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Asymptotic form for random walk survival probabilities on three-dimensional lattices with traps

(exciton transfer/mean trapping times/defect motion/lattice random walk)

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ABSTRACT The problem of calculating statistics of time-to-trapping of a random walker on a trap-filled lattice is of interest in solid state physics. Several authors have suggested approximate methods for calculating the average survival probabilities. Here, an exact asymptotic form for the probability that an n step random walk visits S_n distinct sites is used to ascertain the validity of a simple approximation suggested by Rosenstock. For trap concentrations below 0.05, the relative error in using Rosenstock's approximation is less than 10%.

There has been considerable recent interest in the problem of random walks on lattices with randomly distributed trapping sites (1–6). The original motivation for studying this problem was to model the trapping of mobile defects in crystals with point sinks (1, 2, 7), but many further applications have been found for this model. Rosenstock (2) studied the trapping model in analyzing kinetic experiments on luminescent organic materials, and Montroll (8, 9) considered the same model in connection with the kinetics of the conversion of light energy to oxygen in photosynthesis. Klafter and Silbey (6) give a good set of references to various applications of the random walk trapping model. Shuler *et al.* (10) have also dealt with the relationship between the expected number of distinct sites visited in a random walk and the mean time to trapping, in the context of the Montroll (8, 9) model in which there is one trapping site per unit cell. The present treatment is more general in the sense that it starts from the exact asymptotic distribution of the number of distinct sites visited in an n-step random walk rather than from its expected value.

If the random walk takes place on a regular lattice and the probability that a given site is a trapping point is equal to c, then the probability that trapping occurs after step n is $(1-c)^{S_n}$ where S_n is the number of distinct sites visited during the course of an n-step random walk. Hence the expected time to trapping is

$$\langle n\rangle = \sum_{j=1}^{\infty} \langle (1-c)^{S_n}\rangle. \qquad [1]$$

When $c \ll 1$, one expects that $\langle n\rangle \gg 1$. Rosenstock (2, 3) suggested approximating the term $\langle (1-c)^{S_n}\rangle$ by $(1-c)^{\langle S_n\rangle}$ and then evaluating the series in Eq. 1 by using the asymptotic form for $\langle S_n\rangle$ derived by several authors (11–13). It is the purpose of this note to point out that in three dimensions Jain and Pruitt (14) have derived an asymptotic form for $p(S_n)$, the probability density for S_n, allowing us to find a more accurate expression for $\langle n\rangle$ than that yielded by the Rosenstock approximation. Jain and Pruitt showed that, for symmetric random walks, S_n has a Gaussian distribution with mean equal to Fn, where F is the probability of return to the origin, and variance given by

$$\sigma^2(R_n) \approx a \cdot n \cdot \ln n$$

where

$$a = \frac{(1-F)^4}{2\pi^2}\frac{1}{\sigma_x\sigma_y\sigma_z}. \qquad [2]$$

The parameters σ_x, σ_y, σ_z are standard deviations of the single-step transition probabilities in the x, y, and z directions, respectively.

Under this Gaussian approximation the averaged probability that trapping occurs after step n is asymptotically

$$P_n \approx \int_0^\infty p(S_n)\,(1-c)^{S_n}\,dS_n$$

$$\approx (1-c)^{Fn}\left\{e^{\lambda^2/[2\sigma^2(S_n)]}\,\frac{\phi\left(\frac{F}{\sqrt{a}}\sqrt{\frac{n}{\ln n}} - \lambda\sqrt{an\ln n}\right)}{\phi\left(\frac{F}{\sqrt{a}}\sqrt{\frac{n}{\ln n}}\right)}\right\} \qquad [3]$$

where $\lambda = \ln[1/(1-c)]$ and

$$\phi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x} e^{-u^2/2}\,du \qquad [4]$$

is the error function. The first term on the right-hand side of Eq. 3 is just Rosenstock's approximation and the terms in brackets are the corrections. Fig. 1 shows plots of $\ln P_n$ as a function of c and as a function of n for an isotropic random walk with transitions to nearest neighbors only, on a simple cubic lattice.

One can see from the curves that below $c = 0.01$ the survival probabilities are essentially equal, whereas at higher trap concentrations the more exact survival probability is larger, often by a considerable amount, than that predicted by the Rosenstock approximation. This would seem to rule out the suggestion by Fastenau *et al.* (5) that a more accurate estimate of P_n can be obtained in the form

$$P_n \sim (1-c)^{Fn\ +\alpha\sqrt{n+\beta}} \qquad [5]$$

because the values of α and β given by these authors are positive. When the concentration is fixed but the number of steps is increased, the divergence between the two expressions also increases (Fig. 1 *Right*). In Fig. 2 is plotted the ratio

$$\left(\sum_{n=10}^{\infty} P_n\right)[1-(1-c)^F]\,(1-c)^{-10F} \qquad [6]$$

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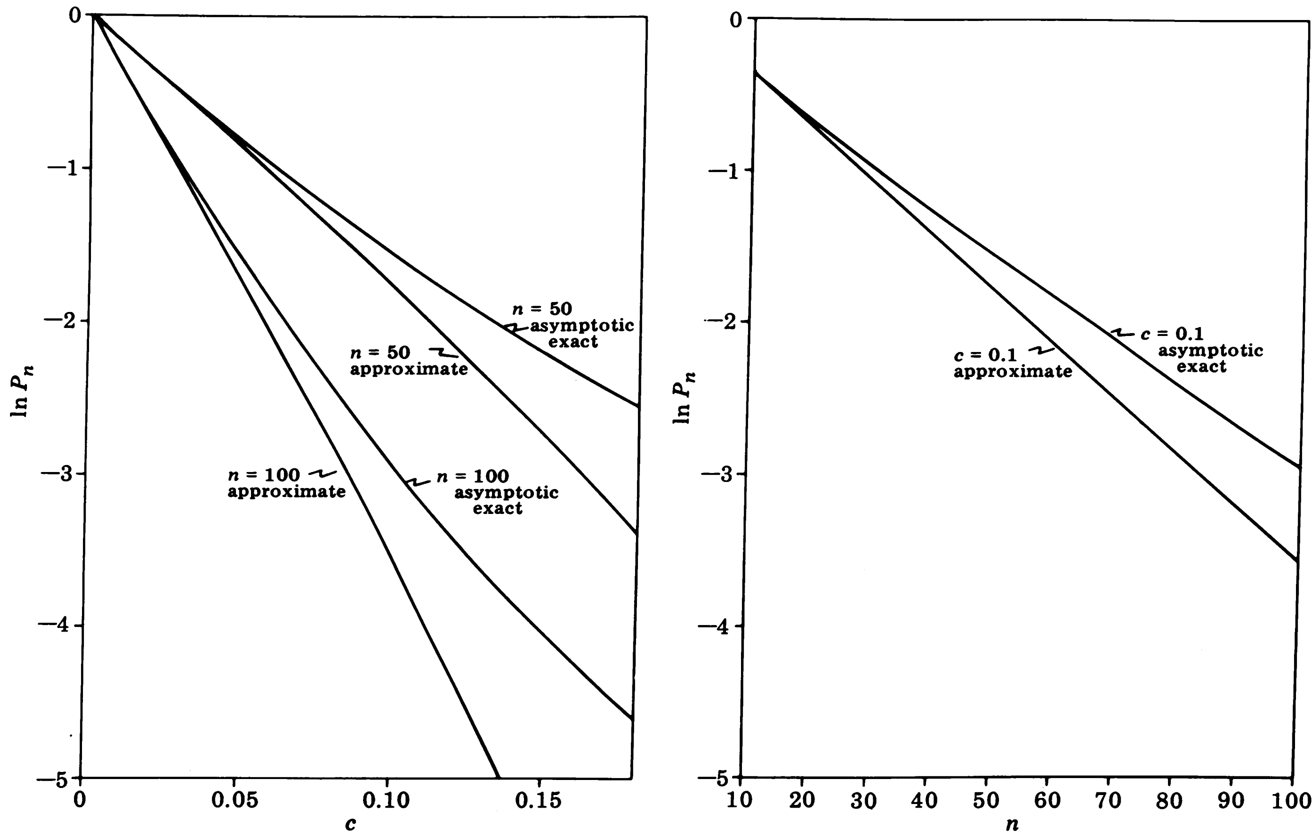

FIG. 1. (*Left*) Curves in ln P_n as a function of c, the concentration of traps, for fixed n. The curves marked "approximate" refer to the use of the approximation ln $P_n = Fn \ln(1 - c)$; the curves marked "asymptotic exact" were computed by using Eq. 3. (*Right*) Curves of ln P_n as a function of n for fixed c.

where the P_n values are taken from Eq. 3. This ratio gives some idea of the discrepancy in $\langle n \rangle$ that is caused by using the approximation $P_n \approx (1 - c)^{Fn}$. Considerably more work would be necessary to find a more exact estimate of the discrepancy because the corrections to Jain and Pruitt's result are unknown at present. In consequence, one does not know the value of n at which the Gaussian approximation becomes valid.

Values of F are known for nearest-neighbor random walks on face-centered and body-centered cubic lattices and lead to results quantitatively similar to those for the simple cubic lattice. However, there is no comparable approximation available for $p(S_n)$ in two dimensions nor is it known whether the Gaussian approximation is valid for the multicomponent lattices studied by Hoshen and Kopelman (15) and Argyrakis and Kopelman (16). We infer from Fig. 2 that the Rosenstock approximation is useful for $c < 0.05$ but leads to errors of the order of 10% or greater for larger concentrations.

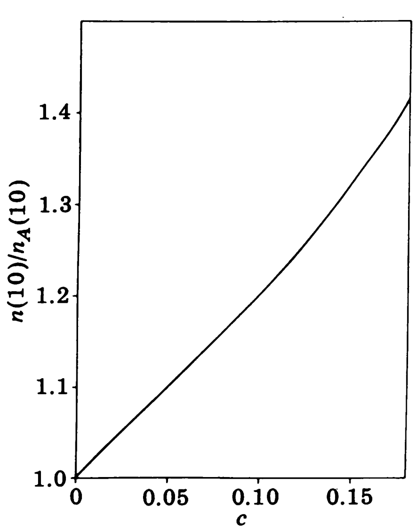

FIG. 2. Curve of the ratio in Eq. 6 that gives an idea of the error in $\langle n \rangle$ as a function of c.

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