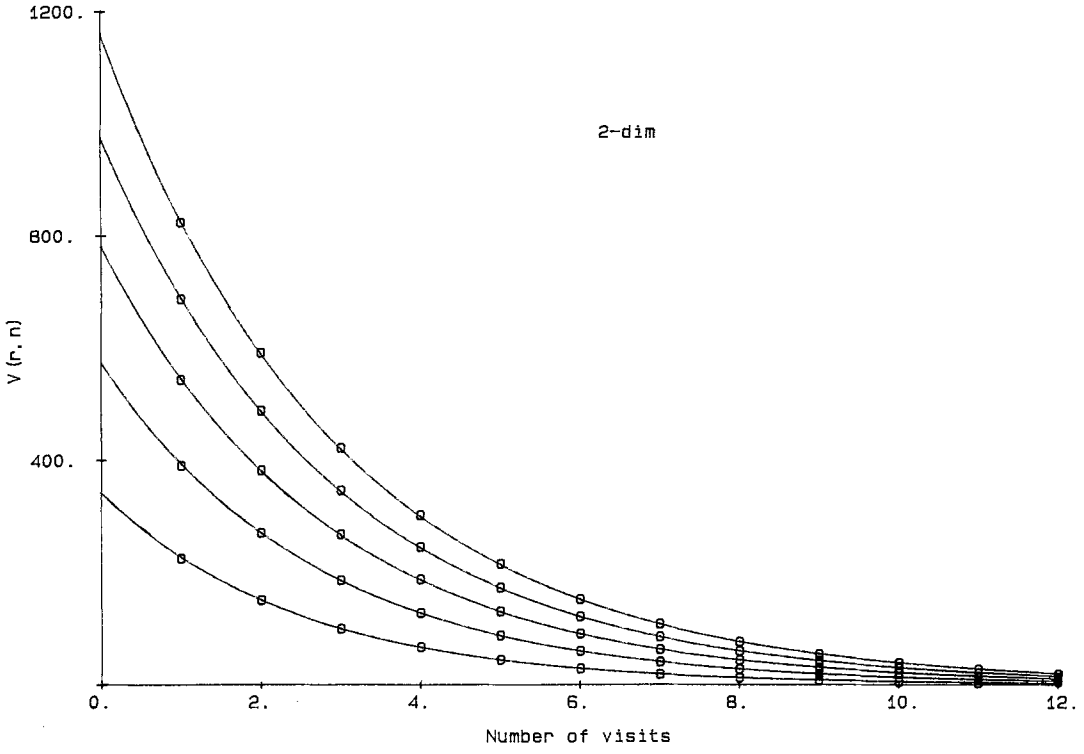

Fig. 2. $V(r, n)$ as a function of r for 2-dim square planar geometry. The solid lines are solutions of (15); the circles are simulation results. Several different n are shown: 10000, 8000, 6000, 4000, and 2000 steps (top to bottom)

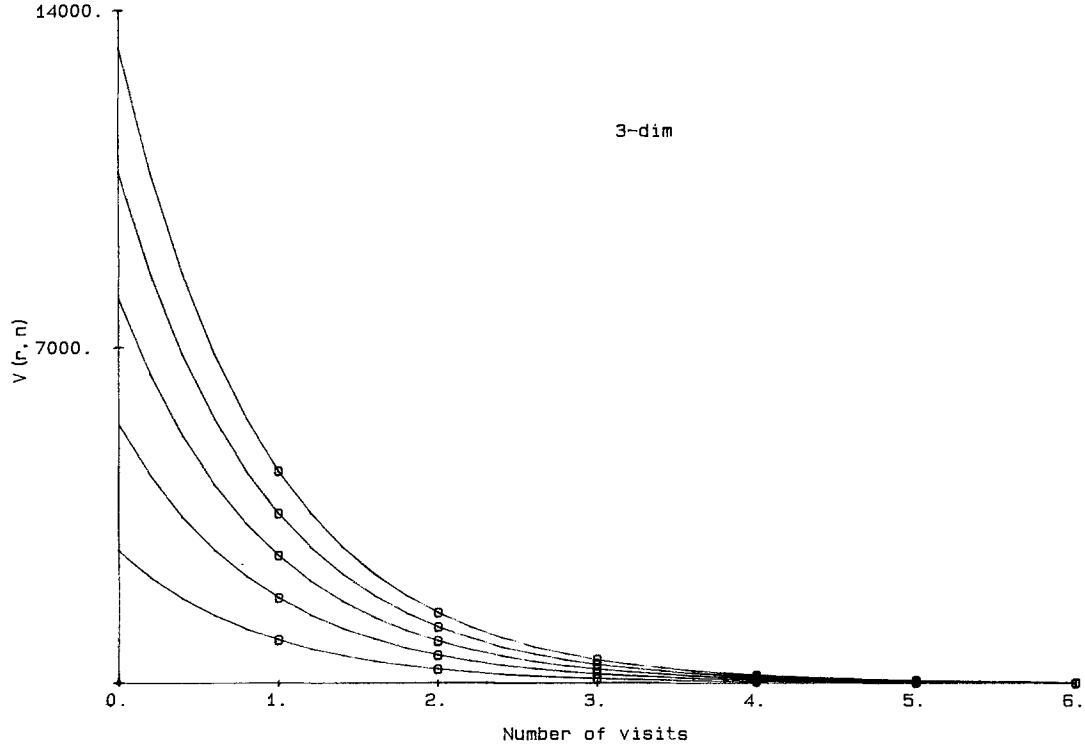

Fig. 3. $V(r, n)$ as a function of r for 3-dim simple cubic geometry. Lines and circles are as in the previous figure

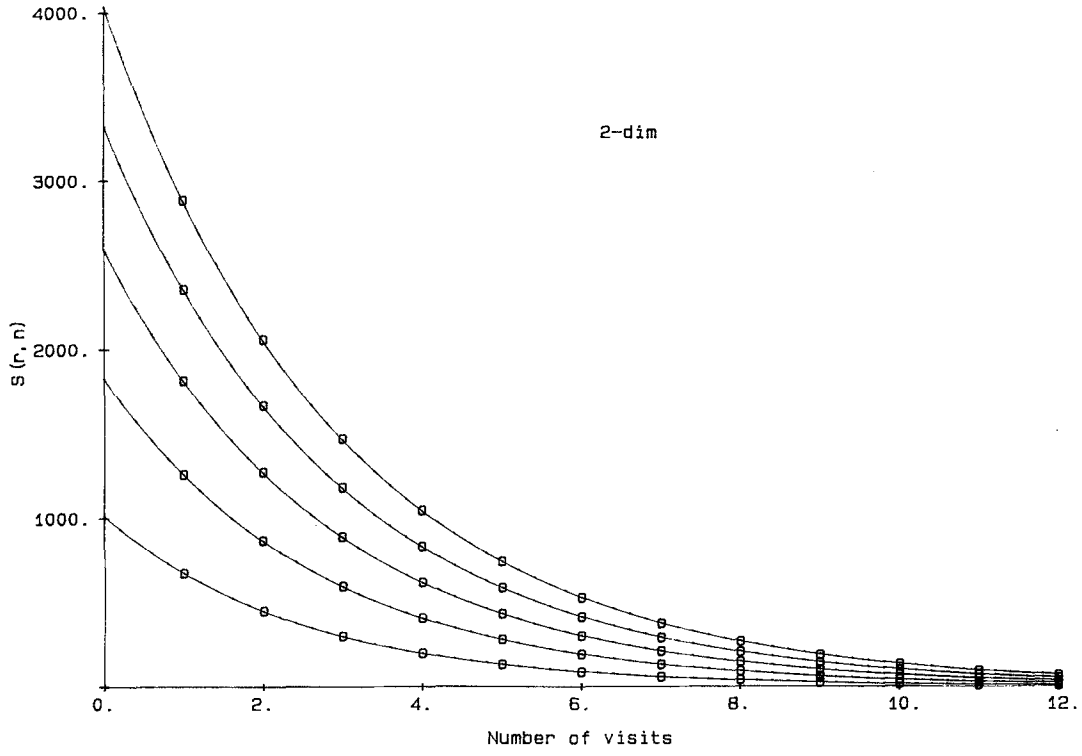

Fig. 4. $S(r, n)$ as a function of r for 2-dim square planar geometry. The solid lines are solutions of (17); the circles are simulation results using (18), with the $V(r, n)$ values taken from the previous calculations. Several different n are shown: 10000, 8000, 6000, 4000, and 2000 steps (top to bottom)

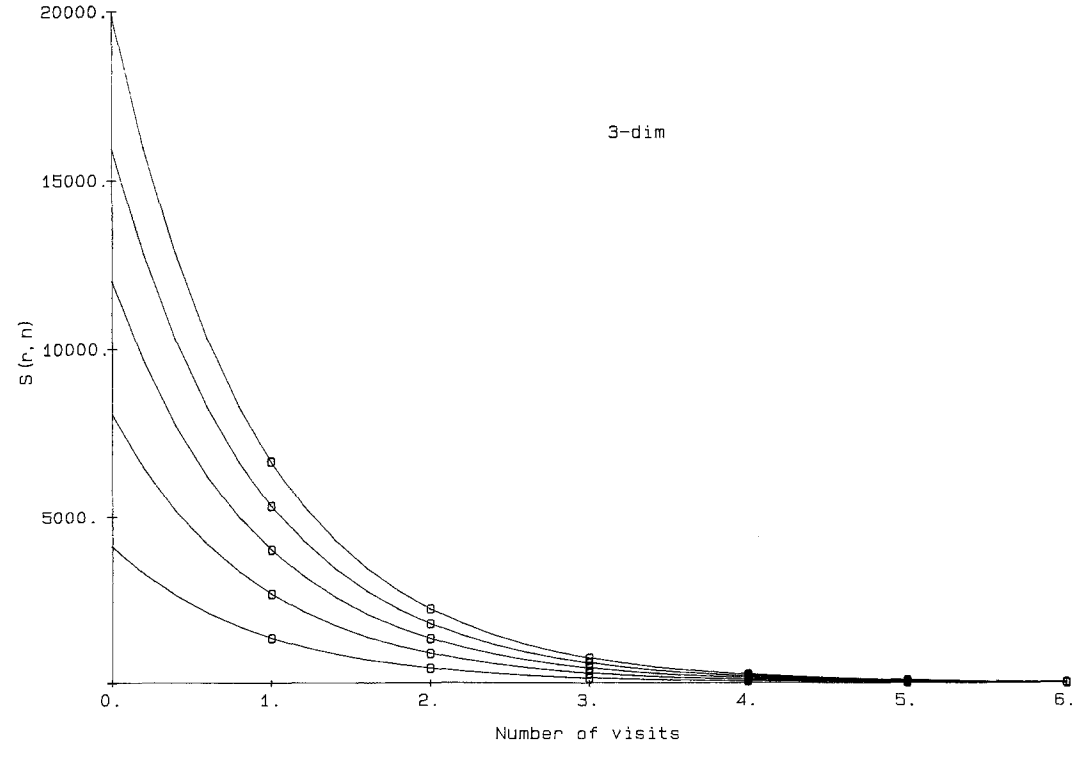

Fig. 5. $S(r, n)$ as a function of r for 3-dim simple cubic geometry. Lines and circles are as in the previous figure

5. Results and discussion

Figures 2 and 3 show the solutions of (15) for $V(r, n)$ as a function of r for several n using the appropriate f, i.e. from (10) and (11), respectively. Since (15) is a smooth function of r we plot $V(r, n)$ continuously and not only at the r = integer points. The simulation data are only at the r = integer values. Excellent agreement is shown to exist with the simulation data over the whole r range. Since the $S(1, n)$ formulae are now satisfactory for any n, we also observe that this carries through to $V(r, n)$, and excellent agreement is also found for any n. For comparison purposes Tables 1 and 2 provide typical values for $V(1, n)$, $S(1, n)$, as well as the $y(n)$ function. We see in these Tables that the agreement is of the order of 0.1% or better.

We also notice the following: the $V(r, n)$ curves in the 3-dim case fall off much more rapidly than the 2-dim case. This is simply a manifestation of the well-known fact that as the dimensionality goes up motion becomes more "free", the probability of escape increases drastically, and the particle returns less and less in previously visited areas.

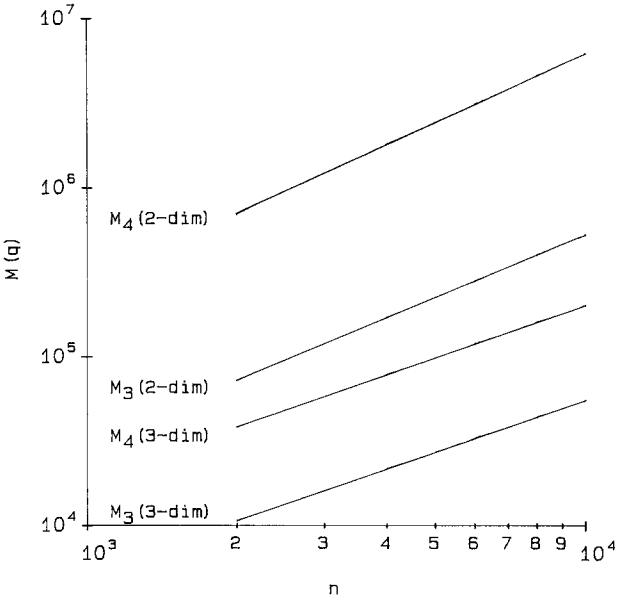

Fig. 6. Plot of M (moments of the $V(r, n)$ quantity) vs. n for $q=3$ and 4. Results for walks on 2-dim and 3-dim lattices are shown. The recursive formula (25) and the analytic expressions in Table 3 are used to make this plot. The resulting slopes of the straight lines are also given in Table 3. Similar lines are received for any q

Table 1. 2-dim square lattice

n	$V(1, n)$ Theoretical	$V(1, n)$ Simulation	$S(1, n)$ Theoretical	$S(1, n)$ Simulation	$y(n)$
2000	226.7	224.8	673.3	673.8	0.7702
4000	393.3	390.4	1254.2	1255.2	0.7903
6000	545.2	543.2	1808.7	1812.8	0.8007
8000	688.7	687.0	2347.2	2353.2	0.8075
10000	826.3	824.3	2874.4	2881.7	0.8112

Table 2. 3-dim simple cubic lattice

n	$V(1, n)$ Theoretical	$V(1, n)$ Simulation	$S(1, n)$ Theoretical	$S(1, n)$ Simulation	$y(n)$
2000	904.7	905.2	1345.2	1346.2	6.4457
4000	1788.5	1786.2	2674.7	2673.6	7.0010
6000	2669.1	2669.0	4001.8	4002.4	7.3446
8000	3547.9	3543.7	5327.6	5325.4	7.5880
10000	4425.7	4423.2	6652.6	6652.3	7.7783

Table 3. Moments and scaling exponents

q	M	$\tau(q)$ 2-dim	$\tau(q)$ 3-dim
0	$n(1-w)$	0.902	0.993
1	n	1	1
2	$n(1+w)(1-w)^{-1}$	1.116	1.010
3	$n(1+4w+w^2)(1-w)^{-2}$	1.235	1.022
4	$n(1+11w+11w^2+w^3)(1-w)^{-3}$	1.355	1.035
5	$n(1+26w+66w^2+26w^3+w^4)(1-w)^{-4}$	1.474	1.047

Figures 4 and 5 show the solutions of (17) for $S(r, n)$ as a function of r for several n using the same parameters as in Figs. 2 and 3. Generally, the same quantitative conclusions are reached as for the $V(r, n)$ function.

Summarizing, we have provided exact analytic solutions for $V(r, n)$ and $S(r, n)$ for perfect lattices in 2 and 3 dimensions. This has been possible due to the highly improved formalism for $S(1, n)$, the random-walk parameter for the number of sites visited at least once in the walk. Our method has been to connect the expressions for $S(r, n)$ and $V(r, n)$ to the $S(1, n)$ formalism. Excellent agreement has been found with computer simulation data that were produced to test the new formulae. Furthermore, we find that the moments of the $V(r, n)$ quantity do scale well with time in a "fractal-type" scaling law (Fig. 6), and the scaling exponents exhibit a constant gap scaling.

References

1. Erdos, P., Taylor, S.J.: Acta Math. Acad. Sci. Hung. **11**, 137 (1960)
2. Montroll, E.W.: Proc. Symp. Appl. Math. Am. Math. Soc. **16**, 193 (1964)

3. Montroll, E.W., Weiss, G.H.: J. Math. Phys. **6**, 167 (1965)
4. Barber, M.N., Ninham, B.W.: Random and restricted walks: theory and applications. London: Gordon and Breach 1970
5. Weiss, G.H., Rubin, R.J.: Adv. Chem. Phys. **52**, 363 (1983)
6. Henyey, F.S., Seshadri, V.: J. Chem. Phys. **76**, 5530 (1982)
7. Zumofen, G., Blumen, A.: J. Chem. Phys. **76**, 3713 (1982)
8. Blumen, A., Zumofen, G.: J. Chem. Phys. **75**, 892 (1981)
9. Argyrakis, P., Kopelman, R.: Chem. Phys. **57**, 29 (1981); **78**, 251 (1983)
10. Montroll, E.W.: J. Math. Phys. **10**, 753 (1969)
11. Argyrakis, P.: Phys. Rev. Lett. **59**, 1729 (1987)
12. Argyrakis, P.: In: Structure and dynamics of molecular systems. Daudel, R., Korb. J.P., Lemaistre, J.P., Maruani, J. (eds.), p. 209. Dordrecht: Reidel 1986
13. Amitrano, C., Coniglio, A., Liberto, F. di: Phys. Rev. Lett. **57**, 1016 (1986)

G.L. Bleris, Panos Argyrakis
Department of Physics 313-1
University of Thessaloniki
GR-54006 Thessaloniki
Greece