Comment on "Diffusion and Drift of Charge Carriers in a Random Potential: Deviation from Einstein's Law"

The authors of Ref. 1 have studied numerically the problem of an assembly of (charge e) random walkers in a three-dimensional random environment when an external (electric) field E is present. Their simulation gives the average velocity $V(E)$, and the diffusion (dispersion) constant $D(E)$, which is found to be finite (diffusion is indeed not expected to be anomalous in their situation[2]). They claim to find a novel and unexplained result as they observe strong deviations from Einstein's relation {which reads $V(E)=[D(E)/kT]eE$} even for relatively small fields E (small enough to ensure linear response $V=\mu E$, i.e., $\epsilon \equiv Ea/kT \ll 1$, where a is the lattice spacing). They note that the deviation is an increasing function of both E and the disorder, while the mobility μ is nearly independent of both.

It is, however, well known, in particular by people studying flows in porous media (see, e.g., Ref. 3 and references therein), that the dispersion constant indeed depends on the average flow rate V. The mechanism leading to such a dependence can be inhomogeneities in the flow field ("geometrical dispersion"[3]) or the trapping of the particle in regions of the medium "at rest" ("dead ends," low-permeability zones, etc.[3]). A very simple[4] model leads to (see also Ref. 3)

$$D(V)-D_m=Vl_d+\alpha V^2\langle\tau^2\rangle/\langle\tau\rangle\,, \qquad (1)$$

where D_m is the molecular diffusion constant, l_d is the "dispersion length," α is some constant, and $\langle\cdots\rangle$ means the average over the local trapping-time (τ) distribution. This result only quantifies the fact that there is an additional spreading of the packet due to those particles which are delayed by a local fluctuation of the flow rate or trapping time. If geometrical dispersion dominates, deviations from Einstein's relation are observed for flow rates larger than D_m/l_d, which can be very small for large disorder. The phenomenon observed in Ref. 1 is precisely the same, as will be argued quantitatively below.

In order to be more specific, we shall consider a one-dimensional hopping model, for which V and D may be computed exactly for any choice of the hopping rates.[5] As the problem addressed here is biased by E, the difference between three and one dimension is not crucial. The local hopping rates $W_{n+1,n}$ are, for simplicity, slightly different from those of Ref. 1, but this will only affect the details of the laws obtained, and not the main trends. Hence we take

$$W_{n\pm1,n}=\exp[(\Delta_{n,n\pm1}\pm Ea)/2kT]\,,$$

with $\Delta_{n,n+1}=\Delta_{n+1,n}$ distributed according to a Gaussian function $(2\pi\sigma^2)^{-1/2}\exp[-(\Delta^2/2\sigma^2)]$. From the general expressions of Ref. 5, one obtains, *in the low-field limit* $\epsilon \ll 1$,

$$V=\epsilon a/\tau_1\,, \qquad (2)$$

$$D=a^2/\tau_1+\tfrac{1}{2}Va(\tau_2/\tau_1^2-1)+O(V^2)\,, \qquad (3)$$

with $\tau_p \equiv \langle W(E=0)^{-p}\rangle$ [note the similarity with (1)]. For the model considered, one thus has

$$D(E)-D(0)\sim E\exp[3\sigma^2/8(kT)^2]\,,$$

which is precisely the dependence found in Ref. 1. [Their Fig. 2 shows the linear dependence of $\ln(D)$ on $(\sigma/kT)^2$.] Note, in particular, that the crossover field above which strong "violations" of Einstein's law are observed is exponentially small in $(\sigma/kT)^2$, and thus can be very much smaller than the pure lattice crossover field, kT/a, below which μ is indeed constant.

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[2]For the general conditions for anomalous diffusion, see J. P. Bouchaud and A. Georges (to be published). We may, in particular, refer the reader to Part V of this paper where the status of Einstein's relation and linear response in disordered media is fully discussed.

[3]For a recent review, see, e.g., the papers of J. F. Brady and J. P. Hulin, in *Proceedings of the Conference on Disorder and Mixing,* edited by E. Guyon, J. P. Nadal, and Y. Pomeau (Kluwer Academic, Hingham, 1988).

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