Comment on "Diffusion of Ionic Particles in Charged Disordered Media"

In a recent Letter, Mehrabi and Sahimi discuss motion of ions in charged disordered media, presenting a variety of results obtained by Monte Carlo simulation on a lattice [1]. Their observations of mean square displacements $R^2(t)$ suggest that this model exhibits anomalous diffusion in three dimensions,

$$R^2(t) \sim (\text{const}) t^{1-\delta} \quad \text{as } t \to \infty . \tag{1}$$

They observe the same behavior in one and two dimensions, but do not present results for δ. Mehrabi and Sahimi also make the physically surprising claim that a suitably defined diffusivity can actually *increase* with increasing disorder strength (see Fig. 3 of Ref. [1]). Exact bounds, renormalization group calculations, and previous numerical simulations are inconsistent with these results in three dimensions.

At low concentrations of mobile ions, the Green function for a diffusing ion should obey the diffusion equation,

$$\frac{\partial c_v(\mathbf{r}, t)}{\partial t} = D_0 \nabla^2 c_v + \beta D_0 \nabla \cdot [c_v \nabla v(\mathbf{r})] . \tag{2}$$

Here c_v is the Green function of a single ion in a given realization of the quenched random potential v, D_0 is the "bare," short-time diffusivity, and β is the inverse temperature. The mean square displacement is given by $R_v^2(t) = \int d^d\mathbf{r} |\mathbf{r}|^2 c_v(\mathbf{r}, t)$. The observable mean square displacement is given by an average over all realizations of the disorder: $R^2(t) = \langle R_v^2(t) \rangle$. The effective diffusion coefficient is defined in d dimensions by $D = \lim_{t\to\infty} R^2(t)/(2dt)$.

Mehrabi and Sahimi model the disorder by a quenched Gaussian random potential field. The statistics of this potential field are chosen so that they obey bulk charge neutrality: $\hat{\chi}_{vv}(\mathbf{k}) = \gamma/[k^2(k^2 + \kappa^2)]$. Here the potential-potential correlation function is $\chi_{vv}(\mathbf{r}) = \langle v(\mathbf{0}) v(\mathbf{r}) \rangle$, κ is an inverse correlation length, and γ is a measure of the density of defects. The Fourier transform in d dimensions is given by $\hat{f}(\mathbf{k}) = \int d^d\mathbf{r}\, f(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r})$.

The single-ion, random diffusion model is a well-studied one in statistical physics, and a variety of exact results are known. First, there is an exact bound for the diffusivity in this system in any dimension [2],

$$\frac{D}{D_0} \geq \exp[-\beta^2 \chi_{vv}(0)] . \tag{3}$$

Calculating this bound in three dimensions, one finds $D/D_0 \geq \exp[-\beta^2\gamma/(4\pi\kappa)]$. This result implies that the motion is diffusive in three dimensions, i.e., $D > 0$. The motion is also diffusive at finite ion concentrations, since the dynamical exponent is 2 [3]. Therefore, the motion should be asymptotically diffusive in three dimensions. Indeed, previous careful simulations by Dean, Drummond, and Horgan on related models have confirmed the bound [4]. Moreover, these simulations have shown that Deem and Chandler's single-ion prediction [5]

$$\frac{D}{D_0} = \exp[-\beta^2 \chi_{vv}(0)/d] \tag{4}$$

is accurate to at least moderate disorder strength. In fact, this equation is correct to second order in $\beta^2 \chi_{vv}(0)$ in all dimensions and is exact in one dimension. Note that, as expected physically, the diffusion constant *decreases* with increasing disorder strength.

The situation is more interesting in two dimensions, where anomalous diffusion can occur [the bound in Eq. (3) vanishes, and the predicted diffusivity in Eq. (4) is zero]. Indeed, field-theoretic treatments have shown that the exponent in Eq. (1) is continuously variable and is given exactly by $\delta = 1/[1 + 8\pi\kappa^2/(\beta^2\gamma)]$ [6]. This scaling has been confirmed by numerical simulations [7]. At finite ion concentrations, the anomalous diffusion persists at high temperature [3], although the mobile ions may partially screen the disorder. A Kosterlitz-Thouless transition can occur at low temperature [3].

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