PERCOLATION PATHS THROUGH SIMULATED GRANULAR SUPERCONDUCTORS

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ABSTRACT. A method is presented to determine the superconducting percolation paths through granular superconductors showing re-entrant resistivity peaks. It introduces an original approach capable of an effective reduction of intermediate data handling and, although originated from such a specific problem, it can be used as an effective method to determine percolation paths through more general networks.

1 Introduction

Based on Josephson junctions array and Coulomb blockage, a model capable to explain re-entrant resistivity peaks in diamond-like carbon-silicon films containing tungsten was presented by Chudinov et al. [1, 2]. Such granular superconductors present one or two re-entrant (or quasi-re-entrant) resistivity peaks at lower temperatures than the critical ones T_c. The hypothesis was investigated that the phenomenon was due to a competition between the Coulombian blockage arising from the inter-granular capacitance of nearest neighboring grains and the unblocking process related to tunneling junctions coupling, this competition determining the presence or the absence of percolation paths on superconducting grains crossing the entire system. Computer simulations confirmed with clear evidence the experimental data. The method devised to determine the presence of superconducting percolation paths in simulated granular systems was a direct derivation from the one developed and implemented for the ring perception problem (a method to gain detailed information on rings and chains of atoms in the analysis of medium-range order in computer-simulated solids) [3–5]. Its key features are the *path messages* propagation and reduction of information handling. Although it was developed fairly long ago, it remained unpublished up to now; anyway, at the best of the author's knowledge, it still constitutes an original approach for the determination of percolation paths.

2 The physical background

A metallic granular systems is a superconductor if it is entirely crossed by Cooper pairs moving from grain to grain. In order to obtain a superconducting shunt in a percolative system, there must be a path consisting of superconducting connected grains. The absence of such a path at temperatures lower than T_c characterizes the appearance of re-entrant resistivity peaks. According to theoretical analyses [6–8], superconducting metallic granular systems are governed -at low temperatures- by the competition between two energies E_c and E_J, being E_c the energy of the Coulombian blockage acting

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on grains i and j:

$$E_c^{i,j} = \frac{1}{2}\frac{Q_i Q_j}{C_{ij}}, \tag{1}$$

(with C_{ij} the inter-granular capacitance, Q_i and Q_j the charges excess in the grains i and j due to Cooper pairs (charge 2e)) and E_J the characteristic energy of Josephson junction coupling for nearest neighboring grains ($i = j \pm 1$):

$$E_J^{i,j}(T) = \frac{\pi\hbar}{4e^2}\frac{1}{R_N^{i,j}}\Delta(T)\tanh(\frac{\Delta(T)}{2k_BT}) \tag{2}$$

where $\Delta(T) = \Delta(0)(1 - \frac{T}{T_c})^{\frac{1}{2}}$ is the superconducting gap at temperatures $T < T_c$, Δ_0 the superconducting gap at $T = 0K$ [9], $R_N^{i,j}$ the resistance for single electron tunneling between neighboring grains and k_B the Boltzman constant. Finally, taking into account all energies involved at each temperature $T < T_c$, (namely E_c, E_J and k_BT), two granules are connected -or activated- when one of the conditions

$$(a) \quad k_BT \geq E_c^{i,j} \quad (b) \quad k_BT < E_c^{i,j} \text{ and } zE_J^{i,j} > E_c^{i,j} + k_BT \tag{3}$$

holds with z -the nearest neighbors average number- accounting for shielding effect. For each couple of connected grains (i, j) a critical super-current $I_c^{i,j}$ and its associate density $J_c^{i,j}$ are defined which depend on the grains distance and radii R_i, R_j according to the relations:

$$I_c^{i,j} = \frac{\pi}{2eR_N^{i,j}}\Delta(T)tanh(\frac{\Delta(T)}{2k_BT}) \quad \text{and} \quad J_c^{i,j} = \frac{I_c^{i,j}}{\pi\,(R_{min}^{i,j})^2} \tag{4}$$

where $R_{min}^{i,j}$ is the smallest radius of the two grains.

3 The model

A numerical representation of a disordered granular system was generated positioning spherical grains in a simulation box, their radii and mutual distances distributed gaussianly around known experimental values. Two opposite sides of the box were chosen to be the injection (source) and ejection (drain) electrodes, constituted by their closest grains. In correspondence of a given temperature $T < T_c$ a graph was then built associating a node to each grain and an edge to each couple of activated grains (conditions 3). As a first data-reduction task, subsequent searches and removals of nodes linked by a single edge were performed.

4 The method

The search for paths in a graph is a problem that rises from a great variety of problems from many different fields, stimulating continuous interest since many years (see [10–12] and references therein). Here we present the method we devised to achieve our goal. It represents an exact, original - and hopefully interesting- approach to the problem. As anticipated, it was derived from the method we proposed for the determination of a smallest set of smallest rings in a graph, based on an analogy to a communication network letting *path-messages*, conveying information on their walk through the network, propagate by means of *transceivers* and communication channels during alternate, synchronous *send* and *receive* states of the network ([3, 4]).

5 Basic definitions

- An $edge\ sequence$ of length (size) $k-1$ in a graph is a finite sequence of edges (n_1,n_2), (n_2,n_3), (n_3,n_4), ..., (n_{k-1},n_k), where each edge is denoted by the pair of nodes it connects. If n_1=n_k or $n_1 \neq n_k$ the edge sequence is $closed$ or $open$, respectively.
- An edge sequence of distinct edges constitutes an $edge\ train$.
- An open edge train in which all nodes are distinct is called a $path$.
- An edge train containing a closed edge sequence will be indicated as a $collapsed\ path$.

Together with the common standard definitions given above, the following ones will prove useful to ease future descriptions:

- A physical record of a path, stored as the sequence of the nodes it traversed $(n_1, n_2, ..., n_k)$, will be indicated as a *path-message*.
- A path-message that can be propagated will be indicated as an *active path-message*.
- A path-message containing a closed edge sequence will be indicated as a *collapsed path-message*.
- A node traversed by a path-message will be indicated as a *visited node*
- An edge traversed at most once will be indicated as an *active edge* .
- An edge traversed in both directions will be indicated as an *exhausted edge*.
- A node whose edges are all exhausted will be indicated as an *exhausted node*.

6 Process overview

The initial graph is abstracted to a synchronous communication network by the association of each node to a *transceiver* and considering each edge a *communication channel*. Each transceiver consists of a receive and a send buffer. A node and its transceiver constitute a $Tnode$. Tnodes receive and send *path-messages* containing the sequence of nodes they crossed. $Tnodes$ belonging to the electrodes are reserved a different approach: the source ones act as pure transmitters, the drain ones as pure receivers. A Tnode is said *active* when it contains at least a path-message. The process of determining the percolation paths is based on a "post office" similitude: the underlining idea is that all active Tnodes, during alternating, synchronous send/receive cycles propagate their path-messages through the communications channels linking adjacent nodes. The key feature of our method is constituted by ***deferred path-messages***: the path-messages contained in the send buffers of visited Tnodes. They will be indicated by a trailing hyphenation, e.g. (1,7,12,-). It is important to note that a Tnode becomes a visited one as soon as its first path-message is sent.

6.1 Sending

During the send cycles, Tnodes forward path-messages in such a way that:

1. (a) edges can be traversed no more than once in both direction;

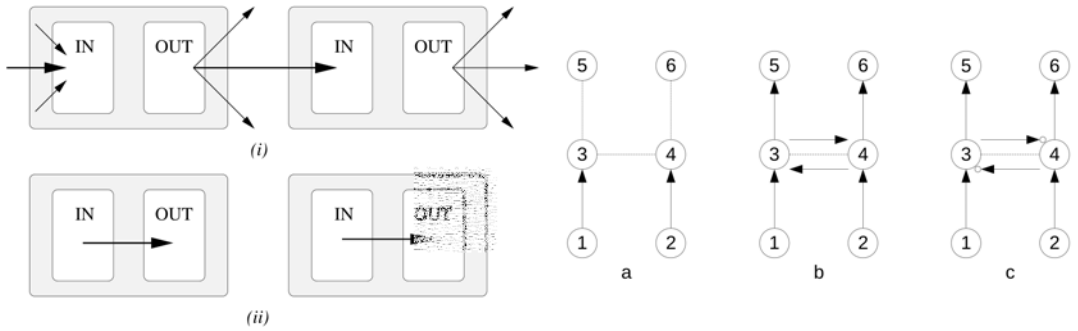

Figure 1: Transceivers sending (*i*) and receiving (*ii*) path-messages. Path-messages propagation (*a*),(*b*),(*c*).

(b) any path-message sent from node m and received by node n is forwarded by n to all the other connected nodes (so that there are no collapsed path- messages);

(c) path-messages are cleared as soon as they are sent;

(d) deferred path-messages are removed from the send process and stored.

6.2 Receiving

During the receiving cycles each transceiver updates -adding itself- the path-messages in its incoming buffer and move them to the outgoing one.

6.3 Initialization

The communication network initialization is done putting in the send buffer of each source Tnode a path-message consisting in the sole indication of the source itself. A scheme of the send and receive phases is given in Fig. 1 (*i*),(*ii*).

6.4 Execution

The entire process is such that, at any stage, all active path-messages are the same length, this length being increased each time messages are re-transmitted; path-messages reaching the drain receivers are then collected and processed in increasing length. Basically, the whole process consists of four phases:

1. initialize the communication network;
2. as long as there are active Tnodes:
   (a) send path-messages;
   (b) receive path-messages;
   (c) identify complete paths;
3. build complete paths from intersecting complete and deferred path-messages.

Fig.1 (*a*),(*b*),(*c*) illustrates the entire process of path-messages propagation in a simple communication network in which electrodes are constituted by the Tnodes 1,2,5,6 and Tnodes 3 and 4 are standard ones (Tnodes are processed in ascending order). In Fig.1.a, at the end of the first send cycle, we have two paths: (1,3) and (2,4); in Fig.1.b we have two active nodes: 3 and 4. After the first transmission from node 3, we have the path (1,3,4) and the node 3 as a visited one. At the end of the transmission from the node 3, we have the paths (1,3,4), (1,3,5); at the end of the transmission from the node 4 we have two active paths:(1,3,4),(2,4,3), two complete ones: (1,3,5),(2,4,6), two visited nodes: 3,4 and an exhausted edge: (3,4). In Fig.1.c, the send cycle individuates the two deferred paths (1,3,4-),(2,4,3,-) and no active path remains. Now we have two complete paths c_1=(1,3,5),c_2=(2,4,6) and two deferred ones d_1=(1,3,4-),d_2=(2,4,3,-). Combining the intersecting complete and deferred paths we have the two additional complete paths (2,4,3,5) from c_1,d_2 and (1,3,4,6) from c_2,d_1. We have then individuated all the percolation paths: (1,3,5),(2,4,6),(2,4,3,5),(1,3,4,6). In large networks, the impact of deferred paths on the number of propagate messages is dramatically effective, in particular when deferred paths are nested.

7 Results and conclusions

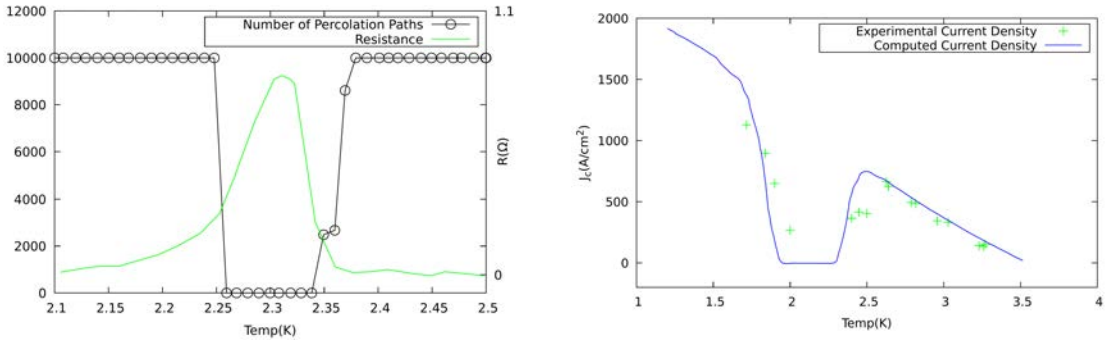

Figure 2: Left: re-entrant resistivity and percolation paths. Right: experimental and computed current densities.

A comparison of experimental and computer simulations results for a sample of diamond-like carbon-silicon film containing tungsten are shown in Fig.2. On the left, the number of percolation paths in the re-entrant resistivity peak region is shown. On the right, the measured value for the maximum current density allowed for the film while retaining its superconducting state, and its value obtained from the simulation network. Notice how the mechanism of paths propagation and rebuilding from deferred paths allow to manage the number of the processed paths avoiding growth beyond reasonable time and hardware resources (Fig.2, left, a limit of 10000 is used as the maximum number of reconstructed complete paths). Even though the simulation sample was constituted by only 1000 grains, the agreement of experimental and computed results is particularly strict and clear.

8 Computational resources

The calculations were performed using the facilities and services available at the ENEA GRID infrastructure (Italy). The simulation software was written in Fortran90 and compiled using the GNU and

Intelcompilers available on CRESCO4 cluster. 800GB of disk storage has been granted on the PFS file system.

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