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Random Walks on Lattices with Traps

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We consider random walks on simple cubic lattices containing two kinds of sites: ordinary ones and "traps" which, when stepped on, absorb the walker. We study two related problems: (a) the probability of returning to the origin and (b) the situation in which the particle can meet its end, not only by absorption at a trap, but also by a process, called spontaneous emission, which has a constant probability per step. In problem (b), we ask for the probability that emission, rather than absorption, occurs. The solution to (a) is known for 1 dimension, and given here for the 3-, 4-, $\cdots$ dimensional cases; the 2-dimensional case remains unsolved. The solution to (b) is known for the 1-, 3-, 4-, $\cdots$ dimensional cases; we give it for 2-dimensional case.

I. INTRODUCTION

A random walk (RW) on a space lattice provides a model for many situations and processes encountered in statistical mechanics, solid state theory (e.g., diffusion of electrons, excitons, energy transfer, conductivity, dislocations), as well as in probability theory and related fields in pure mathematics. Here we consider a particle performing a symmetrical RW on a lattice (of dimension to be specified later). There are two kinds of lattice sites, ordinary ones and "traps" or "absorbers"; whenever the particle steps on a "trap," it gets absorbed, and the walk ends. We consider two related problems: (a) the probability of returning to the origin (Sec. II) and (b) the situation in which the particle can meet its death, not only by absorption by a trap, but also by spontaneous emission, a process defined to have a constant probability per step (Sec. III); in that case, we ask for the probability that the walk end by emission, rather than by absorption.

The solution to problem (a) is known[1] in 1 dimension; we give it here for 3 dimensions (Sec. II). The solution to problem (b) is known for 1 dimension[2,3] and for 3 and more dimensions[4]; we fill in the gap, the 2-dimensional case (Sec. III). It is interesting that the 2-dimensional case presents the greatest difficulties for both problems. The possibility of extending the treatment to different situations is discussed also. Results are summarized in Sec. IV.

II. PROBABILITY OF RETURNING TO THE ORIGIN BEFORE STEPPING ON A TRAP

Consider a particle performing an RW in a D-dimensional simple cubic lattice. Let traps be located, at random, on a fraction q of the lattice sites. We ask for the probability that the particle return to its origin (i.e., before being trapped). This problem was proposed by Montroll and Weiss[1] and solved in 1 dimension. We solve it here for $D \geq 3$, valid for small q, using a line of reasoning essentially due to Rudemo.[4]

Let the quantity of interest be $r^{(q)}$, the probability of returning to the origin, given a density q of traps; and let $r_t^{(q)}$ equal the probability of *first* return (fr) to the origin at step t, given a density of traps q. Then,

$$r^{(q)} = \sum_t r_t^{(q)}. \tag{1}$$

If we define $\xi_q(t, w_i)$ as the probability that for a given walk w_i of length t $[1 \leq i \leq (2D)^t]$ trapping not take place (at any trap) before step t, given a density of traps q, then we can write

$$r_t^{(q)} = (2D)^{-t} \sum_{i=1}^{(2D)^t} \delta_{\mathrm{fr},t}(w_i)\xi_q(t, w_i), \tag{2}$$

where $\delta_{\mathrm{fr},t}(w_i)$, somewhat analogous to a Kronecker delta, is unity for the walks that first return to the origin at t, and zero for all others.

Now let $V(t, w_i)$ equal the number of different points visited in the t steps of walk w_i, in the absence of traps. Then, the probability that none of the points visited in t steps be a trap is

$$\xi_q(t, w_i) = (1 - q)^{V(t,w_i)}. \tag{3}$$

Substitution of (3) into (2) and that in turn into (1) then gives

$$r^{(q)} = \sum_t (2D)^{-t} \sum_i \delta_{\mathrm{fr},t}(w_i)(1 - q)^{V(t,w_i)}. \tag{4}$$

Now for any "transient" RW we have asymptotically[5]

$$V(t) \rightarrow (1 - F)t, \tag{5}$$

[1] E. W. Montroll and G. H. Weiss, J. Math. Phys. **6**, 167 (1965), Sec. VI.
[2] H. B. Rosenstock, J. Soc. Ind. Appl. Math. **9**, 169 (1961).
[3] N. Levinson, J. Soc. Ind. Appl. Math. **10**, 442 (1962).
[4] M. Rudemo, SIAM J. Appl. Math. (formerly J. Soc. Ind. Appl. Math.) **14**, 1293 (1966).
[5] L. Spitzer, *Principles of Random Walk* (Van Nostrand, Inc., New York, 1964), pp. 35–38.

where F is defined as the probability of eventual return to the origin[6] (in absence of traps). F is a number whose value for the RW under consideration is easily obtained numerically, as we shall see later in connection with Eq. (12); for $D = 3$, F is known[7] to be 0.340537. Equation (5) is not accurate for small values of t, i.e., for short walks; short walks will, however, make a negligible contribution to (4) when q is small—the physically interesting situation. For small q we substitute (5) into (4), take the $(1 - q)$ term outside the i sum, and note that

$$(2D)^{-t} \sum_{i}^{(2D)^t} \delta_{\mathrm{tr},t}(w_i)$$

is just $r_t^{(0)}$, the probability of first return to the origin at step t in the absence of traps:

$$r^{(q)} = \sum_t r_t^{(0)}(1 - q)^{(1-F)t} \tag{6}$$

or

$$r^{(q)} = \sum_t r_t^{(0)} p^t, \tag{7}$$

with

$$p = (1 - q)^{1-F}. \tag{8}$$

We recognize the right-hand side of (7) as the generating function $F(p)$ for first returns to the origin,

$$r^{(q)} = F(p). \tag{9}$$

[Observe in passing that the quantity F used in Eq. (5) is, in fact, $F(1)$.] In general, this generating function for first return is related to the generating function G for return (not necessarily first) to the origin by[8]

$$F(p) = 1 - G^{-1}(p); \tag{10}$$

hence, we finally obtain

$$r^{(q)} = 1 - G^{-1}(p). \tag{11}$$

Now G is a known function[9] expressible as

$$G(p) = (D/p)\int_0^\infty e^{-Dz/p} I_0^D(z)\, dz, \tag{12}$$

where D is the dimension of the lattice and I_0 the zero-order Bessel function of pure imaginary argument. For any given D, the evaluation of (12) can be done numerically, using Simpson's rule and the convergent series for I_0 for z smaller than some z_1, and the asymptotic one for larger z.[10] We have carried this out for $D = 3$; the dividing point was chosen as $z_1 = 9$. The results are shown in the accompanying Fig. 1. A rough check on the precision of the calculation is provided by the number $F = F(1)$, which appears both in the input [in Eq. (12) via (8)] and the output ($r^{(q)}$ must equal F for physical reasons when $q = 0$). The input value was 0.340537, the output 0.340344, suggesting 3- to 4-figure accuracy. We can also find the behavior of $r^{(q)}$ for very small q from the analytic behavior of I_0; we find a negatively infinite slope, in agreement with our figure, viz.,

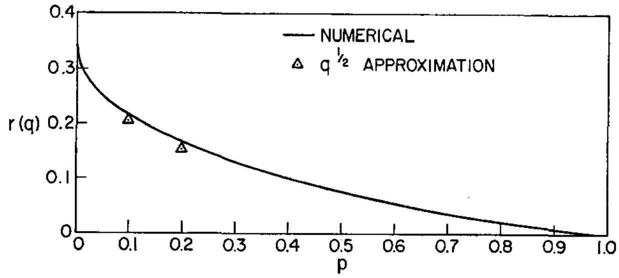

FIG. 1. Probability of return to the origin in 3 dimensions, as a function of trap density q.

$$r^{(q)} \cong F - D^{\frac{3}{2}}(1 - F)^{\frac{5}{2}} 2^{-\frac{1}{2}} \pi^{-1} q^{\frac{1}{2}} + \cdots. \tag{13}$$

In the 3-dimensional case this becomes

$$r^{(q)} = 0.3405 - 0.4130 q^{\frac{1}{2}},$$

which is in good agreement (see Fig. 1) with the numerical results.

The 2-dimensional case is appreciably more difficult. To be sure, the generating function is known—merely substitute $D = 2$ into (12). But (5) does not hold for recurrent[6] RW's; instead we have[11]

$$V(t) \cong \pi t/\ln t. \tag{14}$$

If this, instead of (5), is put into (4), the result is

$$r^{(q)} = \sum_t r_t^{(0)}(1 - q)^{\pi t/\ln t} \tag{15}$$

and not simply the known generating function for the coefficients $r_t^{(0)}$. We would, therefore, have to go through the procedure of explicitly computing the expansion coefficients from the generating function before being able to evaluate (15). A straightforward computation of $r_1, r_2, r_3, \cdots$ is, of course, possible; but we have been unable to obtain an expansion for r_k asymptotically valid for large k and, therefore, we have failed to evaluate (15).

III. SPONTANEOUS EMISSION

Let $\alpha =$ const be the probability per step of spontaneous disappearance ("emission") of the walker

[6] An RW is called "transient" if $F < 1$, "recurrent" if $F = 1$. Symmetric RW's on simple cubic lattices are recurrent in 1 dimension and 2 dimensions, but transient in higher dimensions.
[7] E. W. Montroll, J. Soc. Ind. Appl. Math. 4, 241 (1965), Eq. (4.5).
[8] Ref. 7, Eq. (3.4).
[9] Ref. 7, Eq. (2.11b).
[10] H. B. Dwight, *Tables of Integrals* (Macmillan, New York, 1947), formulas 813.1 and 814.1.
[11] Ref. 1, Eq. (III.15.b).

from the lattice. (We may visualize this walker as a radioactive or otherwise unstable particle capable of decay with constant probability in time.) We ask for the probability that the walk end by spontaneous emission rather than by stepping on a trap. (Physically, this is the probability that emission be observed.) To obtain a formal solution in 2 dimensions we follow the reasoning of Rudemo[4] rather than that of earlier workers[2,3] which seems useful for 1 dimension only.

Let $P^{(q)}$ be the probability of emission if the density of traps is q, and let $P_t^{(q)}$ be the probability that this happen at step t. Then

$$P^{(q)} = \sum_t P_t^{(q)}. \tag{16}$$

Defining ξ as in Eq. (2) and $\delta_{\text{emis},t}$ as unity if emission takes place at step t and zero otherwise, we obtain, as for (2),

$$P_t^{(q)} = (2D)^{-t} \sum_{i=1}^{(2D)^t} \delta_{\text{emis},t}(w_i)\xi_q(t, w_i). \tag{17}$$

If q is small, ξ can be taken out of the i sum, since V and, hence, ξ will asymptotically become independent of w_i; $(2D)^{-1} \sum_i \delta_{\text{emis},t}$ then becomes just the probability of emission at step t in absence of traps, viz.,

$$P_t^{(0)} = (1 - \alpha)^t \alpha \tag{18}$$

(failure to emit at steps $0, 1, 2, \cdots, t - 1$, followed by success at step t). Substitution of (17) into (16) then gives

$$P^{(q)} = \alpha \sum_t (1 - \alpha)^t (1 - q)^{V(t)}. \tag{19}$$

In evaluating this, we confine ourselves to the limit in which both the trap density q and the emission probability per step α are small, though their ratio remains unrestricted. In that situation, the factor α assures us that the early terms in (19) will not contribute appreciably; we can, therefore, use the asymptotic value (14) for the mean number of distinct points visited in a 2-dimensional RW throughout the range. Furthermore, since adjacent terms will not vary greatly in magnitude, we can replace the sum by an integral:

$$P^{(q)} = \alpha \int_1^\infty dt (1 - \alpha)^t (1 - q)^{\pi t / \ln t}.$$

Neglecting terms of order α^2 and q^2, we obtain finally

$$P^{(q)} = \alpha \int_1^\infty dt \exp\,[-\alpha t - (\pi q t / \ln t)]. \tag{20}$$

This should be evaluated for arbitrary values of the ratio α/q. We were unable to do this in closed form, but obtained separate expressions valid for small and for large α/q.

When $\alpha/q \gg 1$, the first term in the exponent is the dominating one throughout the range of integration. We, therefore, let $\alpha t = y$ and rewrite (20) as

$$P^{(q)} = \int_\alpha^\infty dy \exp\left[-y\left(1 + \frac{\pi q/\alpha}{\ln y + \ln (1/\alpha)}\right)\right]. \tag{21}$$

Here $\ln (1/\alpha)$ is a large number, much larger than y in all regions except those in which y itself is so large as to cause the leading term $\exp^{-y}$ to make the integrand negligible. The $\ln y$ term can, therefore, be neglected, and we obtain

$$\begin{aligned} P^{(q)} &= \{1 + [\pi q/\alpha \ln (1/\alpha)]\}^{-1} \\ &\quad \times \exp\,(-\alpha\{1 + [\pi q/\alpha \ln (1/\alpha)]\}) \\ &\cong (1 - \alpha)\{1 - [\pi q/\alpha \ln (1/\alpha)]\}. \end{aligned} \tag{22}$$

In the other extreme $\alpha/q \ll 1$, the second term in the exponential in (20) will be the larger when t is small [i.e., for values of $t < \exp\,(q/\alpha)$], but the first one when t is larger. However, if α/q is small enough, the crossover point will occur for t so large that the entire integrand is negligible beyond. We, therefore, set $\pi q t = z$ and write (20) as

$$P = (\alpha/\beta) \int_\beta^\infty dz e^{-g(z)}, \tag{23}$$

where

$$g(z) = (\alpha/\beta) z + z[\ln z + \ln (1/\beta)]^{-1} \tag{24}$$

with $\beta = \pi q$. Even though α/β is small, β is itself small. Hence, $\ln (1/\beta)$ is a large number, and $\ln z$ will be comparably large only for values of z so large that the entire integrand is negligible. Therefore, we expand g as follows:

$$g = \frac{z}{\ln (1/\beta)}\left(1 - \frac{\ln z}{\ln (1/\beta)}\right) + \frac{\alpha}{\beta} z$$

or, introducing $c = \ln (1/\beta)$, $w = z/c$,

$$g = w(1 + \alpha c/\beta) - (w/c) \ln cw.$$

Inserting this in (23) and expanding $\exp\,[-(w/c) \ln cw]$ in a Taylor series then gives

$$P^{(q)} = \frac{\alpha c}{\beta}\left[\int_{\beta/c}^\infty dw e^{-w(1+\alpha c/\beta)} + \int_{\beta/c}^\infty w\, dw e^{-w}(\ln c + \ln w)\right].$$

Now replace the lower limit by zero, thereby increasing second-order errors only. The first two integrals are then elementary, and the last one[12] is $1 - \gamma = 0.423$,

[12] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products* (Academic Press, New York, 1965), formulas 4.352.2 and 9.73.

TABLE I. Summary of solutions of problems (a) and (b).

Dimensionality D	Problem (a)—return to origin	Reference	Problem (b)—spontaneous emission	Reference
1	$q(1-q)^{-1}\ln(1/q)$	1	$1-\tau_1^2\int_0^\infty \exp(-\tau_1 u)\tanh u\,du$ $\cong 1-\tau_1+O(\tau_1^2)$, small τ_1, $\cong 2\tau_1^{-2}+O(\tau_1^{-4})$, large τ_1, with $\tau_1 = 2^{\frac{1}{2}}q/\alpha^{\frac{1}{2}}$	3 2 2
2	not known		$\alpha\int_1^\infty \exp[-\alpha t - (\pi q t/\ln t)]\,dt$ $= 1-\alpha-[\pi\tau_2/\ln(1/\alpha)]+O(\tau_2^2)$, small τ_2, $= (\pi\tau_2)^{-1}[\ln(1/\pi q)+\ln\ln(1/\pi q)$ $+ 0.423 + O(1/\ln \pi q)] + O(\tau_2^{-2})$, large τ_2, with $\tau_2 = q/\alpha$	0 0 0
≥ 3	$(D/P)\int_0^\infty \exp(-Dz/p)I_0^D(z)\,dz$ $\cong F - D^{\frac{3}{2}}(1-F)^{\frac{5}{2}}2^{-\frac{1}{2}}\pi^{-1}q^{\frac{1}{2}} + O(q^{\frac{3}{2}})$, with $p = (1-q)^{1-F}$	0 0	$[1+(1-F)\tau_2]^{-1}$	4

γ being Euler's constant. So we finally obtain

$$P^{(q)} = (\alpha/\beta)[c + \ln c + 0.423 + O(c^{-1})] + O((\alpha/\beta)^2). \tag{25}$$

Since the derivation involves integration over a region in which previous expansions are not formally valid, this is an asymptotic, rather than a convergent, series. Summarizing (22) and (25), we have

$$\begin{aligned} P^{(q)} &= 1 - \alpha - [\pi q/\alpha \ln(1/\alpha)], & \frac{\pi q}{\alpha} \text{ small}, \\ &= \frac{\alpha}{\pi q}\left[\ln\frac{1}{\pi q} + \ln\ln\frac{1}{\pi q} + 0.423 \right. \\ &\quad \left. + O\left(1\Big/\ln\left(\frac{1}{\pi q}\right)\right)\right] + O\left(\left(\frac{\alpha}{\pi q}\right)^2\right), & \frac{\pi q}{\alpha} \text{ large}. \end{aligned} \tag{26}$$

Direct numerical evaluation of (20) gives good agreement with (26). For example, direct evaluation of (20) gives 0.00924 and 0.00121, respectively, for $(\alpha, \pi q) = (10^{-6}, 10^{-3})$ and $(10^{-8}, 10^{-4})$, whereas the second line of (26) gives 0.00926 and 0.00119 for these situations. Similarly, direct evaluation of (20) gives 0.99883 and 0.99758, respectively, for $(\alpha, \pi q) = (10^{-3}, 10^{-6})$ and $(10^{-3}, 10^{-5})$, whereas the first line of (26) gives 0.99885 and 0.99755. The general behavior of P as a function of α and πq is illustrated in Fig. 2.

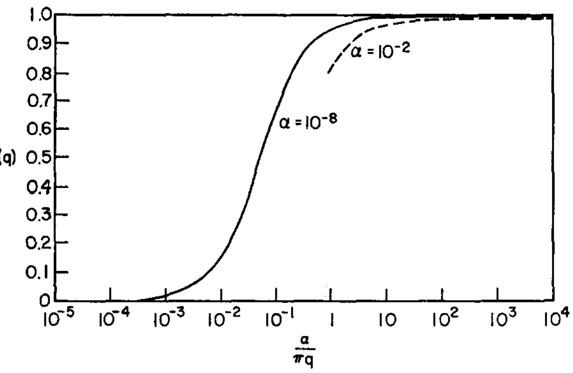

FIG. 2. Probability of spontaneous emission in 2 dimensions, for various trap densities q and spontaneous emission probabilities α per step.

REVIEW

The known results for both problems discussed in this paper are summarized in Table I, where q and α, as previously defined, are, respectively, the trap density and the emission probability per step; F, the return probability in absence of both traps and emission, is a number whose value depends on the dimensionality. The "reference" column refers to our footnotes; Ref. 0 means the present paper. The functional dependence of the calculated probabilities is seen to be quite strongly determined by the dimensionality.