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LETTER TO THE EDITOR

Diffusion in random media as a problem of interacting Bose and Fermi fields

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Abstract. Diffusion on a percolative lattice is formulated as a theory of interacting Bose–Fermi fields. The effective medium approximation (EMA) of Odagaki and Lax is obtained directly from the functional integral and is used to provide an EMA approximation for the diffusion constant and the DC conductivity. Simple corrections to the usual EMA produce exponents near the percolation threshold that agree with the best available data for $d=2$ and 3. This agreement reveals a strong connection between the dynamics of percolative diffusion and percolation itself.

Fortuin and Kasteleyn (1972) exhibit the deep connection between the Potts model and problems of bond percolation and resistor networks. They show how the percolation quantities of interest can be obtained as the $q \to 1$ limit of a q-state Potts model, while the $q \to 0$ limit is used to calculate the DC resistivity of a non-random network. Dasgupta *et al* (1978) extend this approach to the random resistor network and treat the problem using ε expansions about six dimensions within a Wilson–Kadanoff renormalisation scheme. Subseqent attempts have been made to improve upon these results. (See Sahimi *et al* (1983a) and references therein.)

It is believed that near the percolation threshold the DC conductivity σ varies as

$$\sigma_{DC} \propto (p - p_c)^{\mu} \tag{1}$$

where μ is the conductivity critical exponent, p is the bond (resistor) probability (concentration), and p_c is the percolation threshold probability. In two dimensions Derrida and Vannimenus (1982) use transfer matrix methods and finite size scaling to obtain $\mu_2 = 1.28 \pm 0.03$. In three dimensions experimental data of Abeles *et al* (1975) and series expansion estimates of Fisch and Harris (1977) yield $\mu_3 = 1.95 \pm 0.03$. This letter provides a simple theory of these exponents. The method used applies only for distances larger than a correlation length. The approach considers the general problem of diffusion in random media with the random resistor network being a special case.

Consider the standard problem of hopping on a d-dimensional hyperlattice as described by the equation of motion

$$\partial P_n(r)/\partial t = \sum_m T_{nm} P_m(t) \tag{2}$$

with $P_n(t)$ the probability of being at site n at time t and T_{nm} the hopping matrix.

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The initial conditions are taken as $P_n(0) = \delta_{n0}$. The hopping matrix is subject to the constraint

$$\sum_n T_{nm} = 0 \tag{3}$$

in the absence of trapping. This constraint plays an important role in the subsequent analysis. When the T_{mn} are random numbers, we are ultimately interested in the average $\langle P_n(t)\rangle_0$ over a random ensemble of the T_{nm}. The Laplace transformation of (2) gives

$$(s\boldsymbol{I} - \boldsymbol{H})\boldsymbol{P}(s) = \boldsymbol{I}_0 \tag{4}$$

with s the Laplace variable conjugate to t, $\boldsymbol{P}(s)$ the transform of $\boldsymbol{P}(t)$, $\boldsymbol{I}$ the unit matrix, $\boldsymbol{I}_0 = \delta_{n0}$, and the constraint (3) implies $\boldsymbol{H}$ is defined by

$$H_{mn} = (1 - \delta_{mn})T_{mn} - \delta_{mn} \sum_{m(\neq n)} T_{mn}. \tag{5}$$

For simplicity, consider the symmetric case of $T_{mn} = T_{nm}$.

The random resistor problem follows upon the replacement of $T_{nm} \to \sigma_{nm}$, where σ_{nm} is the conductivity between sites n and m and $\sigma_{nm} = \sigma_{mn}$. The matrix $\boldsymbol{H}$ has the essential property

$$\sum_m H_{nm} = \sum_n H_{nm} = 0, \tag{6}$$

similar to the constraint (3). Equation (6) implies $\det \boldsymbol{H} = 0$, and the equality of all cofactors of $\boldsymbol{H}$ (Harary 1969). Hence, when $s = 0$ in (4), the matrix $s\boldsymbol{I} - \boldsymbol{H} \to \boldsymbol{H}$ does not have an inverse, an important fact omitted in the recent attempt by Carton (1983) to combine Bose and Fermi fields to describe the percolation problem.

In random diffusion problem considered here, the quantity of interest is the average

$$G(s) = \langle (s\boldsymbol{I} - \boldsymbol{H})^{-1}\rangle_0 \equiv \langle \boldsymbol{K}^{-1}\rangle_0 \tag{7}$$

with $\langle P_n(t)\rangle_0$ the inverse Laplace transform of $G_{n0}(s)$. The $s = 0$ case is of relevance to the DC resistivity of a non-random resistor network (Fortuin and Kasteleyn 1972, Wu 1982). In the DC problem the matrix $\boldsymbol{H}$ does not have an inverse, and cofactors of $\boldsymbol{H}$ are all equal to the number of spanning trees which can be constructed from a graph related to the matrix $\boldsymbol{H}$ (Harary 1969). This observation has been used by Fortuin and Kasteleyn (1972) to present the non-random network problem as the $q \to 0$ limit of a Potts model, while Dasgupta *et al* (1978) add the replica trick to extend the description to the random case. This latter work, however, ignores the constraint $T_{nm} = T_{mn}$ for symmetric hopping (or $\sigma_{nm} = \sigma_{mn}$) when the average is performed. This feature is readily incorporated with possibly only minor numerical changes, but no alteration of exponents. Stephen (1978) treats the $s \neq 0$ case when the matrix $(s\boldsymbol{I} - \boldsymbol{H})$ does not have the property (6), so it is unclear *a priori* how the Potts model can be applied in this case. Stephen claims that the $s \neq 0$ case produces the exponents lying within the same universality class as the $s = 0$ case. This is a plausible assumption, but unfortunately no explicit proof of the statement has been given to date, so the question still remains open as does the calculation of the conductivity exponent μ.

Given the inverse matrix (7), the mean square displacement is obtained as

$$\langle \boldsymbol{R}^2(t)\rangle_0 = \mathscr{L}^{-1}\left(\sum_n n^2 \langle \boldsymbol{P}_n(s)\rangle_0\right) \tag{8}$$

where $\mathscr{L}^{-1}$ denotes an inverse Laplace transform. The diffusion coefficient is then obtained as (Gefen *et al* 1983)

$$\mathscr{D}_\infty \propto \lim_{t\to\infty} \frac{\mathrm{d}}{\mathrm{d}t}\langle R^2(t)\rangle_0, \tag{9}$$

and the DC conductivity follows from the Einstein relation

$$\sigma_{\mathrm{DC}} = e^2 n \mathscr{D}_\infty / T \tag{10}$$

with n the carrier concentration, e its charge, and T the temperature in energy units. Electrons can only contribute to σ_{DC} if they belong to an infinite percolative cluster, so the fraction of available carriers is given by $n \propto (p-p_c)^\beta$ for $p \to p_c$. Combining this fact with (1) and (10) yields the result

$$\mathscr{D}_\infty \propto (p-p_c)^{\mu-\beta} \tag{11}$$

where β is known but μ remains to be determined.

Here we evaluate D_∞, enabling μ to then be determined from (11). Begin with the two identities (Efetov 1983)

$$\int \prod_i \mathrm{d}\varphi_i^* \, \mathrm{d}\varphi_i \exp(-\boldsymbol{\varphi}^* \boldsymbol{K} \boldsymbol{\varphi} + \boldsymbol{\mathcal{J}}^* \boldsymbol{\varphi} + \boldsymbol{\varphi}^* \boldsymbol{\mathcal{J}}) = [\det \boldsymbol{K}]^{-1} \pi^n \exp[\boldsymbol{\mathcal{J}}^* \boldsymbol{K} \boldsymbol{\mathcal{J}}], \tag{12}$$

$$\int \prod_i \mathrm{d}\psi_i^* \, \mathrm{d}\psi_i \exp(-\boldsymbol{\psi}^* \boldsymbol{K} \boldsymbol{\psi}) = \det \boldsymbol{K}, \tag{13}$$

where ϕ and ψ are complex Bose and Fermi fields. These identities enable (7) to be transformed to

$$\langle K_{ij}^{-1} \rangle_0 = \pi^n \int \prod_l \mathrm{d}\varphi_l^* \, \mathrm{d}\varphi_l \prod_m \psi_m^* \psi_m \varphi_i \varphi_j \left\langle \exp\left(-\sum_{ij} K_{ij} A_{ij} \right) \right\rangle_0 \tag{14}$$

where $A_{ij} = \varphi_j^* \varphi_i + \psi_j^* \psi_i$, and the constraint (3) must be incorporated when the average $\langle\ \rangle_0$ is applied.

First we derive the effective medium approximation (EMA) from (14) by introduction of the non-random matrix $\boldsymbol{M}$ such that $\langle \boldsymbol{M} \rangle_0 = \boldsymbol{M}$. Consider the quantity

$$Z = \langle\langle \exp[-(\boldsymbol{K}-\boldsymbol{M})\boldsymbol{A} - \boldsymbol{M}\boldsymbol{A} + \boldsymbol{\mathcal{J}}^* \boldsymbol{\varphi} + \boldsymbol{\varphi}^* \boldsymbol{\mathcal{J}}] \rangle\rangle_0 \tag{15}$$

where $\langle \ldots \rangle$ denotes the functional average over φ_i^*, φ_i, ψ_i^* and ψ_i, and (14) is obtained via $\partial \ln Z / \partial y_i \partial y_j^* |_{y=y^*=0}$ in the usual way. Let $\langle\ \rangle_{\boldsymbol{M}}$ represent the functional average with weight $Z_{\boldsymbol{M}}^{-1} \exp(-\boldsymbol{M}\boldsymbol{A} + \boldsymbol{y}^* \boldsymbol{\phi} + \boldsymbol{\phi}^* \boldsymbol{y})$ so that $\langle 1 \rangle_{\boldsymbol{M}} = 1$. Then we may write

$$Z = Z_M \langle\langle \exp[-(\boldsymbol{K}-\boldsymbol{M})\boldsymbol{A}] \rangle_M \rangle_0. \tag{16}$$

If s is chosen as real, (16) produces the inequality

$$Z \geqslant Z_M \exp[-\langle\langle (\boldsymbol{K}-\boldsymbol{M})\boldsymbol{A} \rangle_M \rangle_0]. \tag{17}$$

The best approximation results when

$$0 = \langle\langle (\boldsymbol{K}-\boldsymbol{M})\boldsymbol{A} \rangle_M \rangle_0 |_{y^*=\dot{y}=0} = \langle \boldsymbol{M}^{-1} - \boldsymbol{K}^{-1} \rangle_0, \tag{18}$$

which is just the conventional EMA condition (Odagaki and Lax 1981). Using the

percolative-like distribution,

$$w(T_{ij}) = p\delta(T_{ij} - K_{ij}^0) + (1-p)\delta(T_{ij}) \tag{19}$$

for the jump probabilities, the EMA condition (18), and the constraint (3) yields (Sahimi *et al* 1983b)

$$\lim_{t\to\infty} \langle R^2\rangle_0 \propto (p - p_c)t \tag{20}$$

for $d = 2$ and 3 with $p_c = p_c^{EMA} = (2/z)$ and z the lattice coordination number. The EMA result (20) and the definition (9) can be used to provide an approximation for the diffusion constant, but this simple result may readily be improved by noting that below p_c propagation is confined to some of the clusters of various sizes. At p_c at least one infinite cluster is formed, and diffusional propagation requires that the particle initially be on this infinite cluster. Over length scales L for which $a \ll L \ll \xi$, with a the lattice constant and ξ the fractal (percolation) correlation length $\xi \propto (p - p_c)^{-\nu}$, we have the case of fractal diffusion (Gefen *et al* 1983). Ordinary diffusional motion (20) occurs only for $L \gg \xi$, while for $a \ll L \ll \xi$ the fractal dimension enters into the calculation of $\langle R^2(t)\rangle_0$. The cross over between these regimes remains to be described, but evidently the EMA applies only for $L \gg \xi$.

Using (9) and (20) produces the naively EMA prediction $\mathscr{D}_\infty \propto (p - p_c)$. However, equations (4) and (7) imply that this naive result implicitly presumes that the particle begins motion on some particular site **0**. The random nature of the lattice requires that we perform an average over all possible initial lattice sites. Then contributions to this site average yield the form (20) *only for initial sites lying on the infinite cluster*, so (20) must be multiplied by the fraction of initial sites which belong to the infinite cluster. Since this fraction is proportionl to $(p - p_c)^\beta$, equations (9), (20) and this factor yield

$$\mathscr{D}_\infty \propto (p - p_c)^{1+\beta}. \tag{21}$$

Equating the exponent in (21) to that in (11) produces

$$\mu = 1 + 2\beta. \tag{22}$$

Stauffer (1979) gives $\beta = 0.14$ for $d = 2$, while Sahimi *et al* (1983a) have $\beta = 0.46 \pm 0.05$ in $d = 3$. Hence we obtain the values $\mu_2 = 1.28$ and $\mu_3 = 1.92 \pm 0.1$ for $d = 2$ and 3, respectively, in remarkable agreement with the most accurate two-dimensional calculations (Derrida and Vannimenus 1982) $\mu_2 = 1.28 \pm 0.03$ and in excellent agreement with three-dimensional experiments (Abeles *et al* 1975) $\mu_3 = 1.9 \pm 0.2$ and the most reliable series estimate $\mu_3 = 1.95 \pm 0.03$ (Fisch and Harris 1977). Recent Monte Carlo calculations for D_∞ on percolation clusters by Havlin *et al* (1983) obtain the diffusion exponents 1.05 ± 0.05 for $d = 2$ and 1.5 ± 0.1 for $d = 3$ in good agreement with our predictions of $1 + \beta$. This remarkable agreement is not coincidental. It reveals a strong connection between diffusion on a percolative lattice and the underlying percolation phenomenon. Our analysis employs p_c^{EMA}, but this choice does not affect the calculated exponents. A better estimate of p_c requires the treatment of fluctuations about the mean fluid solution. We plan to provide such a generalisation in a subsequent paper.

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