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Trap-controlled conduction in disordered materials: Self-organized criticality at play?

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Charge transport in disordered insulators and semiconductors is generally agreed to occur by transferring of charge (electrons, holes or ions) between localized states or traps that act as potential wells with respect to the conduction-band level [1]. Crucial to the dynamics is the trap occupancy, which is believed to have a significant effect on the current-voltage characteristics [2]. The filling of the traps at higher voltages (strong injections) progressively burns the localized states through the medium, thus offering more sites available for the conduction. As a result, the net mobility of the charge carriers is enhanced as their density increases, a phenomenon which relates to the observed dependence of the conductivity on electron density and electron injection in porous nanocrystalline semiconductors [3], as well as electrical degradation and breakdown in insulating polymers [4].

In this paper we propose a model of charge transport in disordered solid materials that is intended to explore the transition to a macroscopically conducting state due to the trap-filling. Our main finding is the complex and multi-scale character of the transition. Our results can most naturally be explained within a paradigm of self-organized criticality (SOC), perhaps the simplest framework that captures the key signatures of slowly driven evolution processes [5].

Description of the model. − Let us consider a hypercubic d-dimensional lattice, where $d \geq 2$ is an integer number. Charge can be stored on each node. The lattice nodes are intended to mimic the traps of real insulating materials. In our model only one particle (unit charge) is allowed per node. Adding a particle switches the node from insulating to conducting. Particles are added at random according to the following rule. If the node is empty it absorbs the particle, otherwise excess charge (one particle) is transmitted to a nearest neighboring node. If several neighbors are prone to absorb the particle the destination node is a random choice. Tunnelling of charge between the nodes is forbidden. A compensating potential is applied across the lattice in proportion to the number of the absorbed particles. We refer to a setting in which the lattice is confined between two conducting plates exposed to a potential difference. The voltage between the plates is increased at a rate so slow that all particles are absorbed in traps before a new charge is added. The trap-filling is thus adiabatic and the system evolves through a sequence of quasi-stationary states of progressively increasing trap occupancy.

Of interest is a situation when the concentration q of the conducting nodes approaches the percolation threshold, q_c. In this limit, the pair connectedness length (i.e., the size of the biggest conducting cluster) diverges as an inverse power of $q_c - q$ and for q sufficiently close to q_c exceeds the size of the system (i.e., the distance between the plates). The lattice as a whole then turns into a macroscopic conducting state out of the initial insulation state. The insulation is broken to this point.

As soon as the percolation state is reached for $q \to q_c$, a portion of electric charge is transferred from one plate to the other. We argue that the transfer time is short compared to the dielectric relaxation time in the system. In fact, once the percolation is established, the free charges may cross the entire lattice by hopping through only the filled nodes which provide little resistance to the motion. In some sense, the filled nodes offer a runway along which the current carrying particles may walk without rest, all the way through. The transfer time is estimated as the time it takes for an individual particle to cross the conducting cluster along a path of least resistance. On the contrary, the dielectric relaxation time necessitates detrapping of all particles stored through the lattice. This time, which is basically the RC time of the circuit, is typically very long due to the huge (compatible with the total number of the absorbing states) bulk capacity of the medium. A key point is that the two times are scale separated. The argument of scale separation leads one to propose that (i) the early bird charges reach the other conducting plate before the bulk populations are significantly perturbed and (ii) these first portions of the transmitted charge are still small compared to the overall charge stored through the lattice.

Next, we assume that the transmitted charges recombine with the boundaries or external electron acceptors or reach the collecting electrode. Because the particle injection rate is adiabatic, the system is given to dissipate all of the charge which has come through. We now again pursue with the argument of scale separation by requiring that the charge dissipation time (which is defined by the resistance outside the boundaries) is short compared to the dielectric relaxation time of the lattice. Once the transmitted charges are gone, the voltage between the plates diminishes in the proportion. Because the lattice itself cannot store more charge than is permitted by the potential difference, the average trap occupancy through the lattice is posed to decrease to reinstall the equilibrium. This causes a redistribution of the particles between the lattice nodes, with excess charge left out of the boundaries. The lattice then comes into a state with a diminished number of the stored particles.

On the other hand, the particles are sources of the conducting nodes and diminishing the number of the stored particles harms the conduction. If the concentration of the conducting links now falls below the q_c the macroscopic conduction is destroyed and the system turns to insulate. The reinstalled insulation locks the lattice whose overall conductivity switches to zero.

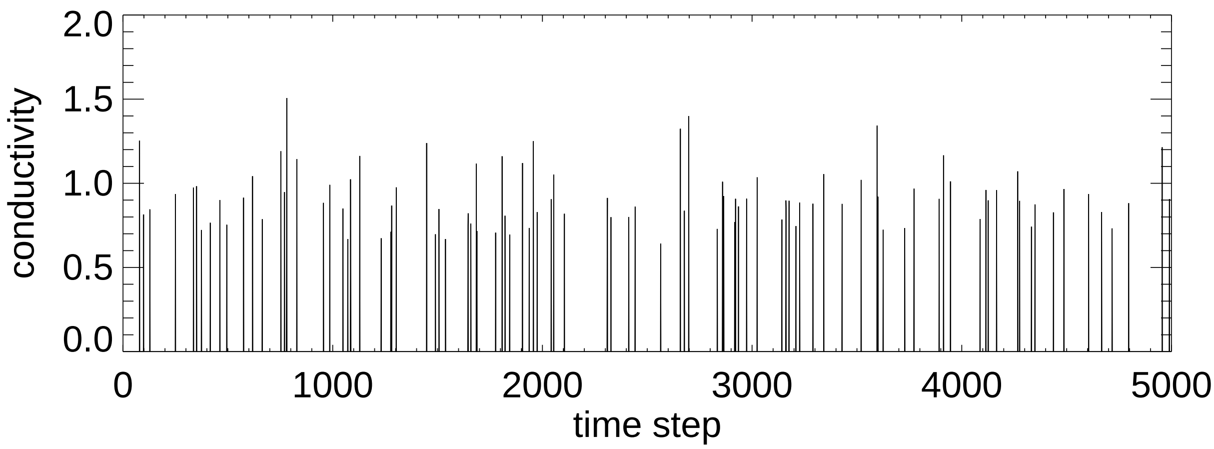

Figure 1: The pulses of nonzero conductivity at the percolation point. The numerical model is set on a square 15×15 lattice which simulates a charge absorbing medium. The percolation is observed when approximately one half of the initially absorbing nodes are activated. The observation is split into 5×10^3 consequent time steps, with an output of 1096 pulses.

More charge cannot be transmitted through the system and the dynamics tend to relax.

The onset of relaxation is a proper moment for the external drive to come into play. Because the plates are constantly exposed to the slowly growing potential difference, the equilibrium trap occupancy now reclaims an increased concentration of the conducting nodes. To respond to the changing external conditions, the lattice attempts a new climb of the percolation threshold. At the end of the day, the circuit unlocks to permit a new release of electric charge. The final state of the system is likewise multi-scale self-adjusting dynamical state which fluctuates near the percolation point. This state bears signatures enabling to associate it with the state of self-organized criticality. A computer realization of the phenomenon is summarized in Figs $1-2$.

References

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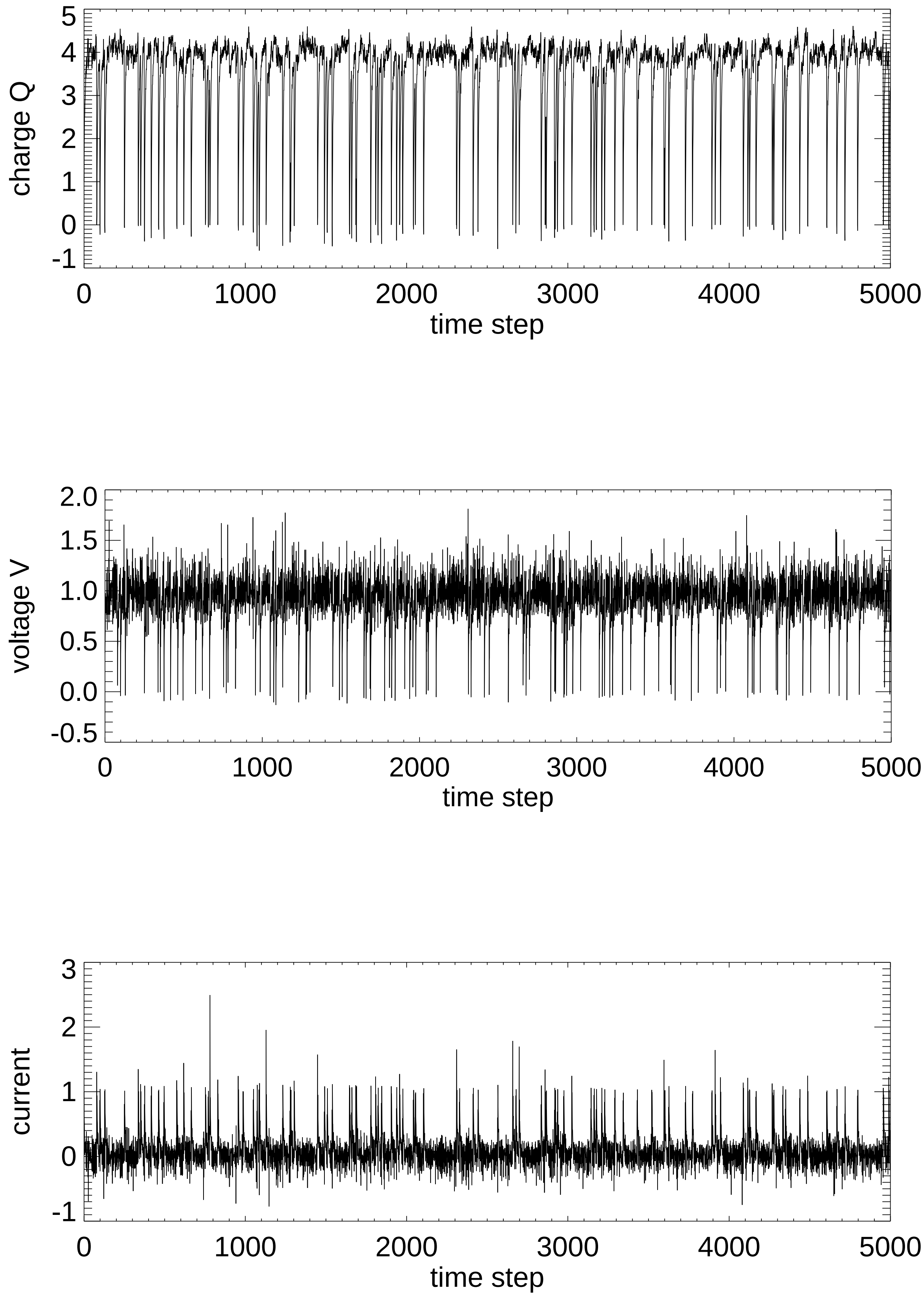

Figure 2: Dynamics of the critical state: Fluctuations of the bulk occupancy (top), potential difference (middle), and cross-lattice electric current (bottom).