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LETTER TO THE EDITOR

Region of validity in theories of diffusion near to the percolation threshold

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Abstract. In theories of classical diffusion near to the percolation threshold two characteristic times can be defined: τ_s for the short time and τ_h for the hydrodynamic behaviour. Physically $\tau_s < \tau_h$ should be fulfilled and we suggest this relation as a criterion of validity in such theories. For the effective medium and the self-consistent current relaxation theory the region where this criterion is violated shrinks with dimension $d \to \infty$, but remains finite for all $d > 2$. $d = 2$ is a marginal case concerning our criterion.

The importance and the theoretical challenge of classical diffusion in disordered media have caused intense research during recent years. The conductor–insulator transition in such systems is closely related to percolation (see e.g. Stauffer 1979). Models describing the essence of this phenomenon can be either of hopping character (see e.g. Mitescu and Roussenq 1983), or continuous Lorentz models, where the static disorder serves as scattering potential (see e.g. Götze 1982). Considerable effort has been made to construct approximation theories for these models. Successful attempts are the effective medium theory (EMT) (Bruggeman 1935) for hopping models (Kirkpatrick 1971, Odagaki and Lax 1981, Summerfield 1981, Webman 1981, Kaski *et al* 1982), and the self-consistent current relaxation theory (SCCRT) (Götze 1978) for the hard sphere Lorentz model (Götze *et al* 1981a). These theories are exact in the weak disorder limit, they give a description of the conductor–insulator transition and some quantities of interest can be calculated with high accuracy in a large range of the disorder parameter (see Kirkpatrick 1971, Götze *et al* 1981b, 1982). A question of fundamental importance is to clarify the region of validity in these theories, as is done by the Ginzburg criterion in the mean field theory of phase transitions.

In this letter we point out the main physical reasons for the breakdown of the theories near the percolation threshold c_p and we suggest a criterion to estimate the region of validity.

The system under consideration consists of allowed and forbidden regions with c being the concentration of e.g. broken links. (In continuum systems the dimensionless scatterer density plays the role of the concentration c. Universality between continuum and lattice systems seems to hold (see e.g. Kertész and Vicsek 1982).) The correlation length ξ, diverging as $|\varepsilon|^{-\nu}$ with $\varepsilon = c_p - c$, is characteristic in both finite and infinite clusters for $\varepsilon > 0$. The characteristic finite clusters with radius $\sim\xi$ give the main contribution to the diverging moments of the cluster distribution (Stauffer 1979). The infinite cluster is homogeneous on length scales much larger than ξ, while it is self

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similar on much shorter length scales (Stanley and Coniglio 1983). This structure is reflected in the diffusion of a particle on percolation clusters. According to the scaling form (Straley 1980, Ben Avraham and Havlin 1982, Gefen *et al* 1983) of the mean square displacement

$$\langle r^2(t)\rangle \propto \varepsilon^{-2\nu+\beta} f(t/\tau) \tag{1}$$

at time t for $\varepsilon \to 0$, where $\tau \propto |\varepsilon|^{-2\nu+\beta-\mu}$ is the characteristic time and μ and β are the critical exponents of the diffusion coefficient $D \propto \varepsilon^{\mu}$ and of the percolation probability. For times $t \ll \tau$ the critical behaviour can be observed, which is anomalous diffusion like at the threshold (Ben Avraham and Havlin 1982, Gefen *et al* 1983). For $t \gg \tau$ the long time asymptotics sets in (Götze 1982, Kertész and Metzger 1983)

$$\langle r^2(t)\rangle/(2d) = Dt + r_0^2 + l(t), \qquad t \to \infty \tag{2}$$

$l(t)$ being determined by the long time behaviour of $K(t)$, the time dependent diffusion coefficient and for $\varepsilon \to 0$, $r_0^2 \propto \varepsilon^{-2\nu+\beta}$. τ of equation (1) can be calculated as $\tau \sim r_0^2/D$. This is the time needed for the particle either to notice the boundaries of a typical finite cluster or to cross a self similar blob (Stanley and Coniglio 1983) in the infinite cluster. In equation (2) the term r_0^2 expresses the fact that the particle 'remembers' even for $t \to \infty$ the typical finite clusters and the structure of the infinite cluster (Kertész and Metzger 1983), i.e. features carrying criticality at c_p. Taking r_0^2 and D from an approximation theory, we can define

$$\tau_s = r_0^2/D \tag{3}$$

as the time characteristic for the short time behaviour.

$l(t)$ is a typical hydrodynamic term. Accepting universality arguments, as they are established in the case of classical liquids (Forster *et al* 1977), we assume

$$l(t) = -at^{-(d/2-1)} \tag{4}$$

where the exponent is taken from the low density limit of the Lorentz model (Ernst and Weyland 1971)†. EMT and SCCRT also predict this behaviour for all $\varepsilon > 0$. A quantity with dimension of time is, therefore, $(a/D)^{2/d}$. Because of equations (1) and (2) this should yield τ again, as far as order of magnitude and divergence properties are concerned. For $t \gg \tau$ one should see the long time asymptotics. According to van Beijeren's (1982) convincing argument, the long time tail of $K(t)$ in the low density limit of the Lorentz model is due to missing randomisation of velocities when the particle comes back to the region where it has started from. Physically the long time tails are always due to memory effects and the time scale where they become observable corresponds to the returning time. If a and D are now taken from an approximation theory, one can define

$$\tau_h = (a/D)^{2/d} \tag{5}$$

as a characteristic time for the hydrodynamic limit. We argue that in the theories the short and long time scales should be separated, i.e.

$$\tau_s < \tau_h \tag{6}$$

† In numerical simulations (Alder and Alley 1978) a density dependent exponent was found. This could be explained because in runs with fixed t only effective exponents can be seen (Götze *et al* 1981b, 1982).

and we propose this relation as a criterion for the region of validity in approximation theories.

The reason for the breakdown of EMT and SCCRT is similar to that of mean field theories in thermal phase transitions: fluctuations are neglected. Both EMT and SCCRT do not contain the non-ergodic singularity due to finite clusters in the conducting phase (Kertész and Metzger 1983). The complicated structure presented at the beginning is approximated in these theories in an overall (effective) medium. Near to c_p fluctuations become important, which have geometrical origin here, and which manifest in the fact that the infinite cluster has a structure (Stanley and Coniglio 1983) and finite clusters are present in the conducting phase.

In order to illustrate how criterion (6) works, we calculate τ_s and τ_h for hypercubic bond percolation in EMT, and for the d-dimensional Lorentz model in the SCCRT framework. First we note that the low frequency behaviour of $K(z)$, the Laplace transform of $K(t)$, is the same in both theories. For EMT it can be read off from Sahimi *et al* (1983) and Haus *et al* (1983). For SCCRT, where it suffices for our purposes to use a simplified version, it can be read off from Leutheusser (1982). One obtains

$$K(z)/D_0 = \mathrm{i}(1-c/c_p) + c/c_p\left(Bz/D - \mathrm{i}A\int_0^{q_0} \mathrm{d}k\, k^{d+1}(z/\mathrm{i}D + k^2)^{-1}\right)$$

where in the last integral only the leading (cut-off independent) non-analyticity is to be taken. c is the density of scatterers with radius unity in the Lorentz model. $c_p = 1 - 1/d$ in EMT and $c_p = d/V_d$ in SCCRT, where V_d is the volume of the d-dimensional unit sphere. D_0 denotes the diffusion constant of the pure system or the Boltzmann approximation in EMT and SCCRT respectively. The dimension dependent numerical factors A and B are for $d>3$: $A = V_d[(1-1/d)(2\pi)^d]^{-1}$, $B = (2d-2)^{-1}\int_0^\infty \mathrm{d}t(\mathrm{e}^{-t}I_0(t))^d$ in EMT, where $I_0(t)$ denotes the modified Bessel function of order 0, and $A = d(2^d\Gamma^2(d/2+1))^{-1}$, $B = [(d+2)\,(d/2-1)]^{-1}$ in SCCRT.

After inverting the Laplace transform, we can identify the quantities needed in our criterion as $r_0^2 = D_0cB/(c_pD)$ and $a = D_0cA\Gamma(d/2-1)/(2c_pD^{d/2})$. Via equations (3), (5), (6) we get the estimate $D^{2/d} \leqslant D$. This relation is violated near to c_p for all $d>2$. There is no dimension above which the critical behaviour could be described by these theories. In fact, it is widely accepted (de Gennes 1976, Stauffer 1979) that for $d \geqslant d_c = 6$, $\mu = 3$, while D goes linearly to 0 in all d in these theories. On the other hand the criterion (6) can be written as

$$c \leqslant c_p(1+x(d))^{-1} \tag{7}$$

where $x(d) = \{4B^d/[A^2\Gamma^2(d/2-1)]\}^{1/(d-2)}$. From this formula one easily deduces that $x(d\to\infty)$ vanishes in both theories. Therefore one can say that the higher the dimension is, the larger is the range of c for which these theories should be valid, but the deviations from experiment should show up more promptly in higher dimensions, if c violates equation (7). We mention that in $d=3$ equation (7) yields $c \leqslant c_p$ 0.20 in EMT and $c \leqslant c_p$ 0.35 in SCCRT. In the first case a factor of three (Kirkpatrick 1971) and in the second case a factor of two (Götze *et al* 1981b) could be allowed. Here we have to emphasise that such a criterion can be taken only as an order of magnitude estimate.

The case $d=2$ requires a separate discussion. Equations (1), (2) and (4) yield

$$\tfrac{1}{4}\langle r_0^2(t)\rangle = Dt + r_0^2 + a\ln(t/\tau) \tag{8}$$

for $t\to\infty$. The same long time behaviour is predicted in both theories with r_0^2 and

$a \propto \varepsilon^{-1}$ (Sahimi *et al* 1983, Haus *et al* 1983, Götze *et al* 1981). This parallel scaling fulfils equation (1), and from that viewpoint, which is a basis of our criterion, these theories are consistent. This could mean that $d = 2$ is the lower critical dimension and $\mu = 1$ with logarithmic corrections (de Gennes 1976). However, in the light of recent numerical results, μ settles at 1.3 (Binder and Stauffer 1983, Pandey *et al* 1983). Discrepancies also show up in r_0^2, which is known to diverge as $\varepsilon^{-2.52}$ (see e.g. Stauffer 1979). This means that the separation of time scales is theoretically held valid with wrong exponents. But the fact that the theories show excellent agreement with the numerical data concerning $D(c)$ in two dimensions (Kirkpatrick 1971, Götze *et al* 1982) underlines the importance of our aspect. Because equation (8) should be generally valid, we suggest to reanalyse some hopping simulations (Mitescu and Roussenq 1983, Pandey *et al* 1983) with taking into account that the linearity in $\langle r^2(t)\rangle$ is only logarithmically approached and not exponentially fast, as assumed in Straley (1980), Mitescu and Roussenq (1983) and Pandey *et al* (1983).

In conclusion, we have given a simple criterion for the region of validity in approximation theories describing diffusion near to the percolation threshold. It has been successfully applied to EMT and SCCRT, thereby emphasising that these theories, although different in origin, describe the critical region in the same manner. Finally we mention that any approximation theory for the models treated here could be tested by our criterion equations (2)–(6).

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