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FRACTAL EXCITON FUSION: SIMULATIONS ON LONG-RANGE PERCOLATION CLUSTERS*

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Computer simulations of exciton fusion on percolating clusters
were performed for interaction distances n=2, 3, and 4. The
data yield slopes less than those expected from
superuniversality (f=2/3) at interaction distances above 2,
when the probability of successively longer hops falls by a
factor of 1/10.

Exciton fusion kinetics in isotopic mixed crystals have been
modeled by Monte Carlo random walks on random binary lattices [1],
giving for both two- and three-dimensional systems of reacting
walkers an effective spectral dimension $d_s=2f$, where $f=2/3$ at the
critical percolation concentration (C_c), $f=1$ at 100%
concentration (classical behavior), and a "crossover" from
fractal to classical regime in between. Fusion occurs when two
walkers occupy the same site simultaneously. The integrated rate
equation for fusion is: $\rho(t)^{-1} - \rho(0)^{-1} = K_0 t^f$, where $\rho(t)$ is
the walker density at time t, and K_0 is a constant. The simu-
lations have here been extended to walks with jumps longer than
nearest-neighbor[2] (see Fig. 1) .   The probability assigned to a
long range jump is a function of the number of ways an exciton
may arrive there and the assigned probability for an interaction
range. Static percolation gave[3] the following: C_c = 0.282, n=2;
C_c= 0.156, n=3; and C_c = 0.099, n=4.

The slopes of the curves in Fig. 2 (n=2), Fig. 3 (n=3), and
Fig. 4 (n=4) correspond to f. Simulations close to C_c were run

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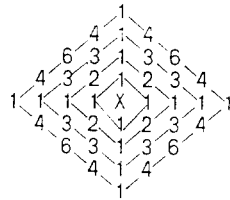| c	f
40/	.823
29/	.687
20%	.719
40%	.853
29/	.665
20/	.335
40%	.774
29%	.645
20%	.315

FIGURE 1

FIGURE 2

Four "diamonds" corresponding
to n=1, 2, 3, and 4, nested
around a walker X. The walker
may choose any diamond with
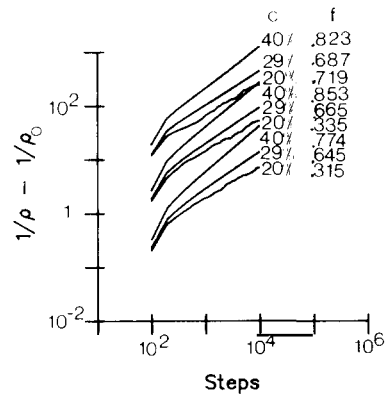assigned probability. The num-
bers are the number of routes
to a site.

n=2. $\text{Log}[1/\rho-1/\rho_0]$
vs. Log Time plotted. 5000 step
random walks on largest cluster
of 250,000 site square lattices.
10% initial concentration of
walkers. 100 runs averaged.
See text for explanation.

somewhat   above C_c,   to   ensure percolation.   Cluster Multiple
Labelling Technique was used to find the largest cluster.   The
three sets of three curves in Fig. 2 are for n=2 with 1/10 ratio
between diamonds, 1/2, and 1/1, top to bottom.   (Top and bottom
sets   are   shifted 1 log cycle   up   and   down   for   clarity.)
Interaction   range n=2   seems   to   conform   to   the   asymptotic
superuniversality hypothesis at criticality.   At 29%, there is a
trend to higher f when all sites are equally probable and a trend
to   lower f when the ratio is 1/10.

In Figs. 3 & 4 the ratio between diamonds was 1/10. These data
show a trend in f toward lower values   as   the   interaction range
increases.   This may be due to walkers   in   inaccessible   regions
not having taken   sufficiently   many   long   hops   to   meet   other
walkers and annihilate.   Indeed, the   20%   curve on the n=4 graph
might   be   viewed   as   if   it   were an   n=2   or   n=3   curve   near
percolation--as if the   longer   hops were not contributing.   Over
the   course   of   100,   000   steps,   a   walker can only perform 100

hops of four lattice spacings (n=4). Therefore the walks should be extended to much longer times to assure that asymptotic f values (for superuniversality) are obtained. Similar behavior was observed in single walker simulations [1].

We note that recent experiments [5] for triplet excitons in naphthalene-perdeuteronaphthalene indicate that "classical" behavior becomes "fractal" behavior between 16% and 12% concentrations, corresponding roughly to n=4.
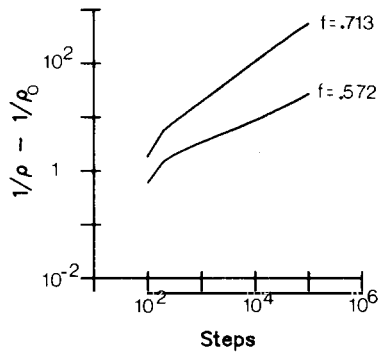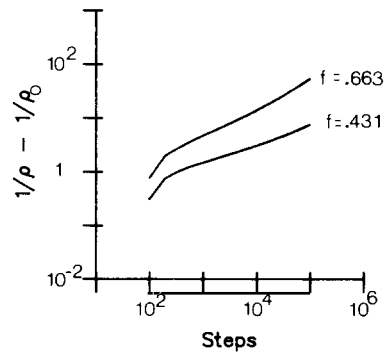

FIGURE 3

FIGURE 4

n=3. 100,000 step random walks.
Top: 30%, 8 runs.
Bottom: 16.5%, 8 runs.

n=4. 100,000 step random walks.
Top: 20%, 5 runs.
Bottom: 10.5%, 14 runs.

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