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LETTER TO THE EDITOR

The number of distinct sites visited by a tracer particle

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Abstract. We calculate the average number of distinct sites visited by a tracer particle in a three- or higher-dimensional lattice gas with vacancy density ρ, in the limit of low density and large times, i.e., $\rho\downarrow 0$ and $\rho t \gg 1$.

We define the tracer particle problem. Consider an infinite d-dimensional hypercubic lattice, with a fraction $1-\rho$ of its sites occupied by identical particles. The remaining sites are empty. *All* particles on the lattice perform Brownian motion, but subject to a 'no double occupany' condition. Alternatively, one may think of the vacancies (empty sites) as performing simple random walks, which in the limit $\rho\downarrow 0$ become independent. Next, one of the particles is selected at random, and is called the *tracer particle*. The object now is to investigate its motion, for example by calculating its diffusion constant.

When studying this problem, the general observation usually made is that many of the properties of the motion of the tracer particle can be found by first considering the corresponding property for a simple random walk on the same lattice and afterwards applying a 'renormalization of time' in the obtained result. For example, the mean square displacement of a simple random walk on a d-dimensional hypercubic lattice and in a distance time $t = 0, 1, \ldots$ is given by

$$\langle r^2\rangle_t = t. \tag{1}$$

For the corresponding tracer particle problem (see, e.g., the review article by Kehr and Binder [1]) one finds for the mean square displacement of the tracer particle, if the step frequency of an isolated vacancy is taken as the unit of time,

$$\langle r_{\rm tr}^2\rangle_t \simeq \rho f(\rho) t \qquad \rho t \gg 1. \tag{2}$$

Obviously, (2) may be obtained from (1) by replacing t by $\rho f(\rho) t$. The factor ρ comes in since the tracer particle can move only when it is reached by a vacancy, which, on average, happens every ρ^{-1} time units. The factor $f(\rho)$ is called the correlation factor and takes into account the characteristic backward correlation effects in the motion of the tracer particle (to see that these effects are there just consider two successive moves of the tracer particle due to the same vacancy). Only for $\rho = 0$ and $\rho = 1$ can its value be calculated exactly, but for general ρ a rather accurate approximation exists [2].

As Czech [3] showed, however, in three and higher dimensions, the 'renormalization procedure' sketched above does *not* work for the calculation of $\langle \mathcal{S}_t \rangle$, the average number of distinct sites visited by the tracer particle at time t. In fact, he found that $\langle \mathcal{S}_t \rangle$ could, asymptotically, be described remarkably well by modelling the tracer particle motion as a special *correlated random walk*, called the backward jump (BJ) model, with appropriately chosen, ρ-dependent, step probabilities (see [3]). The reason for this good agreement was not fully clear. We shall show now that, arguing along the same lines as Czech, one can find the exact answer for $\langle \mathcal{S}_t \rangle$ in the limit $\rho \downarrow 0$ and $\rho t \gg 1$. We shall indeed describe the tracer particle motion as a correlated random walk, with afterwards t replaced by ρt for the reasons given above, but, instead of the BJ model Czech used, we shall use a more general correlated random walk model.

To be specific, we consider a correlated random walk with a one-step memory on a d-dimensional hypercubic lattice in discrete time t. At any instant of time the walker steps to one of its nearest-neighbour sites. Let A denote the probability that two consecutive steps of the walker are in opposite directions, B the probability that they are in the same direction, and C the probability for them to be in any of the other, right-angled, configurations. Then obviously,

$$A + B + 2(d-1)C = 1. \tag{3}$$

The BJ model employed by Czech corresponds to taking $B = C$. Ernst [4] has studied this ABC model and finds

$$\sum_{t=0}^{\infty} P_t(\mathbf{0}) = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \mathrm{d}^d \boldsymbol{q} \frac{\frac{1}{d} \sum_{i=1}^{d} \frac{1 + (A-B)\cos q_i}{1 - 2(B-C)\cos q_i + (B-A)(B+A-2C)}}{1 - 2C \sum_{i=1}^{d} \frac{\cos q_i + A - B}{1 - 2(B-C)\cos q_i + (B-A)(B+A-2C)}} \tag{4}$$

where $P_t(\mathbf{0})$ denotes the probability for the walk to be at its starting point at time t. Formula (4) was in fact first derived by Gillis [5], albeit in a rather complicated way involving a lengthy manipulation of determinants. The average number of distinct sites $\langle S_t \rangle$ visited by a random walk (whether correlated or not) in three and higher dimensions is asymptotically given by [6]

$$\langle S_t \rangle \simeq \frac{t}{\sum_{t=0}^{\infty} P_t(\mathbf{0})} \qquad t \gg 1. \tag{5}$$

Hence, using (4), $\langle S_t \rangle$ is known for the ABC model.

We shall now explicitly treat the three-dimensional tracer particle problem, in order to be able to compare with Czech's results. The procedure is easily generalized to higher dimensions. We first consider a tracer particle and a *single* vacancy on the infinite three-dimensional lattice. The probability B_0 that after a first step the tracer particle will *ever* make a second step in the same direction, as well as the corresponding probabilities A_0 for reversal and C_0 for stepping sideways are known. Sholl [7] states them as

$$\begin{aligned} A_0 &= 0.223\,423\ldots \\ B_0 &= 0.013\,581\ldots \\ C_0 &= 0.025\,883.\ldots \end{aligned} \tag{6}$$

Since $A_0 + B_0 + 4C_0 < 1$ it is not certain that there will be a second step. However, if we now introduce a finite density ρ of vacancies, then the tracer particle will make an infinite number of steps, since vacancies will keep arriving at the site of the particle at a constant rate ρ. In the limit $\rho\downarrow 0$ moves of the tracer particle due to different vacancies are uncorrelated. If a given vacancy, after having caused a step of the tracer particle, does not come back to it, then a different vacancy will come in and cause a step in an independent direction. This shows that the *ABC* model applies *exactly* to the tracer particle motion if one chooses the probabilities A, B, and C according to

$$X = X_0+\tfrac{1}{6}(1-A_0-B_0-4C_0) \qquad X = A, B, C, \text{also in } X_0. \tag{7}$$

It is possible to show that with this prescription the low-density limit of the correlation factor $f(\rho)$ has the corect value [7, 8]. Also one may show that

$$A=\tfrac{1}{3} \tag{8a}$$

and that in d dimensions $A=1/d$. For B and C we find from (6) and (7)

$$B=0.123\,49\ldots \qquad C=0.135\,79\ldots. \tag{8b}$$

But then it is clear, B and C being rather close to one another, why the BJ model works so well. In the low-density limit Czech uses the values $A=0.341\,53\ldots$, $B=C=0.131\,69\ldots$, very close to the values in (8a) and (8b), respectively. Evaluating (4) numerically for the three-dimensional case with the values A, B, C of (8a) and (8b), we find

$$\langle \mathscr{S}_t\rangle = 0.4907\ldots\rho t \qquad \rho\ll 1, \rho t\gg 1. \tag{9}$$

This should be compared to Czech's

$$\langle \mathscr{S}_t\rangle \approx 0.4863\ldots\rho t. \tag{10}$$

Our result is ≈0.9% higher than Czech's BJ approximation and is consistent with his simulation results which are systematically somewhat higher than the prediction of the BJ model but where 'the deviations are less than ≈1.5%' [3].

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