Chapter 1

ENTROPY SATURATION AND THE BRINKMANN-RICE TRANSITION IN A RANDOM-TILING MODEL

D. K. Sunko
Department of Physics, Faculty of Science, Bijenička 32, HR-10000 Zagreb, Croatia.

Abstract
The parameter regime in which a Brinkmann-Rice (BR) transition appears near half-filling is investigated for a model of one kind of electrons traversing a plane randomly tiled with CuO$_4$ molecules, simulating the copper-oxide planes of high-$T_c$ superconductors. As the hole doping is increased, the BR transition evolves continuously into a state characterized by Kauzmann-like plateaus in the entropy vs. temperature curves. Despite clear analogies with the glass transition, these are equilibrium properties of the model. This is because the spin interactions, responsible for ordering in real space, are not included.

Introduction. One difficulty in describing the metal-insulator transition, caused by strong electron repulsion, is that there is no obvious classical solution in the limit of infinite repulsion. This is in contrast to ‘strong-coupling’ problems with attractive interactions, which are difficult when the coupling is competitive with the hopping scale, but simplify when it becomes much greater.

Like some other approaches, saddle-point slave-boson [1] and dynamical mean-field theory [2], the random-tiling (RT) model [3] tries to get around this problem by simply postulating a ‘heavy mode’. The RT heavy mode is essentially the one proposed by Gutzwiller: electrons of one spin see those of the other as static. This is implemented as a Falicov-Kimball limit of the three-band Emery model, in which only up-electrons move, by projected hopping. There are no spin interactions in the model. The parameters are the hopping overlap $t$ and copper-oxygen splitting $\Delta_{pd}$.

Brinkmann-Rice regime. Here I concentrate on the limit $t \ll \Delta_{pd}$, which was identified in Ref. [3] as having a crossover of Brinkmann-Rice [4] type. The novelty is in what happens when one moves away from half-filling. In Fig. (1.1), I show the entropy of the mobile spins. There appear saturation
plateaus, reminiscent of Kauzmann plateaus [5] in vitreous liquids. One of the curves even exhibits a ‘Kauzmann paradox’, extrapolation from the high-temperature part yielding a negative entropy at low temperatures. Entropy saturation due to ‘freezing’ of kinetic motion was also observed in $^3$He, and even modelled by the Hubbard model [6].

![Figure 1.1](image)

*Figure 1.1* Entropy of mobile spins, for $t = 0.25$ eV (left three curves), and $t = 0.5$ eV (right four curves). Curves are marked by the corresponding concentration. Saturation plateaus are clearly visible. Here $\Delta_{pd} = 3$ eV, $U = 10$ eV, and $n = 2n_\uparrow = 2n_\downarrow$.

The value of the entropy at the plateaus corresponds to complete static disorder of the tiles, so it is the maximum one-band entropy, the rise beyond being due to the oxygen degrees of freedom. These play a role analogous to classical translation in the case of $^3$He. Once the rise occurs, the oxygen gas rapidly becomes Maxwellian (the chemical potential moves out of the effective band). The plateaus signal ‘pseudogaps’ in the system density of states. The single-particle model on which the problem is mapped reflects this by a very narrow effective band for the parameters in question, so the Maxwellian regime corresponds to the temperature becoming comparable to this effective band-width. The input parameters, as shown, are still on the usual ‘electron’ scale, indicating strong model renormalization when $t/\Delta_{pd} < 1/5$. The effective one-particle density of states shows no pseudogaps.

For realistically large values of the hopping overlap, e.g. $t = 1$ eV for $\Delta_{pd} = 3$ eV, the entropy has a fairly smooth ‘metallic’ rise at finite fillings, and there is no Brinkmann-Rice regime near half-filling, either.

**Discussion.** The Brinkmann-Rice ‘transition’ in the RT model is the endpoint of a continuous range of glass-like crossovers, tuned by doping. The model interpolation, between quantum order at low temperatures and classical
disorder at high ones, is not smooth in this parameter regime, despite the input $t/\Delta_{pd}$ being fairly large, though smaller than suggested by experiment.

The expression ‘glass-like’ is used only conditionally, to describe the shape of the entropy curves. In the absence of spin interactions, there is no spatially ordered state of lower free energy, even at half-filling. In fact, the RT Mott-Hubbard transition occurs slightly below half-filling, immediately producing a less ordered state [7]. This tendency of charge correlations to disorder the system, presumably counteracting spin correlations on the hole-doped side, is one of the more interesting aspects of the RT model.

Experimentally, a pseudogap can be noticed in the temperature dependence of the entropy of LSCO [8]. For underdoped systems, the curve is first flat, then rises, so that extrapolation from the high-temperature part indicates a disappearance of states at the Fermi level. However, the parameter regime needed to obtain the observed values of the entropy in the RT model is the above-mentioned realistic one, $t/\Delta_{pd} \sim 1/3$, where the entropy curves are smooth, not like the ones shown here. This discrepancy of qualitative and quantitative fits is probably due to the overly simplistic Falicov-Kimball limit.

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